Process Optimization

Mathematical Programming and Optimization of Multi-Plant Operations and Process Design

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Process Optimization

- Typical Industrial Problems
- Mathematical Programming Software
- Mathematical Basis for Optimization
- Lagrange Multipliers and the Simplex Algorithm
- Generalized Reduced Gradient Algorithm
- On-Line Optimization
- Mixed Integer Programming and the Branch and Bound Algorithm
- Chemical Production Complex Optimization

New Results

- Using one computer language to write and run a program in another language
- Cumulative probability distribution instead of an optimal point using Monte Carlo simulation for a multi-criteria, mixed integer nonlinear programming problem
- Global optimization

Design vs. Operations

- Optimal Design
  - Uses flowsheet simulators and SQP
  - Heuristics for a design, a superstructure, an optimal design
- Optimal Operations
  - On-line optimization
  - Plant optimal scheduling
  - Corporate supply chain optimization

Plant Problem Size

	Contact 3,200 TPD	Alkylation 15,000 BPD	Ethylene 200 million lb/yr
Units	14	76	~200
Streams	35	110	~4,000
Constraints			
Equality	761	1,579	~400,000
Inequality	28	50	~10,000
Variables			
Measured	43	125	~300
Unmeasured	732	1,509	~10,000
Parameters	11	64	~100

Optimization Programming Languages

- GAMS - **G**eneral **A**lgebraic **M**odeling **S**ystem
- LINDO - Widely used in business applications
- AMPL - **A** **M**athematical **P**rogramming **L**anguage
- Others: MPL, ILOG

optimization program is written in the form of an optimization problem

optimize:	$y(\mathbf{x})$	economic model
subject to:	$f_i(\mathbf{x}) = 0$	constraints

Software with Optimization Capabilities

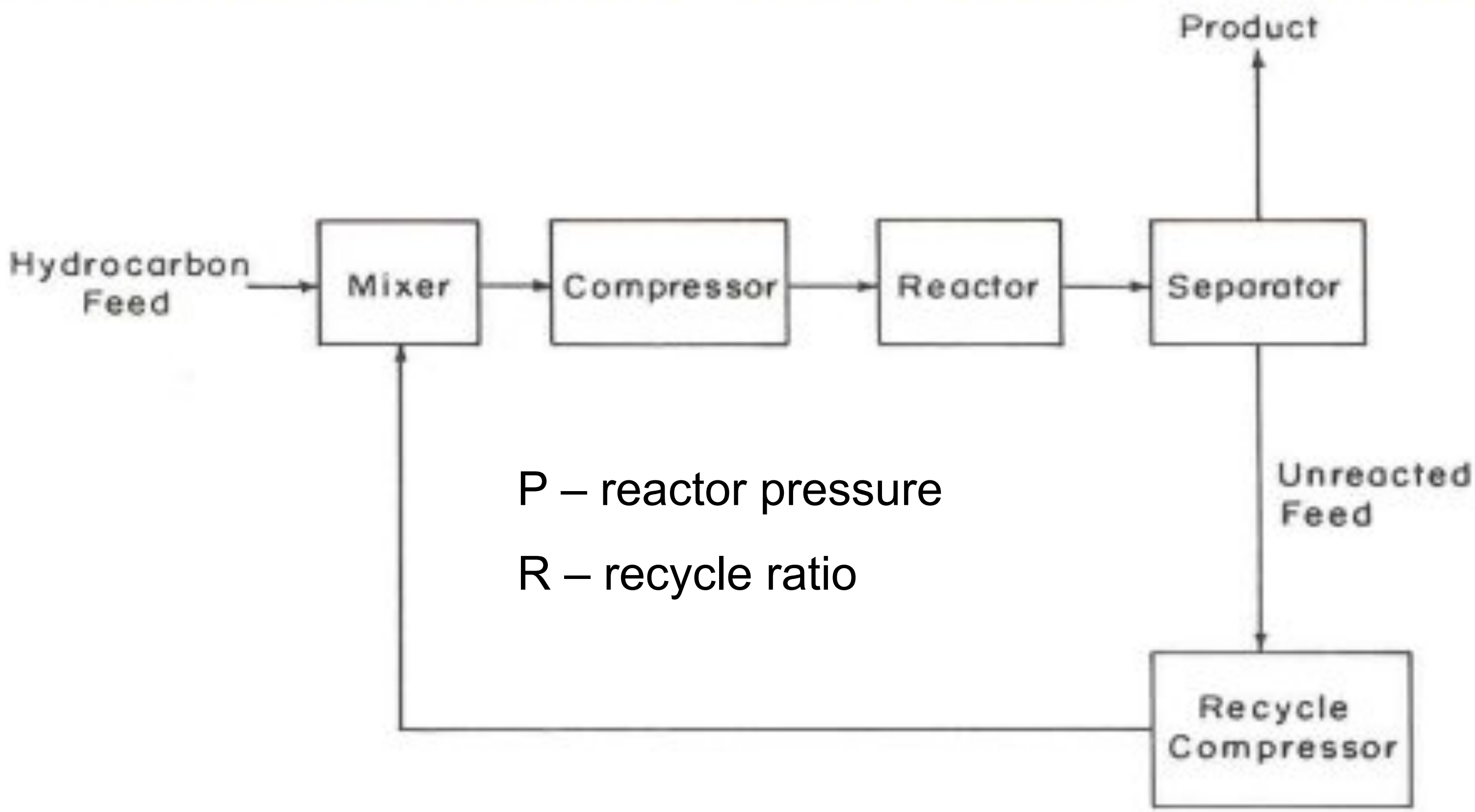
- Excel – Solver
- MATLAB
- MathCAD
- Mathematica
- Maple
- Others

Mathematical Programming

- Using Excel – Solver
- Using GAMS
- Mathematical Basis for Optimization
- Important Algorithms
  - Simplex Method and Lagrange Multipliers
  - Generalized Reduced Gradient Algorithm
  - Branch and Bound Algorithm

Simple Chemical Process

minimize: $C = 1,000P + 4*10^9/P*R + 2.5*10^5R$
subject to: $P*R = 9000$



P – reactor pressure

R – recycle ratio

Excel Solver Example

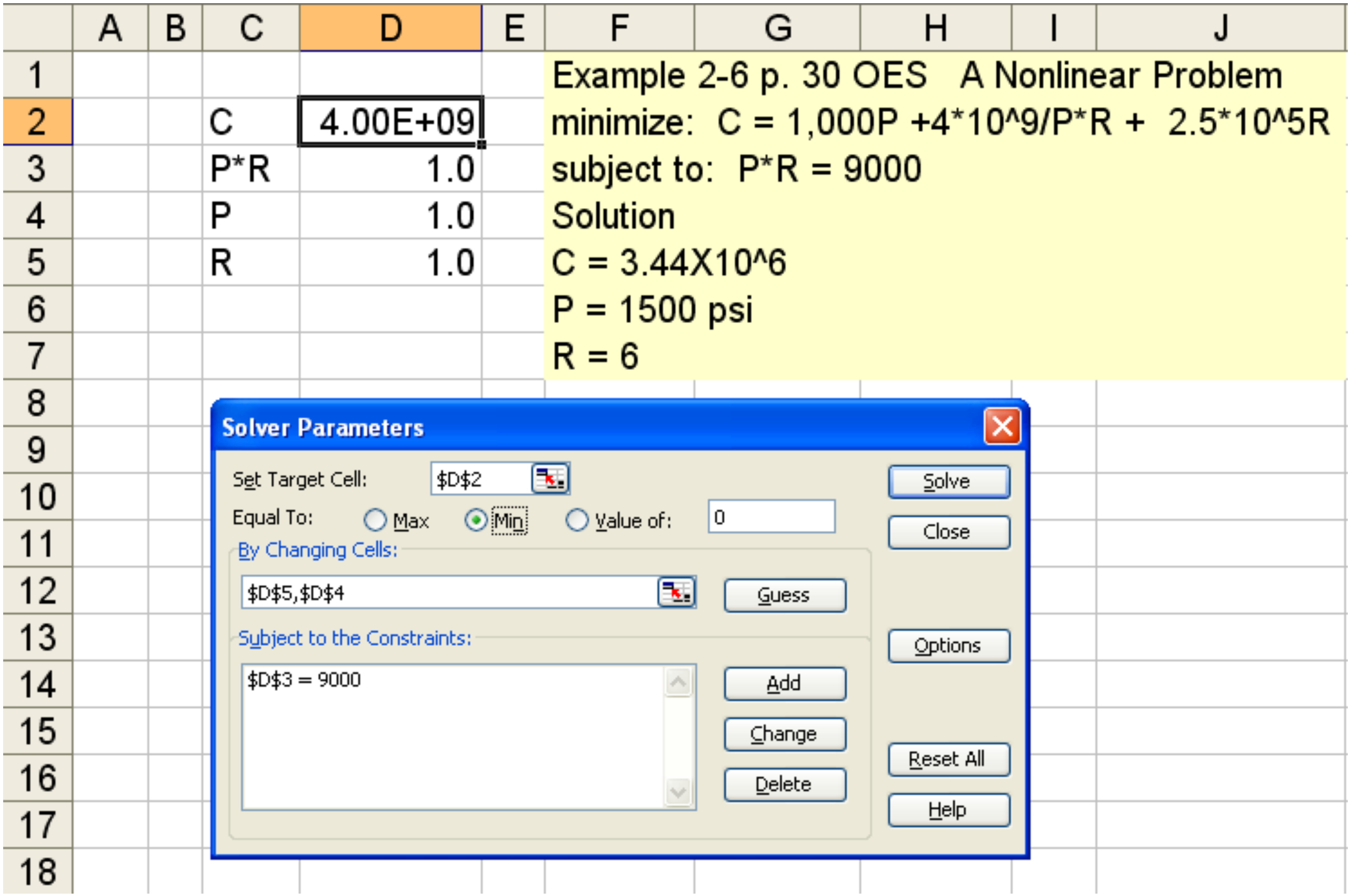
Solver optimal solution

		Example 2-6 p. 30 OES A Nonlinear Problem
C	3.44E+06	minimize: C = 1,000P +4*10^9/P*R + 2.5*10^5R
P*R	9000.0	subject to: P*R = 9000
P	6.0	Solution
R	1500.0	C = 3.44X10^6
		P = 1500 psi
		R = 6

Showing the equations in the Excel cells with initial values for P and R

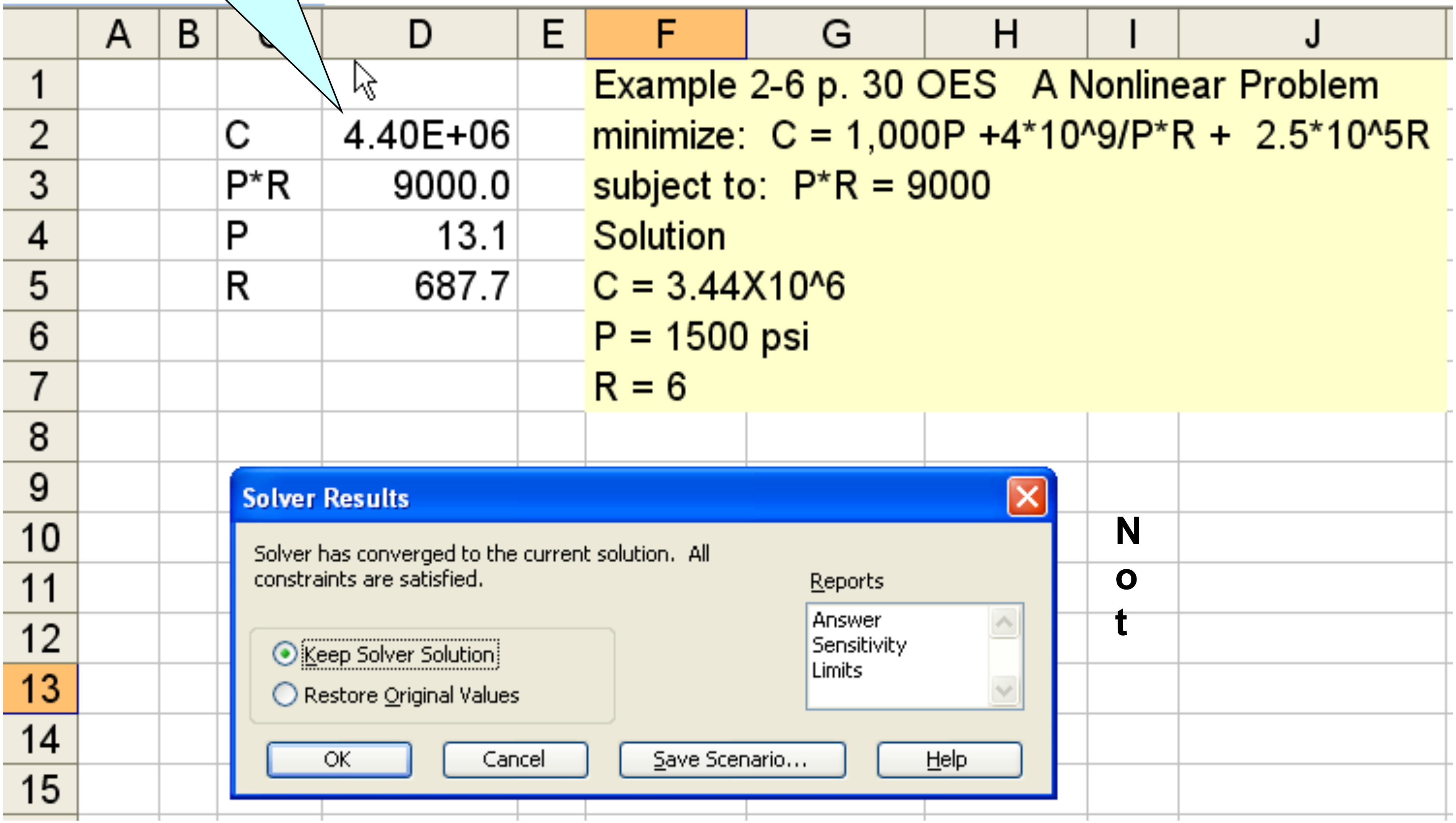
C	=1000*D5+4*10^9/(D5*D4)+2.5*10^5*D4
P*R	=D5*D4
P	1
R	1

Excel Solver Example



Excel Solver Example

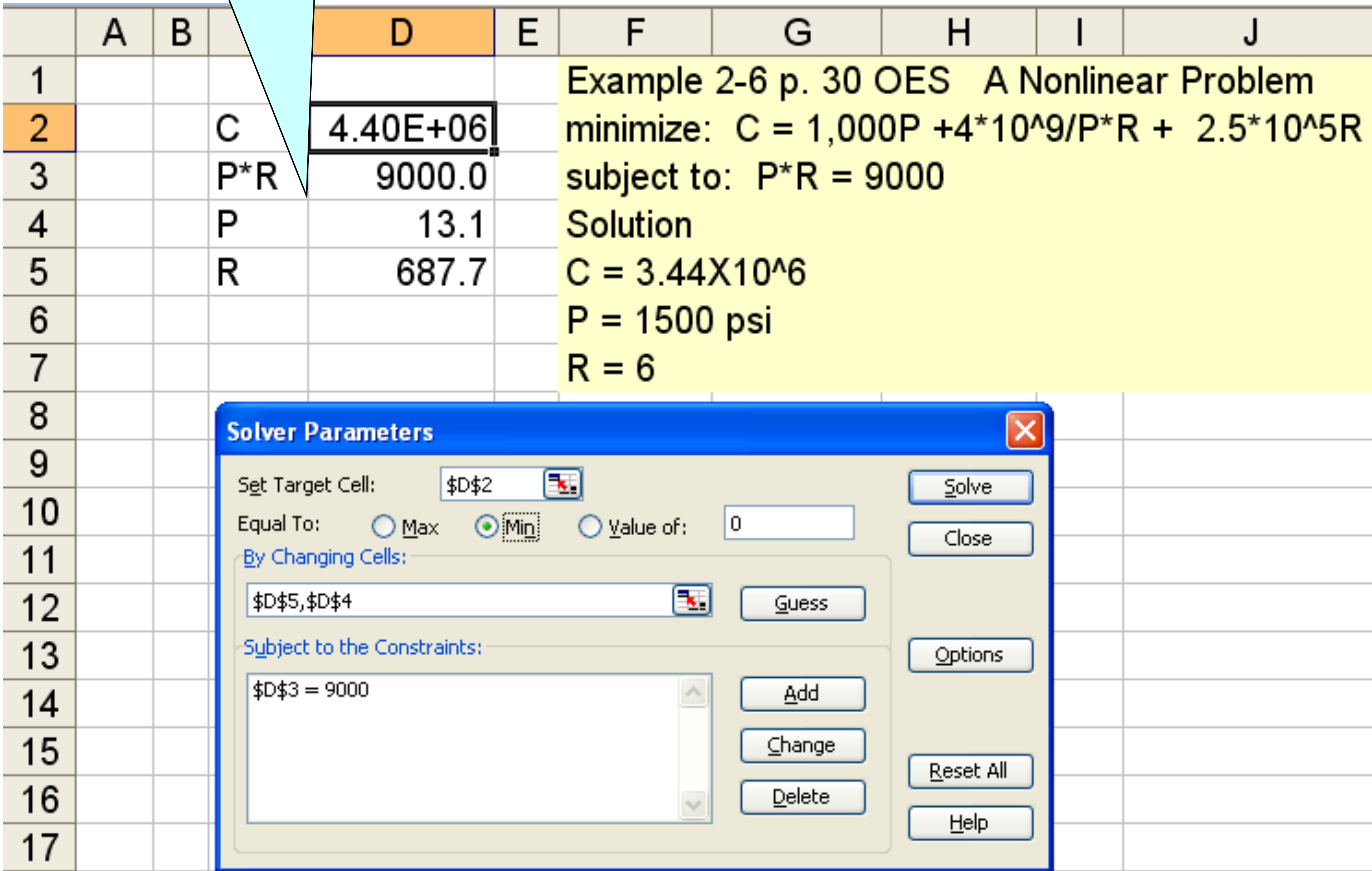
Not the minimum for C



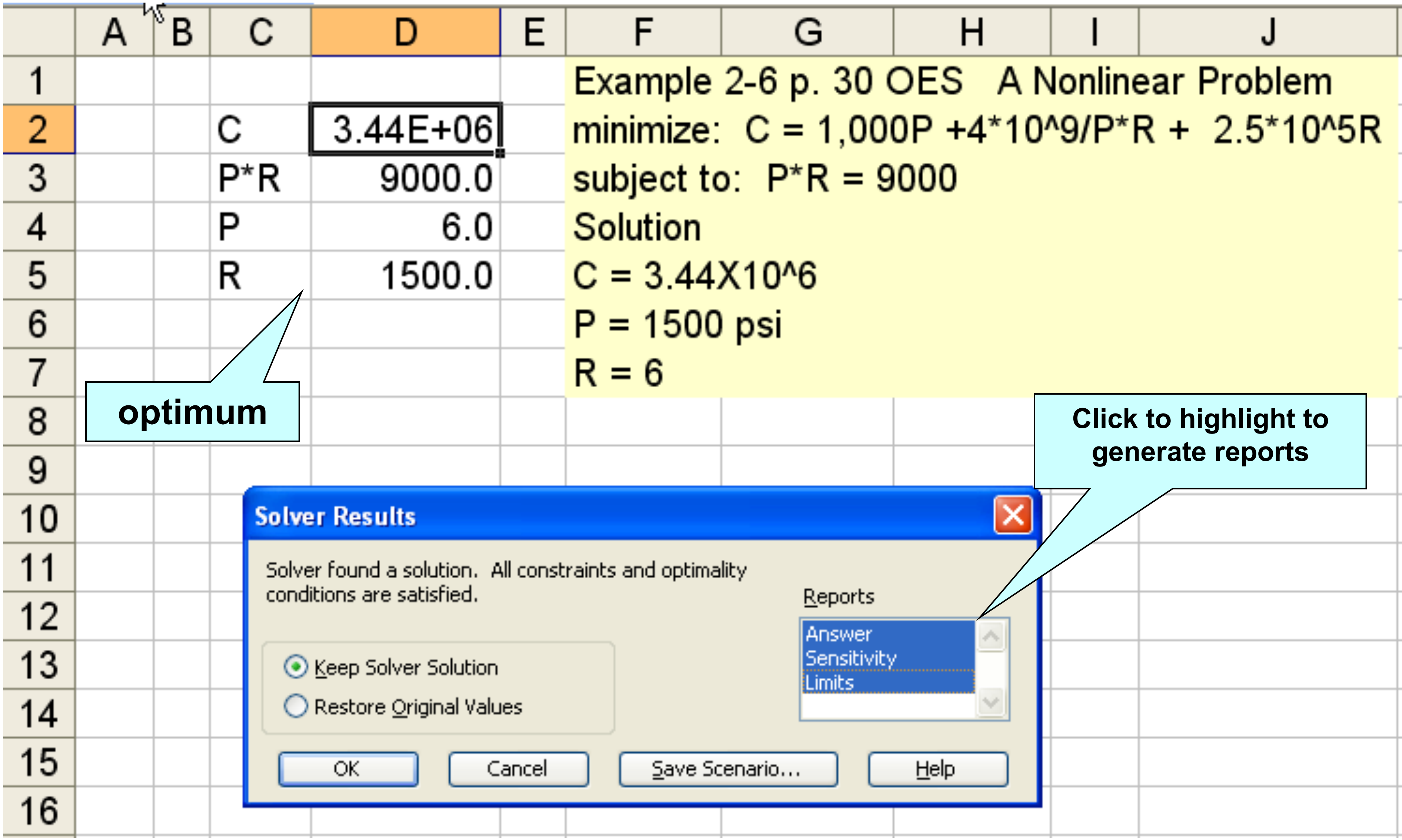
N
o
t

Excel Solver Example

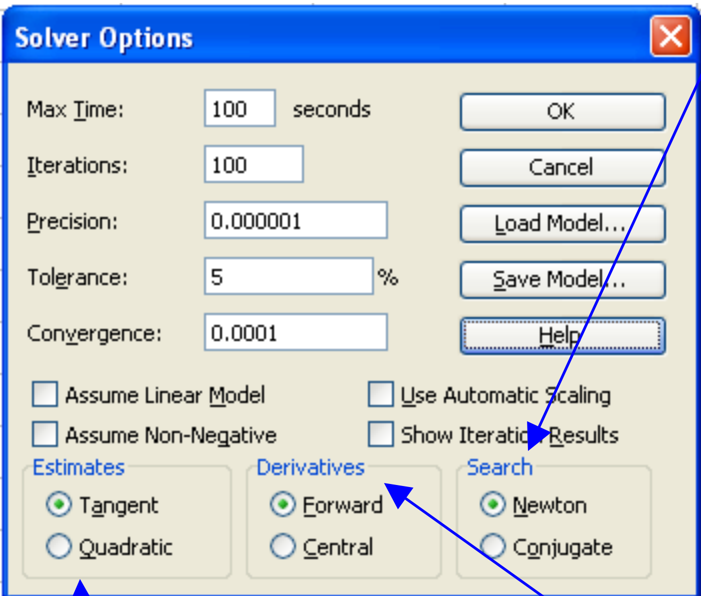
Use Solver with these values of P and R



Excel Solver Example



Excel Solver Example



Search

Specifies the algorithm used at each iteration to determine the direction to search.

Newton Uses a quasi-Newton method that typically requires more memory but fewer iterations than the Conjugate gradient method.

Conjugate Requires less memory than the Newton method but typically needs more iterations to reach a particular level of accuracy. Use this option when you have a large problem and memory usage is a concern, or when stepping through iterations reveals slow progress.

Information from Solver Help is of limited value

Derivatives

Specifies the differencing used to estimate partial derivatives of the objective and constraint functions.

Forward Use for most problems, in which the constraint values change relatively slowly.

Central Use for problems in which the constraints change rapidly, especially near the limits. Although this option requires more calculations, it might help when Solver returns a message that it could not improve the solution.

Estimates

Specifies the approach used to obtain initial estimates of the basic variables in each one-dimensional search.

Tangent Uses linear extrapolation from a tangent vector.

Quadratic Uses quadratic extrapolation, which can improve the results on highly nonlinear problems.

Excel Solver Answer Report

management report format

Microsoft Excel 11.0 Answer Report

Target Cell (Min)

Cell	Name	Original Value	Final Value
D2	C	3.44E+06	3.44E+06

values at the optimum

Adjustable Cells

Cell	Name	Original Value	Final Value
D5	R	1500.0	1500.0
D4	P	6.0	6.0

constraint status

slack variable

Constraints

Cell	Name	Cell Value	Formula	Status	Slack
D3	P*R	9000.0	D3=9000	Not Binding	0

Excel Sensitivity Report

Microsoft Excel 11.0 Sensitivity Report

Adjustable Cells

Cell	Name	Final Value	Reduced Gradient
D5	R	1500.0	0.0
D4	P	6.0	0.0

Constraints

Cell	Name	Final Value	Lagrange Multiplier
D3	P*R	9000.0	117.3

Solver uses the generalized reduced gradient optimization algorithm

Lagrange multipliers used for sensitivity analysis

Shadow prices ($ per unit)

Excel Solver Limits Report

Sensitivity Analysis provides limits on variables for the optimal solution to remain optimal

Microsoft Excel 11.0 Limits Report

Cell	Target Name	Value
D2	C	3.44E+06

Cell	Adjustable Name	Value	Lower Limit	Target Result	Upper Limit	Target Result
D5	R	1500.0	1500.0	3.44E+06	1500.0	3.44E+06
D4	P	6.0	6.0	3.44E+06	6.0	3.44E+06

GAMS

C:\Backup\WPDOCS\OPT\GAMS\Example 2-6 p 30 OES Recycle.gms

Example 2-6 p 30 OES Recycle.gms

```
$TITLE Recycle
$OFFSYMXREF
$OFFSYMLIST
* Example 2-6 on p. 30 of OES

VARIABLES P,R, Z;
POSITIVE VARIABLES P,R;

EQUATIONS CON1, OBJ;

CON1..  P*R =E= 9000;
OBJ.. Z =E= 1000*P + 4*1000000000/(P*R) + 2.5*100000*R;

P.LO=1; R.LO=1;

MODEL Recycle /ALL/;

SOLVE Recycle USING NLP MINIMIZING Z;

DISPLAY P.L, R.L, Z.L;
```

GAMS

S O L V E S U M M A R Y

```
MODEL   Recycle            OBJECTIVE  Z
TYPE    NLP                DIRECTION  MINIMIZE
SOLVER  CONOPT             FROM LINE  18
```

****** SOLVER STATUS   1 NORMAL COMPLETION**
****** MODEL STATUS   2 LOCALLY OPTIMAL**
****** OBJECTIVE VALUE   3444444.4444**

```
RESOURCE USAGE, LIMIT          0.016      1000.000
ITERATION COUNT, LIMIT        14         10000
EVALUATION ERRORS              0             0
```

C O N O P T 3   x86/MS Windows version 3.14P-016-057
Copyright (C)   ARKI Consulting and Development A/S
Bagsvaerdvej 246 A
DK-2880 Bagsvaerd, Denmark

Using default options.

The model has 3 variables and 2 constraints with 5 Jacobian elements, 4 of which are nonlinear.
The Hessian of the Lagrangian has 2 elements on the diagonal, 1 elements below the diagonal, and 2 nonlinear variables.

**** Optimal solution. Reduced gradient less than tolerance.**

GAMS

Lagrange multiplier

	LOWER	LEVEL	UPPER	MARGINAL
---- EQU CON1	9000.000	9000.000	9000.000	117.284
---- EQU OBJ	.	.	.	1.000

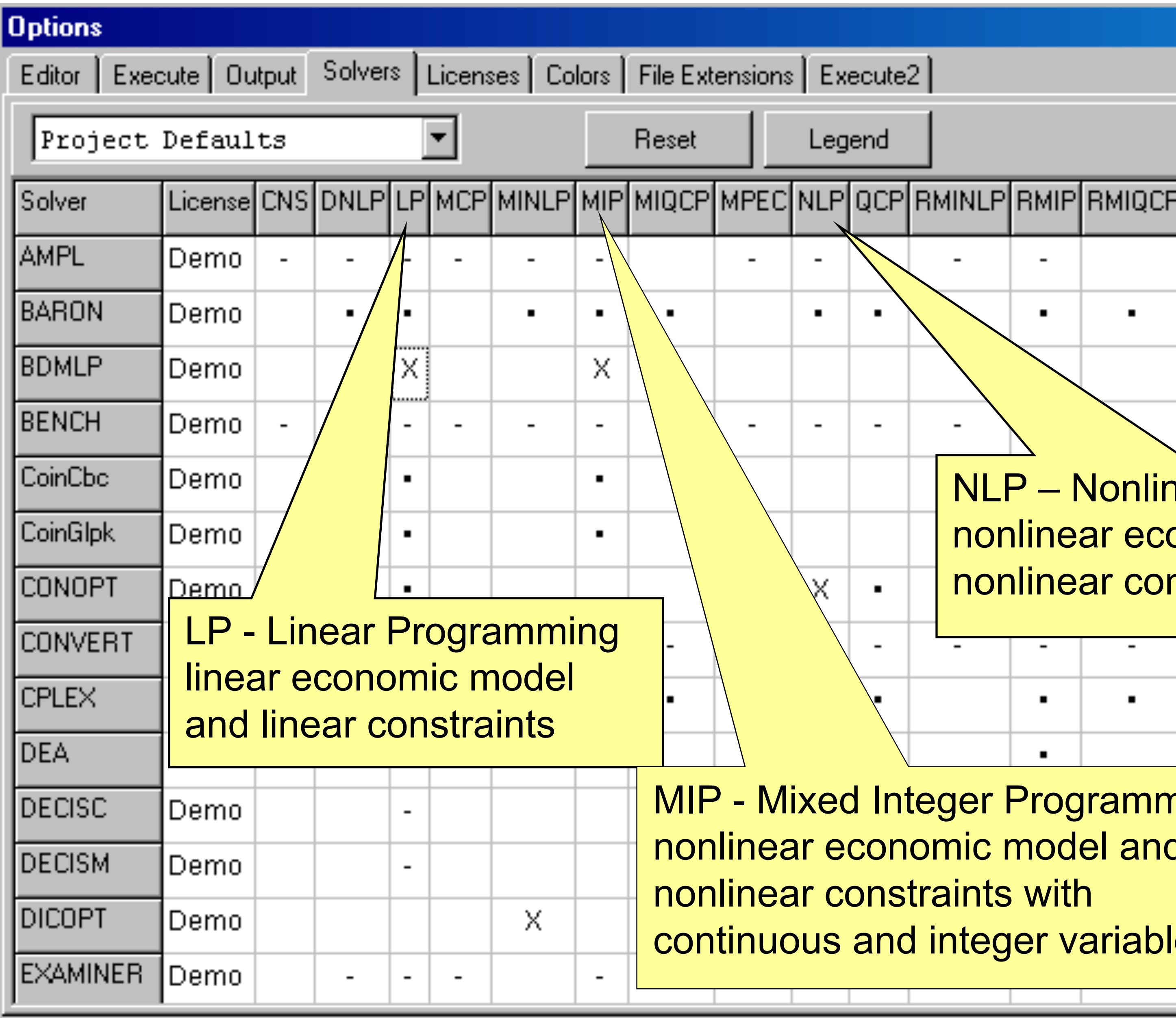
	LOWER	LEVEL	UPPER	MARGINAL
---- VAR P	1.000	1500.000	+INF	.
---- VAR R	1.000	6.000	+INF	EPS
---- VAR Z	-INF	3.4444E+6	+INF	.

values at the optimum

- **** REPORT SUMMARY : 0 NONOPT
- 0 INFEASIBLE
- 0 UNBOUNDED
- 0 ERRORS

900 page Users Manual

GAMS Solvers



13 types of optimization problems

LP - Linear Programming
linear economic model
and linear constraints

MIP - Mixed Integer Programming
nonlinear economic model and
nonlinear constraints with
continuous and integer variables

NLP – Nonlinear Programming
nonlinear economic model and
nonlinear constraints

GAMS Solvers

Options

Editor | Execute | Output | Solvers | Licenses | Colors | File Extensions | Execute2

32 Solvers

Reset | Legend

Solver	License	CNS	DNLP	LP	MCP	MINLP	MIP	MIQCP	MPEC	NLP	QCP	RMINLP	RMIP	RMIQCP
AMPL	Demo	-	-	-	-	-	-		-	-		-	-	
BARON	Demo		■	■		■	■	■		■	■	■	■	■
BDMLP	Demo			X			X						■	

new global optimizer

Solver	License	CNS	DNLP	LP	MCP	MINLP	MIP	MIQCP	MPEC	NLP	QCP	RMINLP	RMIP	RMIQCP
DICOPT	Demo					X								
EXAMINER	Demo		-	-	-		-	-	-	-	-	-	-	-
GAMSBAS	Demo		-	-	-	-	-			-		-	-	
GAMSCHK	Demo		-	-	-	-	-			-		-	-	
KNITRO	Demo		■	■						■	■	■	■	■
LGO	Demo		■	■						■	■	■	■	■
LINGO	Demo		-											
MILES	Demo													
MINOS	Demo		■	■						■	X	X	X	X

DICOPT One of several MINLP optimizers

MINOS a sophisticated NLP optimizer developed at Stanford OR Dept uses GRG and SLP

Mathematical Basis for Optimization is the Kuhn Tucker Necessary Conditions

General Statement of a Mathematical Programming Problem

Minimize: $y(x)$

Subject to: $f_i(x) \leq 0$ for $i = 1, 2, \ldots, h$

$f_i(x) = 0$ for $i = h+1, \ldots, m$

$y(x)$ and $f_i(x)$ are twice continuously differentiable real valued functions.

Kuhn Tucker Necessary Conditions

Lagrange Function

– converts constrained problem to an unconstrained one

$$L(x,\lambda) = y(x) + \sum_{i=1}^{h} \lambda_i \left[f_i(x) + x_{n+i}^2 \right] + \sum^{m} \lambda_i f_i(x)$$

λ_i are the Lagrange multipliers

x_{n+i} are the slack variables used to convert the inequality constraints to equalities.

Kuhn Tucker Necessary Conditions

Necessary conditions for a relative minimum at **x***

1. $\frac{y(\mathbf{x}^*)}{x_j} + {}^{h}_{i=1} \; {}_i \frac{f_i}{x_j}(\mathbf{x}^*) + {}^{m}_{i=h+1} \; {}_i \frac{f_i}{x_j}(\mathbf{x}^*) = 0 \quad \text{for } j = 1,2,..,n$

2. $f_i(\mathbf{x}^*) \quad 0 \qquad \text{for } i = 1, 2, ..., h$

3. $f_i(\mathbf{x}^*) = 0 \qquad \text{for } i = h+1, ..., m$

4. ${}_i \, f_i(\mathbf{x}^*) = 0 \qquad \text{for } i = 1, 2, ..., h$

5. ${}_i \geq 0 \qquad \text{for } i = 1, 2, ..., h$

6. ${}_i$ is unrestricted in sign $\qquad \text{for } i = h+1, ..., m$

Lagrange Multipliers

Treated as an:

- Undetermined multiplier – multiply constraints by λ_i and add to $y(\mathbf{x})$
- Variable - $L(x,\lambda)$
- Constant – numerical value computed at the optimum

Lagrange Multipliers

optimize: $y(x_1, x_2)$
subject to: $f(x_1, x_2) = 0$

$$dy = \frac{\partial y}{\partial x_1} dx_1 + \frac{\partial y}{\partial x_2} dx_2$$

$$0 = \frac{\partial f}{\partial x_1} dx_1 + \frac{\partial f}{\partial x_2} dx_2$$

$$dx_2 = -\frac{\dfrac{\partial f}{\partial x_1}}{\dfrac{\partial f}{\partial x_2}} dx_1$$

Lagrange Multipliers

$$dy = \frac{\partial y}{\partial x_1} dx_1 - \frac{\partial y}{\partial x_2} \frac{\dfrac{\partial f}{\partial x_1}}{\dfrac{\partial f}{\partial x_2}} dx_1$$

Rearrange the partial derivatives in the second term

Lagrange Multipliers

$$dy = \left[\frac{\partial y}{\partial x_1} + \left(\frac{-\dfrac{\partial y}{\partial x_2}}{\dfrac{\partial f}{\partial x_2}} \right) \frac{\partial f}{\partial x_1} \right] dx_1$$

( ) = λ

$$dy = \left[\frac{\partial y}{\partial x_1} + \lambda \frac{\partial f}{\partial x_1} \right] dx_1$$

Call the ratio of partial derivatives in the ( ) a Lagrange multiplier, λ

Lagrange multipliers are a ratio of partial derivatives at the optimum.

Lagrange Multipliers

$$dy = \frac{\partial(y + \lambda f)}{\partial x_1} dx_1 = 0$$

Define L = y +λf , an unconstrained function

$$\frac{\partial L}{\partial x_1} = 0$$

and by the same procedure

$$\frac{\partial L}{\partial x_2} = 0$$

Interpret L as an unconstrained function, and the partial derivatives set equal to zero are the necessary conditions for this unconstrained function

Lagrange Multipliers

Optimize: $y(x_1,x_2)$
Subject to: $f(x_1,x_2) = b$

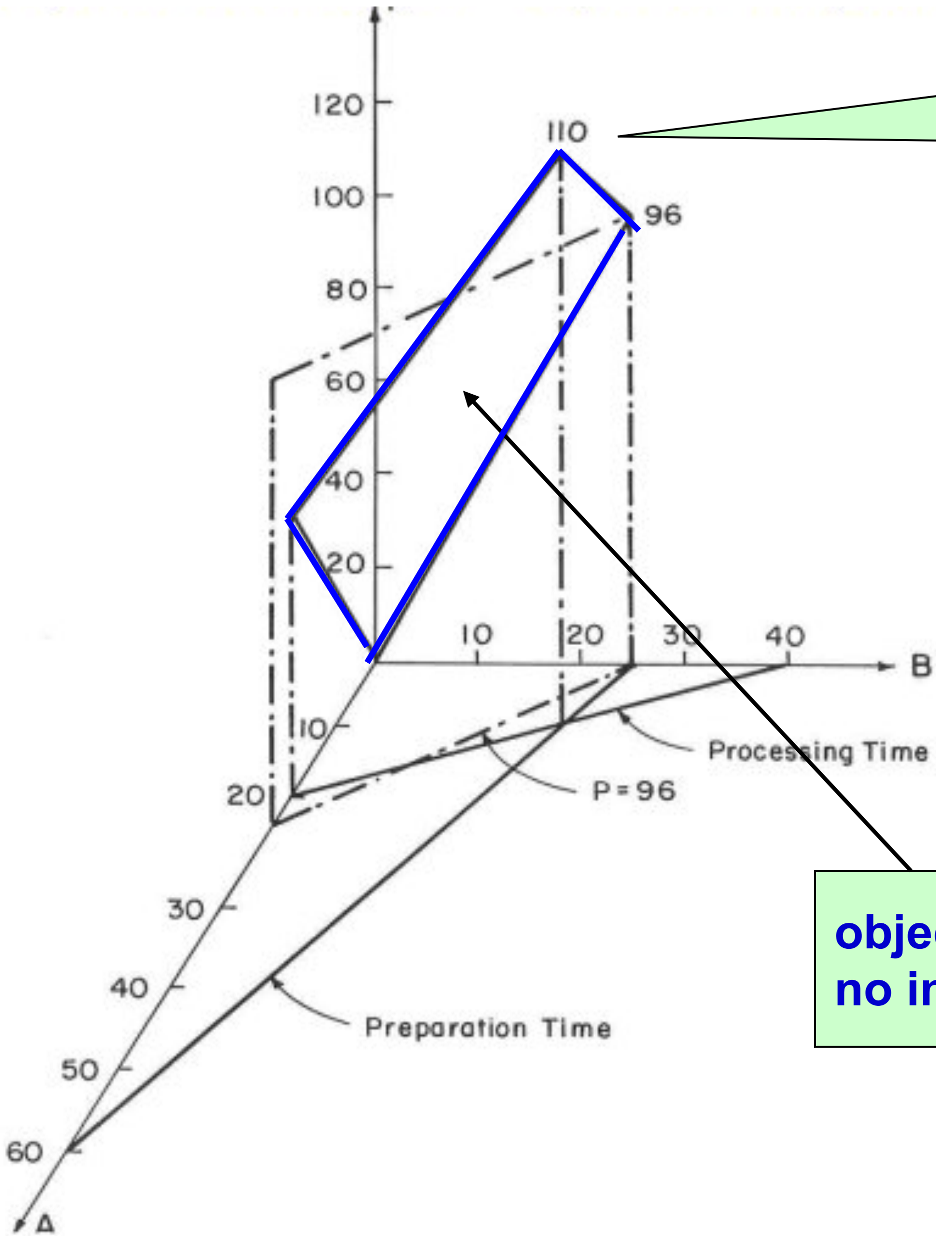
Manipulations give:

$$\frac{\partial y}{\partial b} = -\lambda$$

Extends to:

$$\frac{\partial y}{\partial b_i} = -\lambda_i$$ shadow price (\$ per unit of b_i)

Geometric Representation of an LP Problem



Maximum at vertex
P = 110
A = 10, B = 20

max: $3A + 4B = P$
s.t. $4A + 2B \leq 80$
$2A + 5B \leq 120$

objective function is a plane
no interior optimum

LP Example

Maximize:

$$x_1 + 2x_2 = P$$

Subject to:

$$\begin{aligned}
2x_1 + x_2 + x_3 &= 10 \\
x_1 + x_2 + x_4 &= 6 \\
-x_1 + x_2 + x_5 &= 2 \\
-2x_1 + x_2 + x_6 &= 1
\end{aligned}$$

4 equations and 6 unknowns, set 2 of the x_i =0 and solve for 4 of the x_i.

Basic feasible solution: $x_1 = 0$, $x_2 = 0$, $x_3 = 10$, $x_4 = 6$, $x_5 = 2$, $x_6 = 1$

Basic solution: $x_1 = 0$, $x_2 = 6$, $x_3 = 4$, $x_4 = 0$, $x_5 = -4$, $x_6 = -5$

Final Step in Simplex Algorithm

Maximize: $-3/2\,x_4 - 1/2\,x_5 = P - 10$ $\quad P = 10$

Subject to:

$$
\begin{aligned}
x_3 - 3/2\,x_4 + 1/2\,x_5 &= 2 & \quad x_3 = 2\\
1/2\,x_4 - 3/2\,x_5 + x_6 &= 1 & \quad x_6 = 1\\
x_1 + 1/2\,x_4 - 1/2\,x_5 &= 2 & \quad x_1 = 2\\
x_2 + 1/2\,x_4 + 1/2\,x_5 &= 4 & \quad x_2 = 4\\
& & \quad x_4 = 0\\
& & \quad x_5 = 0
\end{aligned}
$$

Simplex algorithm exchanges variables that are zero with ones that are nonzero, one at a time to arrive at the maximum

Lagrange Multiplier Formulation

Returning to the original problem

$$\text{Max: } (1+2\lambda_1+\lambda_2-\lambda_3-2\lambda_4)\, x_1$$

$$(2+\lambda_1+\lambda_2+\lambda_3+\lambda_4)x_2 +$$

$$\lambda_1 x_3 + \lambda_2 x_4 + \lambda_3 x_5 + \lambda_4 x_6$$

$$-(10\lambda_1 + 6\lambda_2 + 2\lambda_3 + \lambda_4) = L = P$$

Set partial derivatives with respect to $x_{1,}$ x_2, x_3, and x_6 equal to zero (x_4 and x_5 are zero) and and solve resulting equations for the Lagrange multipliers

Lagrange Multiplier Interpretation

$(1+2\lambda_1+\lambda_2-\lambda_3-2\lambda_4)=0$

$(2+\lambda_1+\lambda_2+\lambda_3+\lambda_4)=0$

$\lambda_1=0$

$\lambda_2=-3/2$

$\lambda_3=-1/2$

$\lambda_4=0$

Maximize: $0x_1 + 0x_2 + 0x_3 - 3/2\, x_4 - 1/2\, x_5 + 0x_6 = P - 10 \quad P = 10$

Subject to:

$$x_3 - 3/2\, x_4 + 1/2\, x_5 = 2 \qquad x_3 = 2$$

$$1/2\, x_4 - 3/2\, x_5 + x_6 = 1 \qquad x_6 = 1$$

$$x_1 + 1/2\, x_4 - 1/2\, x_5 = 2 \qquad x_1 = 2$$

$$x_2 + 1/2\, x_4 + 1/2\, x_5 = 4 \qquad x_2 = 4$$

$$x_4 = 0$$

$$x_5 = 0$$

$$-(10\lambda_1 + 6\lambda_2 + 2\lambda_3 + \lambda_4) = L = P = 10$$

The final step in the simplex algorithm is used to evaluate the Lagrange multipliers. It is the same as the result from analytical methods.

General Statement of the Linear Programming Problem

Objective Function:

Maximize: $c_1x_1 + c_2x_2 + ... + c_nx_n \quad = p$ (4-1a)

Constraint Equations:

Subject to: $a_{11}x_1 + a_{12}x_2 + ... + a_{1n}x_n \leq b_1$ (4-1b)

$a_{21}x_1 + a_{22}x_2 + ... + a_{2n}x_n \leq b_2$

$\cdots \qquad \cdots \qquad \cdots$

$\cdots \qquad \cdots \qquad \cdots$

$a_{m1}x_1 + a_{m2}x_2 + ... + a_{mn}x_n \leq b_m$

$x_j \geq 0$ for $j = 1,2,...n$ (4-1c)

LP Problem with Lagrange Multiplier Formulation

Multiply each constraint equation, (4-1b), by the Lagrange multiplier λ_i and add to the objective function

Have x_1 to x_m be values of the variables in the basis, positive numbers

Have x_{m+1} to x_n be values of the variables that are not in the basis and are zero.

equal to zero from $\partial p/\partial x_m=0$

positive in the basis

$$\left[c_1 + \sum_{i=1}^{m} a_{i1}\lambda_i\right]x_1 + \left[c_2 + \sum_{i=1}^{m} a_{i2}\lambda_i\right]x_2 + \left[c_m + \sum_{i=1}^{m} a_{im}\lambda_i\right]x_m + \ldots$$

not equal to zero, negative

equal to zero not in basis

$$+\left[c_{m+1} + \sum_{i=1}^{m} a_{im+1}\lambda_i\right]x_{m+1} + \left[c_n + \sum_{i=1}^{m} a_{in}\lambda_i\right]x_n = p + \sum_{i=1}^{m} b_i\lambda_i$$

Left hand side = 0 and p = - $\sum b_i\lambda_i$

Sensitivity Analysis

- Use the results from the final step in the simplex method to determine the range on the variables in the basis where the optimal solution remains optimal for changes in:
- b_i availability of raw materials demand for product, capacities of the process units
- c_j sales price and costs
- See Optimization for Engineering Systems book for equations at www.mpri.lsu.edu

Nonlinear Programming

Three standard methods – all use the same information

Successive Linear Programming

Successive Quadratic Programming

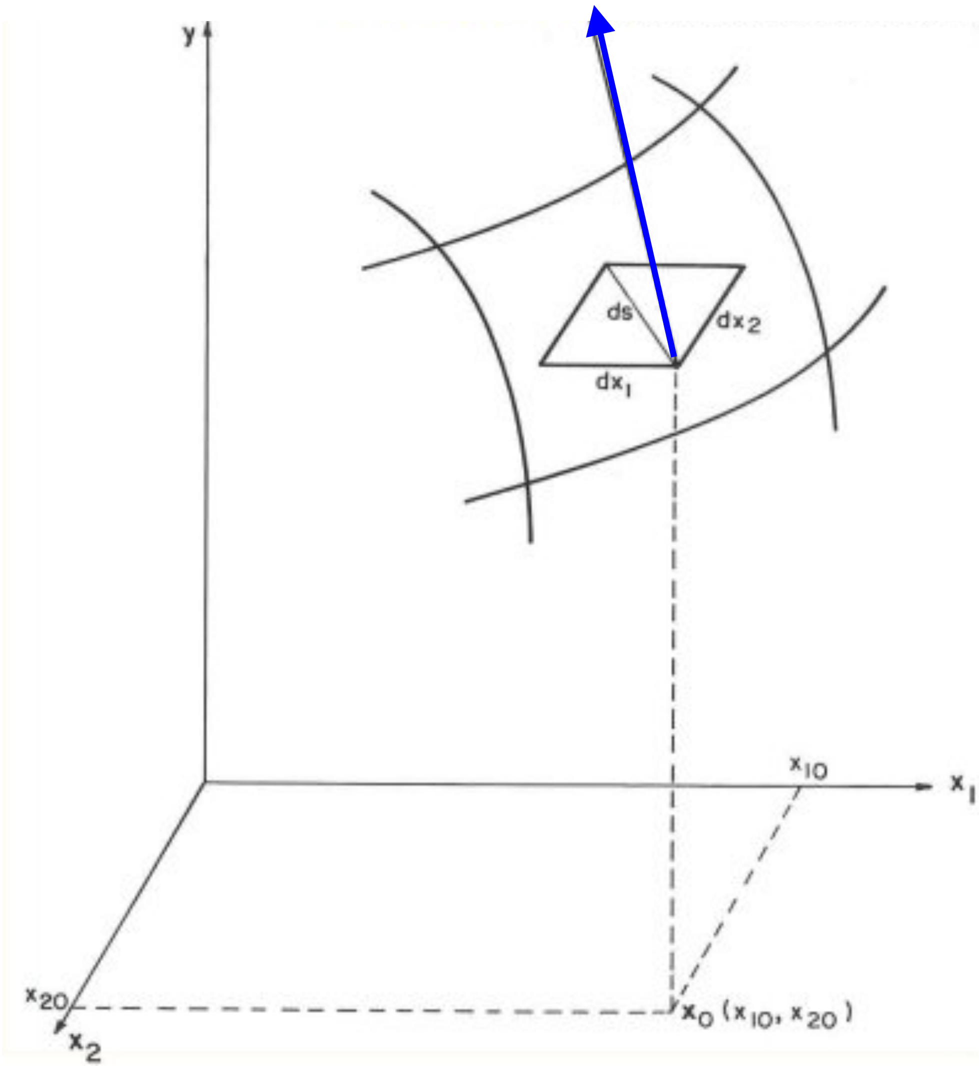
Generalized Reduced Gradient Method

Optimize: $y(\mathbf{x})$ $\mathbf{x} = (x_1, x_2, \ldots, x_n)$

Subject to: $f_i(\mathbf{x}) = 0$ for $i = 1,2,\ldots,m$ $n>m$

$\frac{\partial y(\mathbf{x}_k)}{\partial x_j}$ $\frac{\partial f_i(\mathbf{x}_k)}{\partial x_j}$ evaluate partial derivatives at $\mathbf{x}_k$

Generalized Reduced Gradient Direction



Reduced Gradient Line

Specifies how to change x_{nb} to have the largest change in y(x) at x_k

$$x_{nb} = x_{k,nb} + \alpha \nabla Y(x_k)$$

Generalized Reduced Gradient Algorithm

Minimize: $y(x) = \boldsymbol{y(x)}$ $\quad\quad$ $\boldsymbol{Y}[x_{k,nb} + \alpha \nabla Y(x_k)] = Y(\alpha)$

Subject to: $f_i(x) = 0$

$(x) = (x_b, x_{nb})$ *m basic variables, (n-m) nonbasic variables*

Reduced Gradient

$$\nabla^T Y(x_k) = \nabla^T y_{nb}(x_k) - \nabla y_b(x_k) B_b^{-1} B_{nb}$$

Reduced Gradient Line

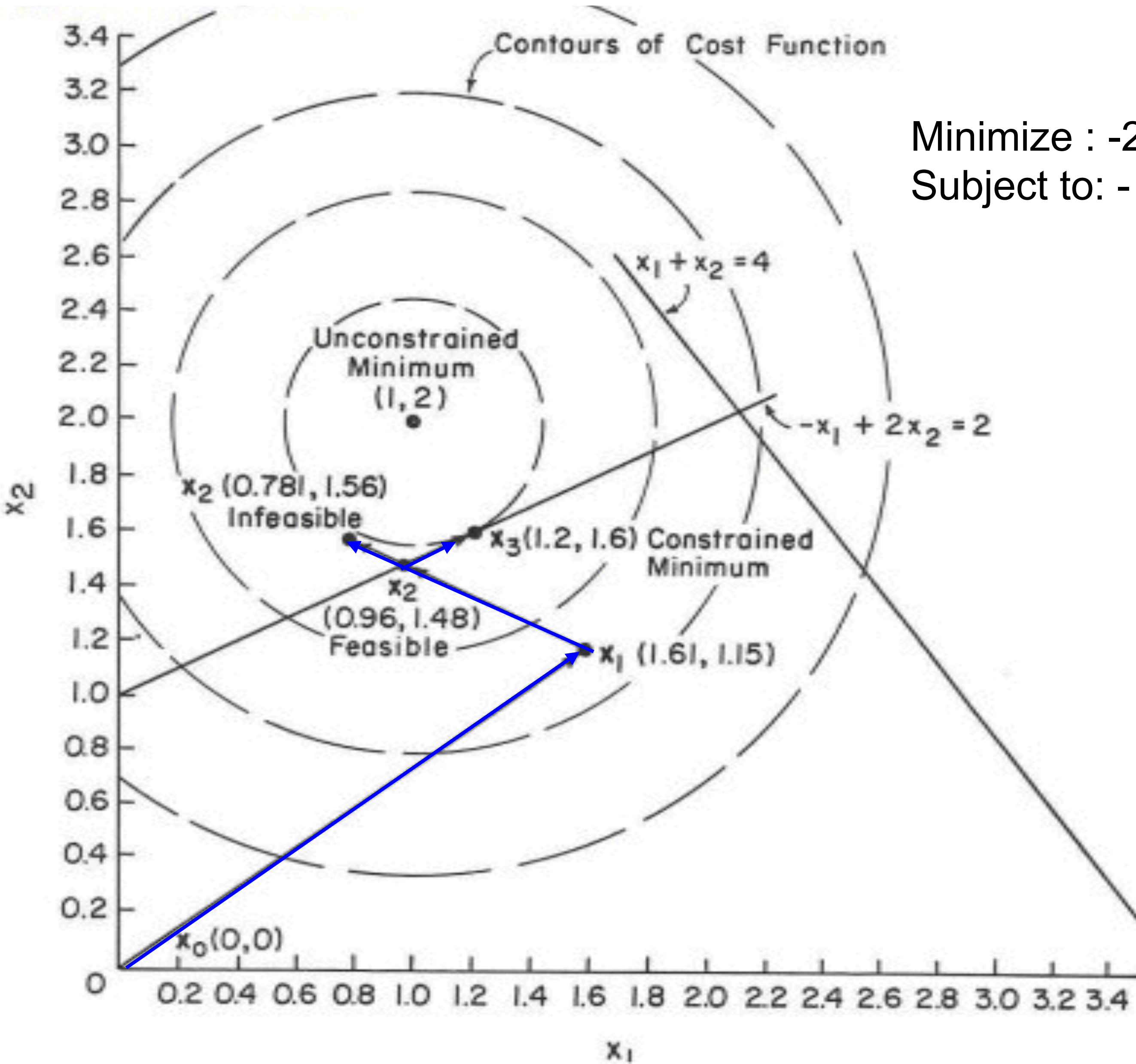
$$x_{nb} = x_{k,nb} + \alpha \nabla Y(x_k)$$

$$B = \frac{\partial f_i(x_k)}{\partial x_j}$$

Newton Raphson Algorithm

$$x_{i+1,b} = x_{i,b} - B_b^{-1} f(x_{i,b}, x_{nb})$$

Generalized Reduced Gradient Trajectory



Minimize : $-2x_1 - 4x_2 + x_1^2 + x_2^2 + 5$

Subject to: $- x_1 + 2x_2 \leq 2$

$x_1 + x_2 \leq 4$

On-Line Optimization

- Automatically adjust operating conditions with the plant's distributed control system

- Maintains operations at optimal set points

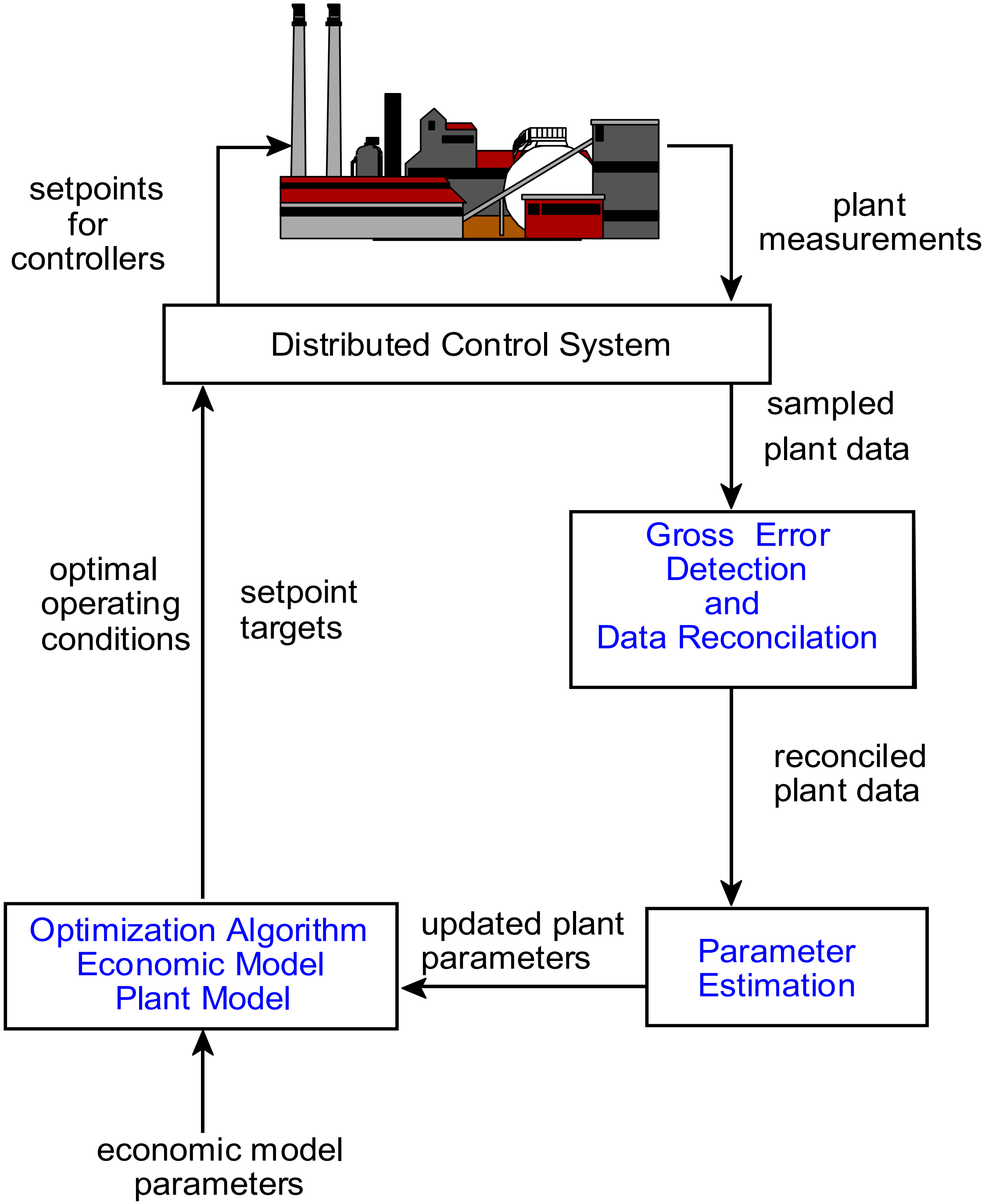
- Requires the solution of three NLP's in sequence
  - gross error detection and data reconciliation
  - parameter estimation
  - economic optimization

BENEFITS

- Improves plant profit by 10%

- Waste generation and energy use are reduced

- Increased understanding of plant operations


setpoints
for
controllers
plant
measurements
Distributed Control System
sampled
plant data
Gross Error
Detection
and
Data Reconcilation
optimal
operating
conditions
setpoint
targets
reconciled
plant data
Optimization Algorithm
Economic Model
Plant Model
updated plant
parameters
Parameter
Estimation
economic model
parameters

Some Companies Using On-Line Optimization

United States	Europe
Texaco	OMV Deutschland
Amoco	Dow Benelux
Conoco	Shell
Lyondel	OEMV
Sunoco	Penex
Phillips	Borealis AB
Marathon	DSM-Hydrocarbons
Dow	
Chevron	
Pyrotec/KTI	
NOVA Chemicals (Canada)	
British Petroleum	

Applications

mainly crude units in refineries and ethylene plants

Companies Providing On-Line Optimization

Aspen Technology - Aspen Plus On-Line
- DMC Corporation
- Setpoint
- Hyprotech Ltd.

Simulation Science - ROM
- Shell - Romeo

Profimatics - On-Opt
- Honeywell

Litwin Process Automation - FACS

DOT Products, Inc. - NOVA

Distributed Control System

Runs control algorithm three times a second

Tags - contain about 20 values for each measurement, e.g. set point, limits, alarm

Refinery and large chemical plants have 5,000 - 10,000 tags

Data Historian

Stores instantaneous values of measurements for each tag every five seconds or as specified.

Includes a relational data base for laboratory and other measurements not from the DCS

Values are stored for one year, and require hundreds of megabites

Information made available over a LAN in various forms, e.g. averages, Excel files.

Key Elements

Gross Error Detection

Data Reconciliation

Parameter Estimation

Economic Model
(Profit Function)

Plant Model
(Process Simulation)

Optimization Algorithm

DATA RECONCILIATION

Adjust process data to satisfy material and energy balances.

Measurement error - **e**

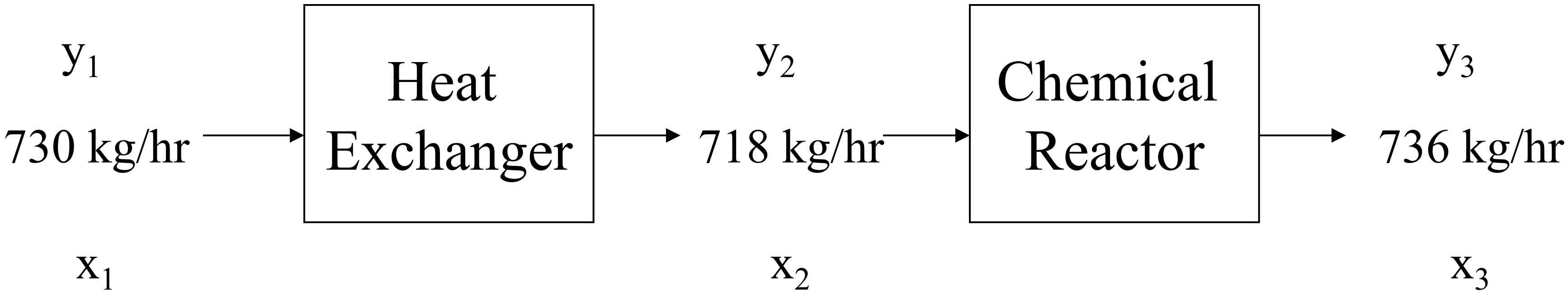
$$\mathbf{e} = \mathbf{y} - \mathbf{x}$$

y = measured process variables
x = true values of the measured variables

$$\tilde{\mathbf{x}} = \mathbf{y} + \mathbf{a}$$

a - measurement adjustment

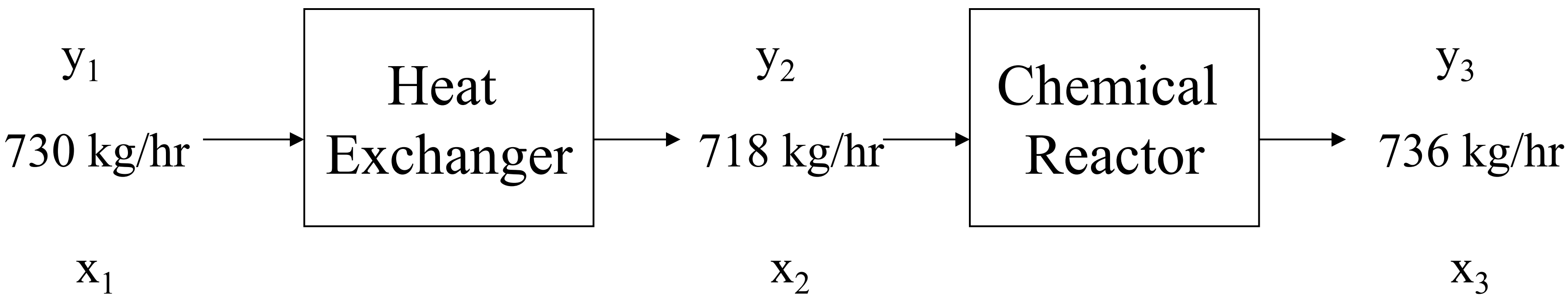
Data Reconciliation



Material Balance $x_1 = x_2$ $x_1 - x_2 = 0$

Steady State $x_2 = x_3$ $x_2 - x_3 = 0$

Data Reconciliation



$$\begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$Ax = 0$$

Data Reconciliation using Least Squares

$$\min_{x} : \sum_{i=1}^{n} \left(\frac{y_i - x_i}{\sigma_i} \right)^2$$

Subject to: $Ax = 0$

$Q =$ diag[🏭$_i$]

Analytical solution using LaGrange Multipliers

$$\hat{x} = y - QA^T (AQA^T)^{-1} Ay$$

$$\hat{x} = [728 \quad 728 \quad 728]^T$$

Data Reconciliation

Measurements having only random errors - least squares

$$\underset{x}{Minimize:}\sum_{i=1}^{n}\left(\frac{y_i - x_i}{\sigma_i}\right)^2$$

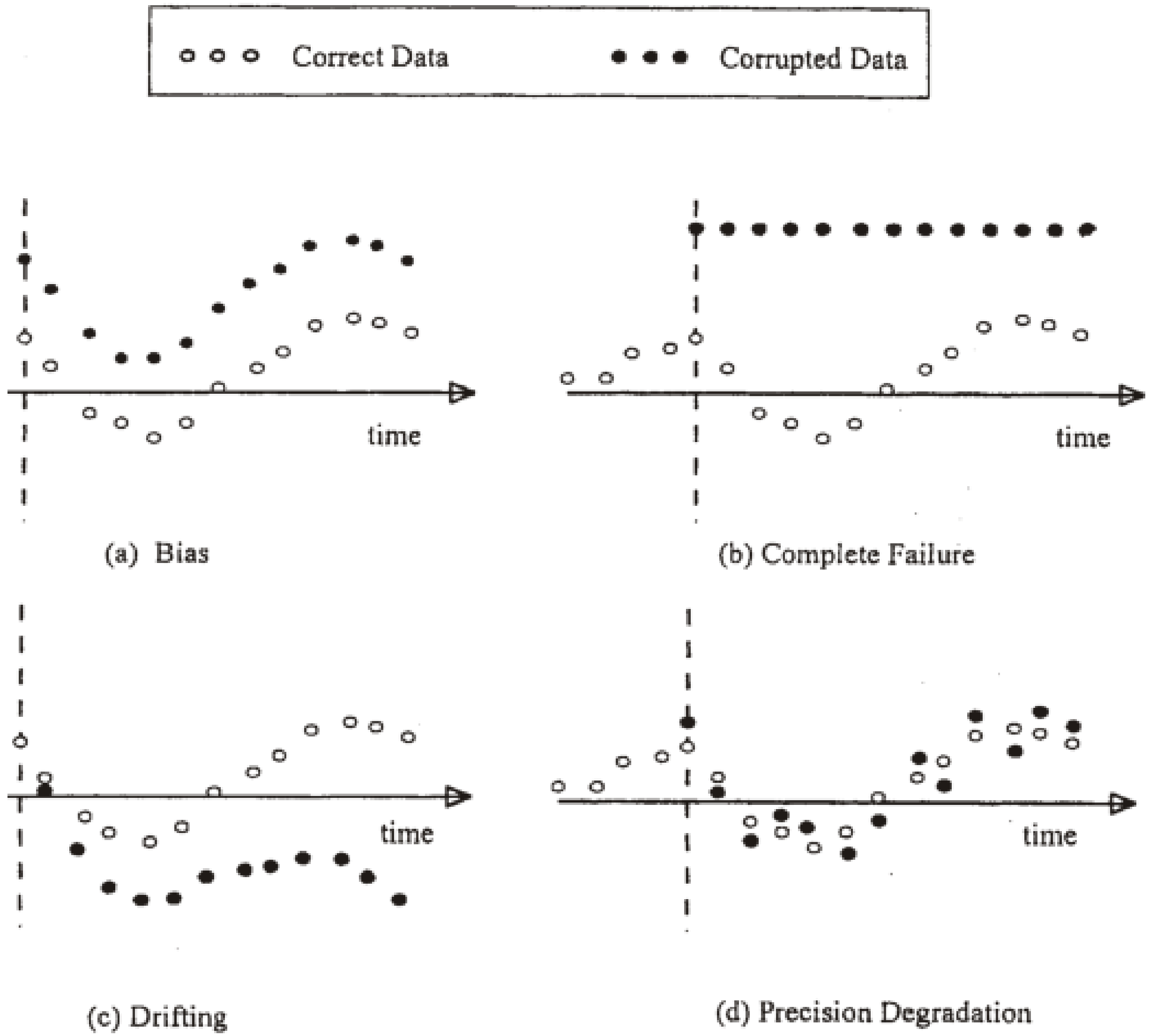
$$Subject\ to: \quad f(x) = 0$$

f(x) - process model

- linear or nonlinear

σ_i = standard deviation of y_i

Types of Gross Errors



Source: S. Narasimhan and C. Jordache, *Data Reconciliation and Gross Error Detection*, Gulf Publishing Company, Houston, TX (2000)

Combined Gross Error Detection and Data Reconciliation

Measurement Test Method - least squares

Minimize: $(\mathbf{y} - \mathbf{x})^T Q^{-1} (\mathbf{y} - \mathbf{x}) = \mathbf{e}^T \mathbf{Q}^{-1} \mathbf{e}$

$\mathbf{x}, \mathbf{z}$

Subject to: $\mathbf{f}(\mathbf{x}, \mathbf{z}, \quad) = 0$

$\mathbf{x}^L \quad \mathbf{x} \quad \mathbf{x}^U$

$\mathbf{z}^L \quad \mathbf{z} \quad \mathbf{z}^U$

Test statistic:

if $e_i = y_i - x_i \ / \quad _i \geq C$ measurement contains a gross error

Least squares is based on only random errors being present Gross errors cause numerical difficulties

Need methods that are not sensitive to gross errors

Methods Insensitive to Gross Errors

Tjao-Biegler's Contaminated Gaussian Distribution

$$P(y_i \quad x_i) = (1\text{-}\eta)P(y_i \quad x_i, R) + \eta\, P(y_i \quad x_i, G)$$

$P(y_i \quad x_i, R)$ = probability distribution function for the random error
$P(y_i \quad x_i, G)$ = probability distribution function for the gross error.
Gross error occur with probability η

Gross Error Distribution Function

$$P(y \quad x, G) \qquad \frac{1}{\sqrt{2\pi} b\sigma}\, e^{\frac{(y \quad x)^2}{2b^2\sigma^2}}$$

Tjao-Biegler Method

Maximizing this distribution function of measurement errors or minimizing the negative logarithm subject to the constraints in plant model, i.e.,

$$\underset{\mathbf{x}}{\text{Minimize:}} \quad {}_{i}\left\{ \ln\left[(1 \quad) e^{\frac{(y_i \quad x_i)^2}{2 \quad {}_i^2}} \quad \frac{}{b} e^{\frac{(y_i \quad x_i)^2}{2b^2 \quad {}_i^2}} \right] \ln\left[\sqrt{2 \quad } \quad {}_i \right] \right\}$$

Subject to: $\mathbf{f}(\mathbf{x}) = 0$ — plant model

$\mathbf{x}^L \quad \mathbf{x} \quad \mathbf{x}^U$ — bounds on the process variables

A NLP, and values are needed for and b

Test for Gross Errors

If P(y_i x_i, G) (1-)P(y_i x_i, R), gross error

probability of a gross error — probability of a random error

$$_i \quad \frac{y_i \quad x_i}{_i} > \sqrt{\frac{2b^2}{b^2 \quad 1} \ln\left[\frac{b(1 \quad)}{} \right]}$$

Robust Function Methods

Minimize: $-\quad[\quad(y_i, x_i)\,]$
$\mathbf{x}\qquad\qquad i$

Subject to: $\mathbf{f}(\mathbf{x}) = 0$

$\mathbf{x}^L \quad \mathbf{x} \quad \mathbf{x}^U$

Lorentzian distribution

$$(\ _i) \qquad \frac{1}{1 \qquad \frac{1}{2}\ {}_i^2}$$

Fair function

$$(\ _i, c) \qquad c^2\left[\frac{\ _i}{c} \qquad \log\left(1 \qquad \frac{\ _i}{c}\right)\right]$$

c is a tuning parameter

Test statistic

$${}_i = (y_i - x_i)/\ \ _i$$

Parameter Estimation
Error-in-Variables Method

Least squares

Minimize: $(\mathbf{y} - \mathbf{x})^T \; ^{-1}(\mathbf{y} - \mathbf{x}) = \mathbf{e}^T \; ^{-1}\mathbf{e}$

Subject to: $\mathbf{f}(\mathbf{x}, \;) = 0$

- plant parameters

Simultaneous data reconciliation and parameter estimation

Minimize: $(\mathbf{y} - \mathbf{x})^T \; ^{-1}(\mathbf{y} - \mathbf{x}) = \mathbf{e}^T \; ^{-1}\mathbf{e}$
$\mathbf{x},$

Subject to: $\mathbf{f}(\mathbf{x}, \;) = 0$

another nonlinear programming problem

Three Similar Optimization Problems

Optimize: **Objective function**
Subject to: **Constraints are the plant model**

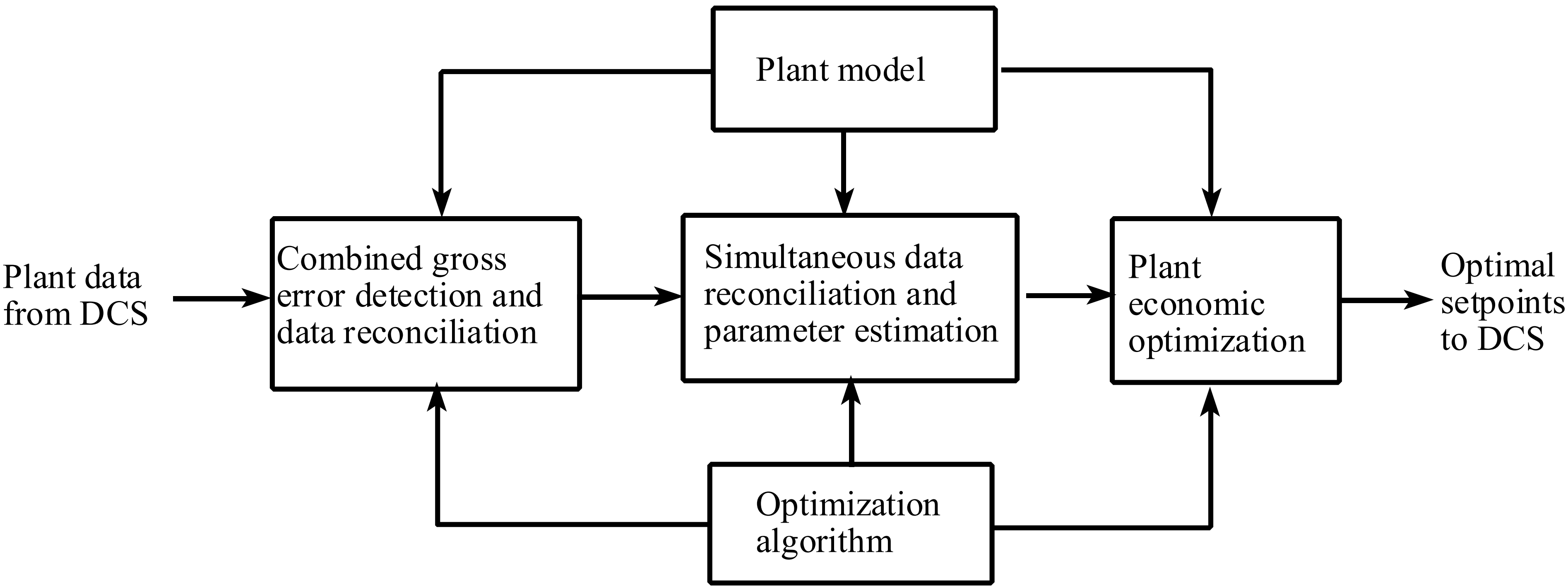
Objective function

data reconciliation - distribution function
parameter estimation - least squares
economic optimization - profit function

Constraint equations

material and energy balances
chemical reaction rate equations
thermodynamic equilibrium relations
capacities of process units
demand for product
availability of raw materials

Key Elements of On-Line Optimization



Interactive On-Line Optimization Program

1. Conduct combined gross error detection and data reconciliation to detect and rectify gross errors in plant data sampled from distributed control system using the Tjoa-Biegler's method (the contaminated Gaussian distribution) or robust method (Lorentzian distribution).

This step generates a set of measurements containing only random errors for parameter estimation.

2. Use this set of measurements for simultaneous parameter estimation and data reconciliation using the least squares method.

This step provides the updated parameters in the plant model for economic optimization.

3. Generate optimal set points for the distributed control system from the economic optimization using the updated plant and economic models.

Interactive On-Line Optimization Program

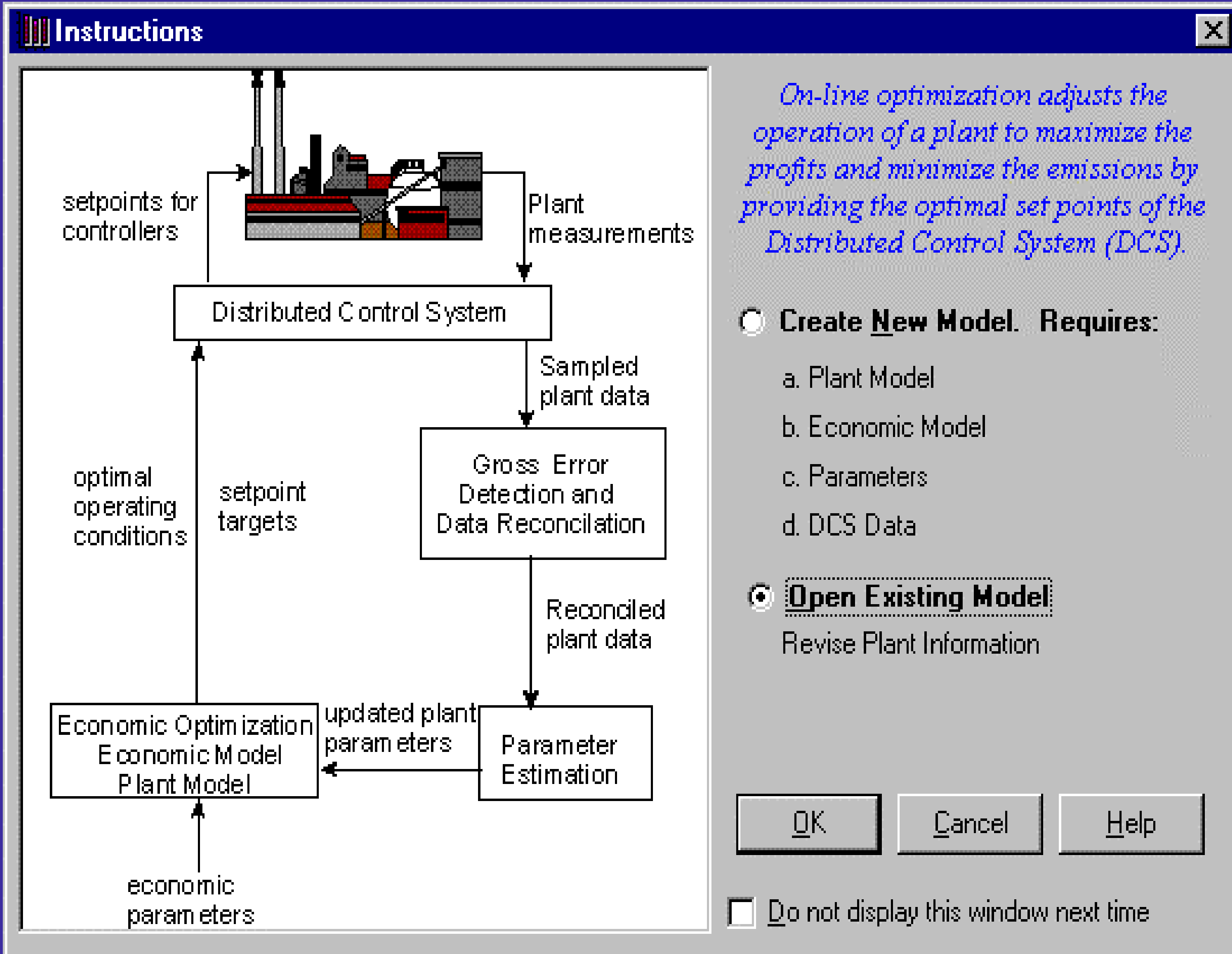
Process and economic models are entered as equations in a form similar to Fortran

The program writes and runs three GAMS programs.

Results are presented in a summary form, on a process flowsheet and in the full GAMS output

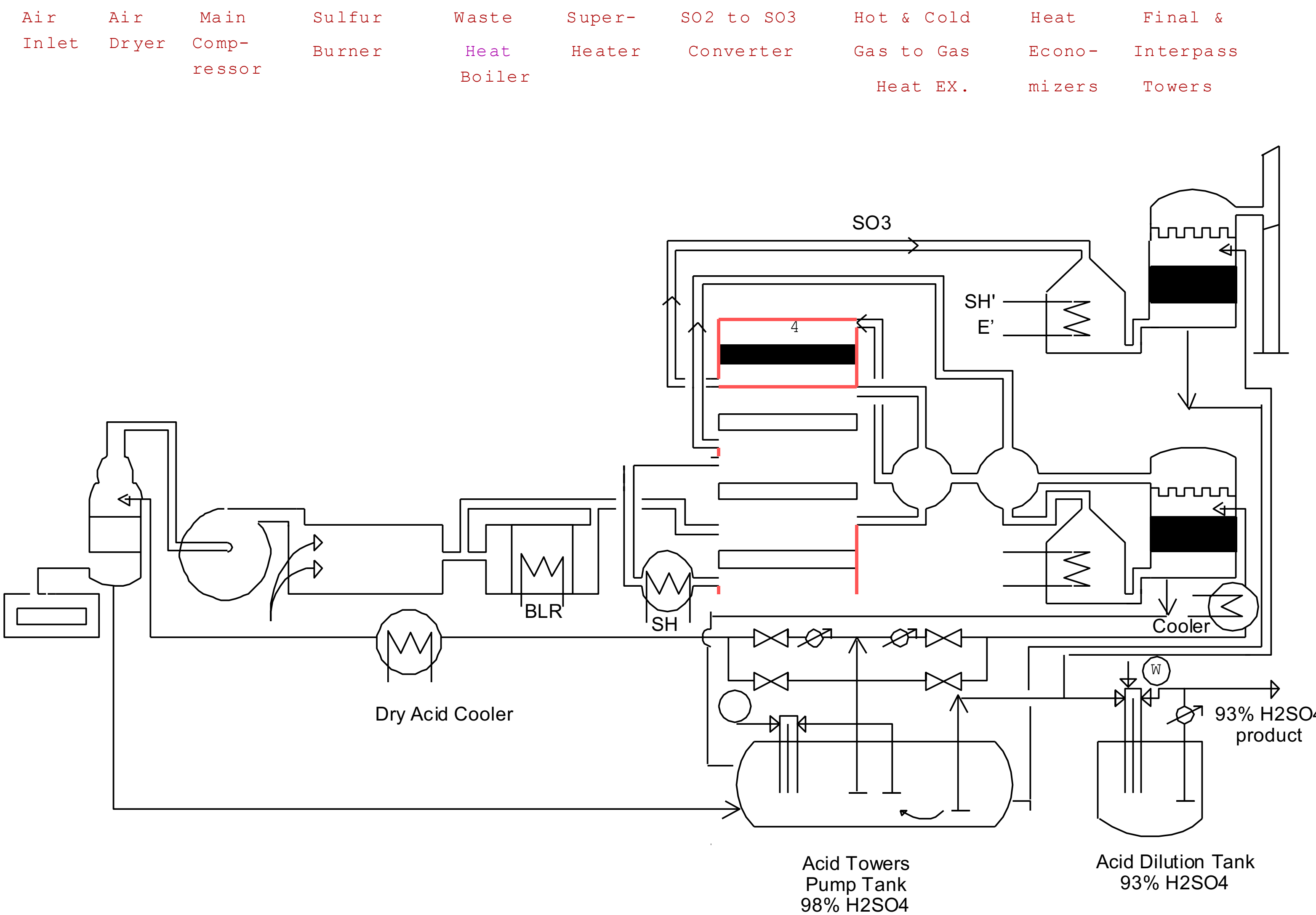
The program and users manual (120 pages) can be downloaded from the LSU Minerals Processing Research Institute web site

URLhttp://www.mpri.lsu.edu


Instructions
setpoints for controllers
Plant measurements
Distributed Control System
Sampled plant data
Gross Error Detection and Data Reconcilation
optimal operating conditions
setpoint targets
Reconciled plant data
Economic Optimization
Economic Model
Plant Model
updated plant parameters
Parameter Estimation
economic parameters
On-line optimization adjusts the operation of a plant to maximize the profits and minimize the emissions by providing the optimal set points of the Distributed Control System (DCS).
Create New Model. Requires:
a. Plant Model
b. Economic Model
c. Parameters
d. DCS Data
Open Existing Model
Revise Plant Information
OK
Cancel
Help
Do not display this window next time

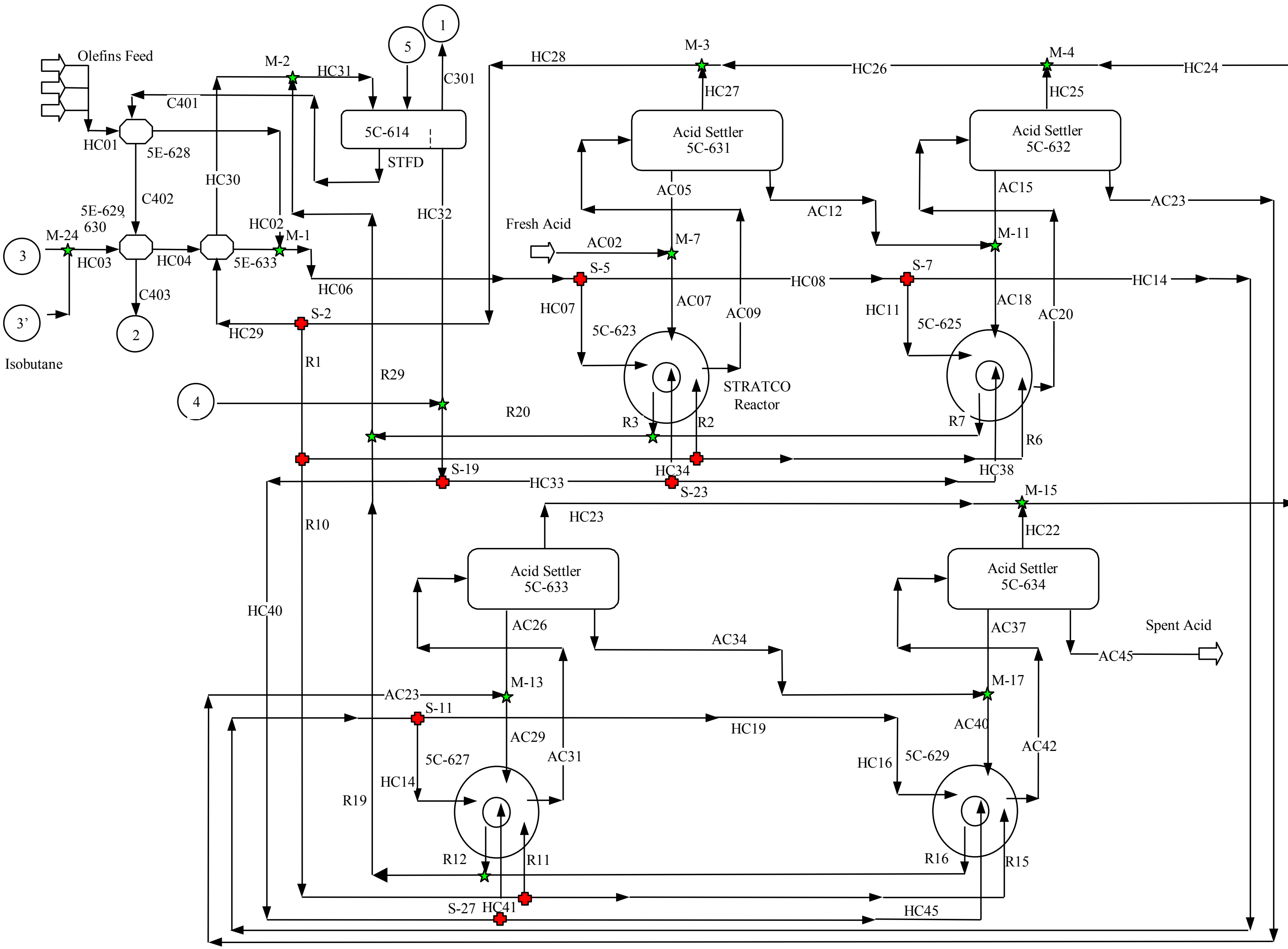
Mosaic-Monsanto Sulfuric Acid Plant

3,200 tons per day of 93% Sulfuric Acid, Convent, Louisiana



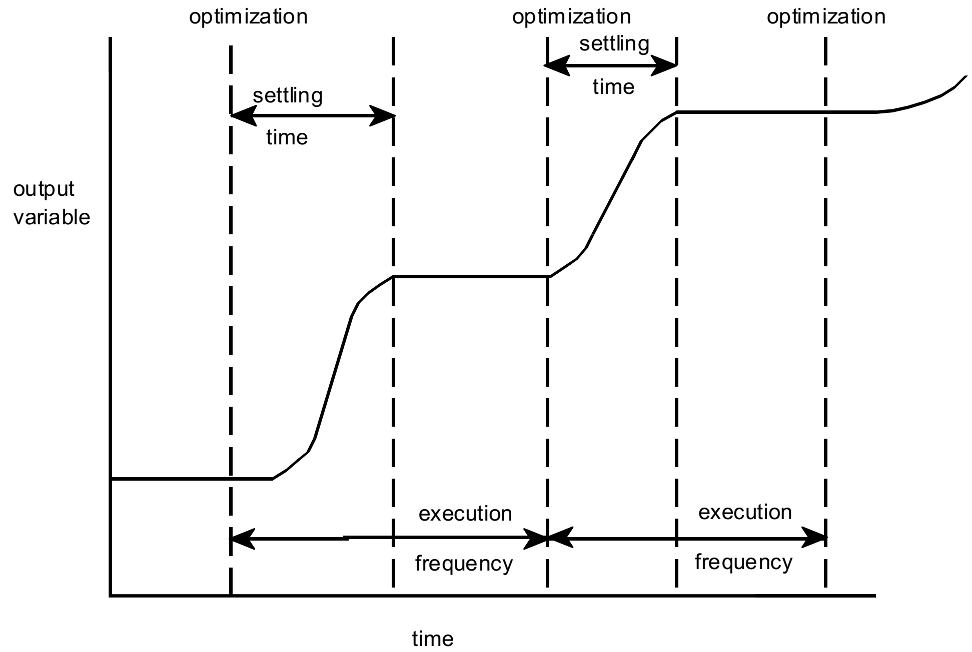
Motiva Refinery Alkylation Plant

15,000 barrels per day, Convent, Louisiana, reactor section, 4 Stratco reactors

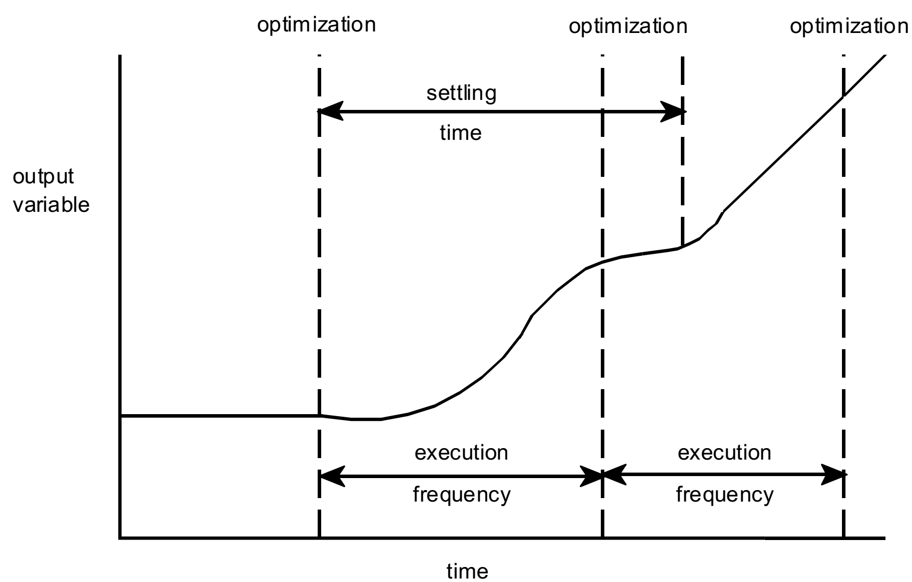


Steady State Detection

Execution frequency must be greater than the plant settling time (time to return to steady state).



a. Time between optimizations is longer than settling time



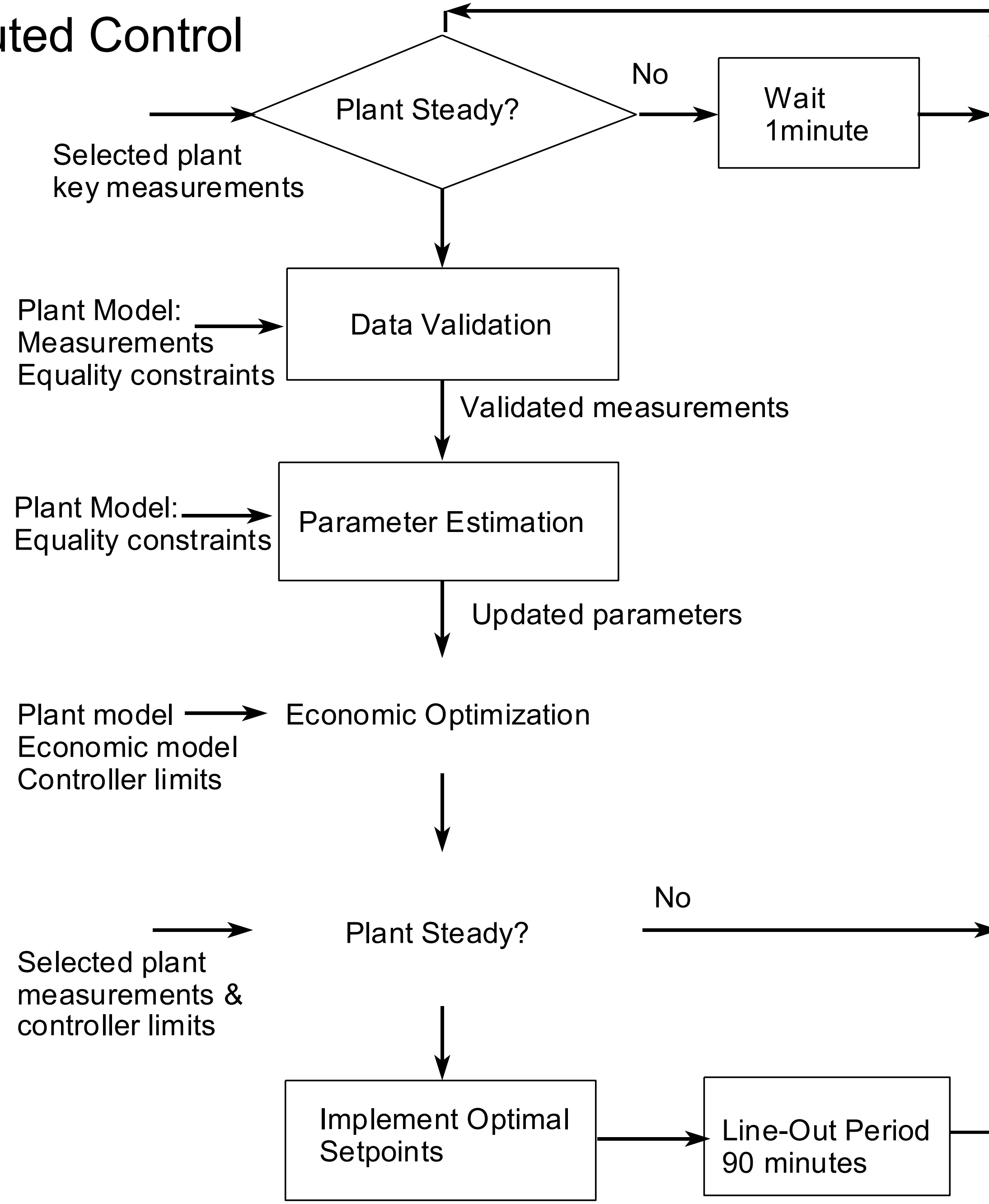
b. Time between optimizations is less than settling time

On-Line Optimization - Distributed Control System Interface

Plant must at steady state when data extracted from DCS and when set points sent to DCS.

Plant models are steady state models.

Coordinator program



Some Other Considerations

Redundancy

Observeability

Variance estimation

Closing the loop

Dynamic data reconciliation and parameter estimation

Additional Observations

Most difficult part of on-line optimization is developing and validating the process and economic models.

Most valuable information obtained from on-line optimization is a more thorough understanding of the process

Mixed Integer Programming

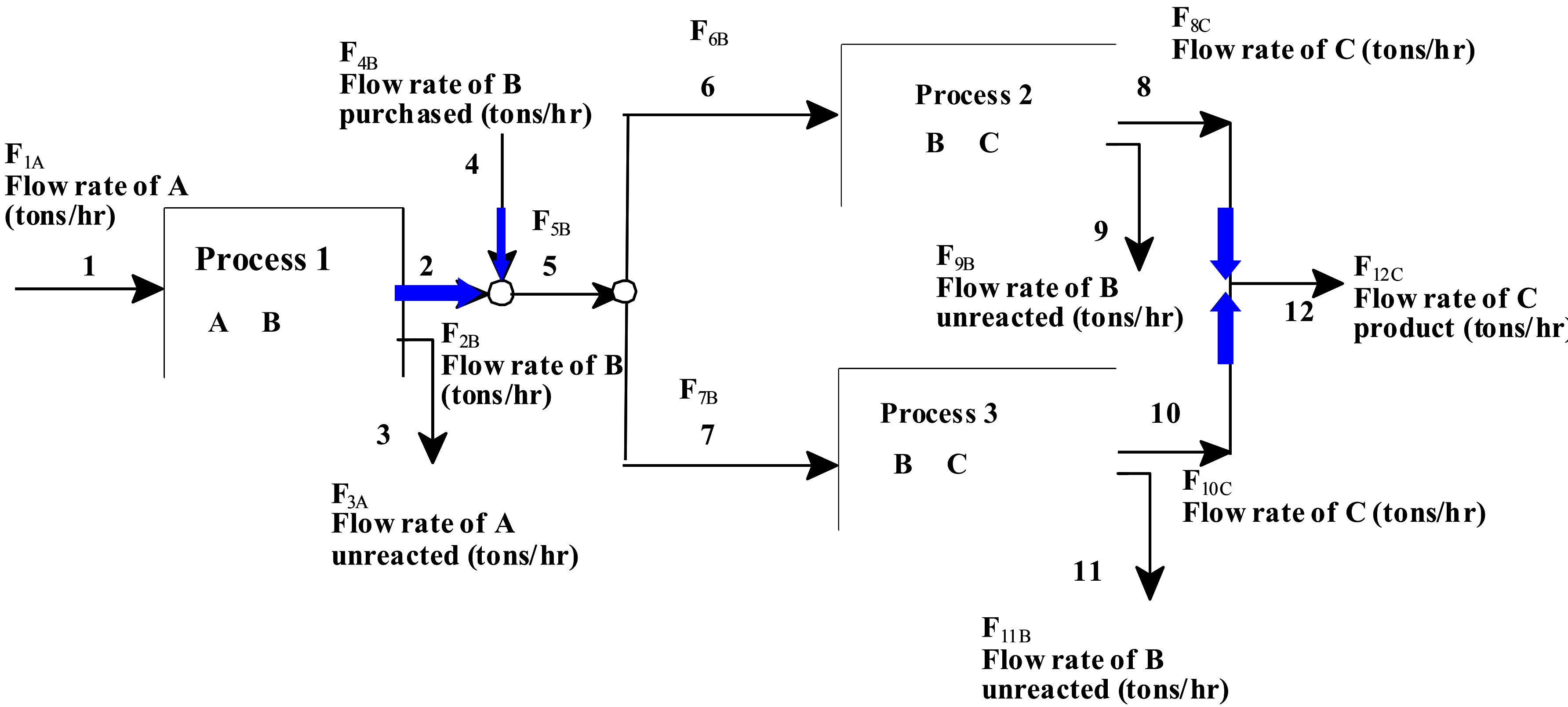
Numerous Applications

- Batch Processing
- Pinch Analysis
- Optimal Flowsheet Structure

Branch and Bound Algorithm

- Solves MILP
- Used with NLP Algorithm to solve MINLP

Mixed Integer Process Example



Produce C from either Process 2 or Process 3

Make B from A in Process 1 or purchase B

Mixed Integer Process Example

operating cost — fixed cost — feed cost — sales

max: $-250 F_1^A - 400 F_6^B - 550 F_7^B - 1{,}000 y_1 - 1{,}500 y_2 - 2{,}000 y_3 - 500 F_1^A - 950 F_4^B + 1{,}800 F_{12}^C$

subject to:

mass yields

$-0.90 F_1^A + F_2^B = 0$

$-0.10 F_1^A + F_3^A = 0$

$-0.82 F_6^B + F_8^C = 0$

$-0.18 F_6^B + F_9^B = 0$

$-0.95 F_7^B + F_{10}^C = 0$

$-0.05 F_7^B + F_{11}^B = 0$

node MB

$F_2^B + F_4^B - F_5^B = 0$

$F_5^B = F_6^B - F_7^B = 0$

$F_8^C + F_{10}^C - F_{12}^C = 0$

availability of A $F_1^A \leq 16 y_1$ **Availability of raw material A to make B**

availability of B $F_4^B \leq 20 y_4$ **Availability of purchased material B**

demand for C $F_8^C \leq 10 y_2$ **Demand for C from either Process 2,**

$F_{10}^C \leq 10 y_3$ **stream F_8^C or Process 3, stream F_{10}^C**

integer constraint $y_2 + y_3 = 1$ **Select either Process 1 or Purchase B**

$y_1 + y_4 = 1$ **Select either Process 2 or 3**

Branch and bound algorithm used for optimization

Branch and Bound Algorithm

LP Relaxation Solution

Max: $5x_1 + 2x_2 = P$ — $P = 22.5$

Subject to: $x_1 + x_2 \leq 4.5$ — $x_1 = 4.5$

$-x_1 + 2x_2 \leq 6.0$ — $x_2 = 0$

x_1 and x_2 are integers ≥ 0

Branch on x_1, it is not an integer in the LP Relaxation Solution

Form two new problems by adding constraints $x_1 \geq 5$ and $x_1 \leq 4$

Max: $5x_1 + 2x_2 = P$

Subject to: $x_1 + x_2 \leq 4.5$

$-x_1 + 2x_2 \leq 6.0$

$x_1 \geq 5$

Max: $5x_1 + 2x_2 = P$

Subject to: $x_1 + x_2 \leq 4.5$

$-x_1 + 2x_2 \leq 6.0$

$x_1 \leq 4$

Branch and Bound Algorithm

Max: $5x_1 + 2x_2 = P$
Subject to:
$x_1 + x_2 \leq 4.5$
$-x_1 + 2x_2 \leq 6.0$
$x_1 \geq 5$
infeasible
no further evaluations required

Max: $5x_1 + 2x_2 = P$
Subject to:
$x_1 + x_2 \leq 4.5$
$-x_1 + 2x_2 \leq 6.0$
$x_1 \leq 4$
LP solution P = 21.0
$x_1 = 4$
$x_2 = 0.5$
branch on x_2

Form two new problems by adding constraints $x_2 \geq 1$ and $x_2 \leq 0$

Max: $5x_1 + 2x_2 = P$
Subject to:
$x_1 + x_2 \leq 4.5$
$-x_1 + 2x_2 \leq 6.0$
$x_1 \leq 4$
$x_2 \geq 1$

Max: $5x_1 + 2x_2 = P$
Subject to:
$x_1 + x_2 \leq 4.5$
$-x_1 + 2x_2 \leq 6.0$
$x_1 \leq 4$
$x_2 \leq 0 = 0$

Branch and Bound Algorithm

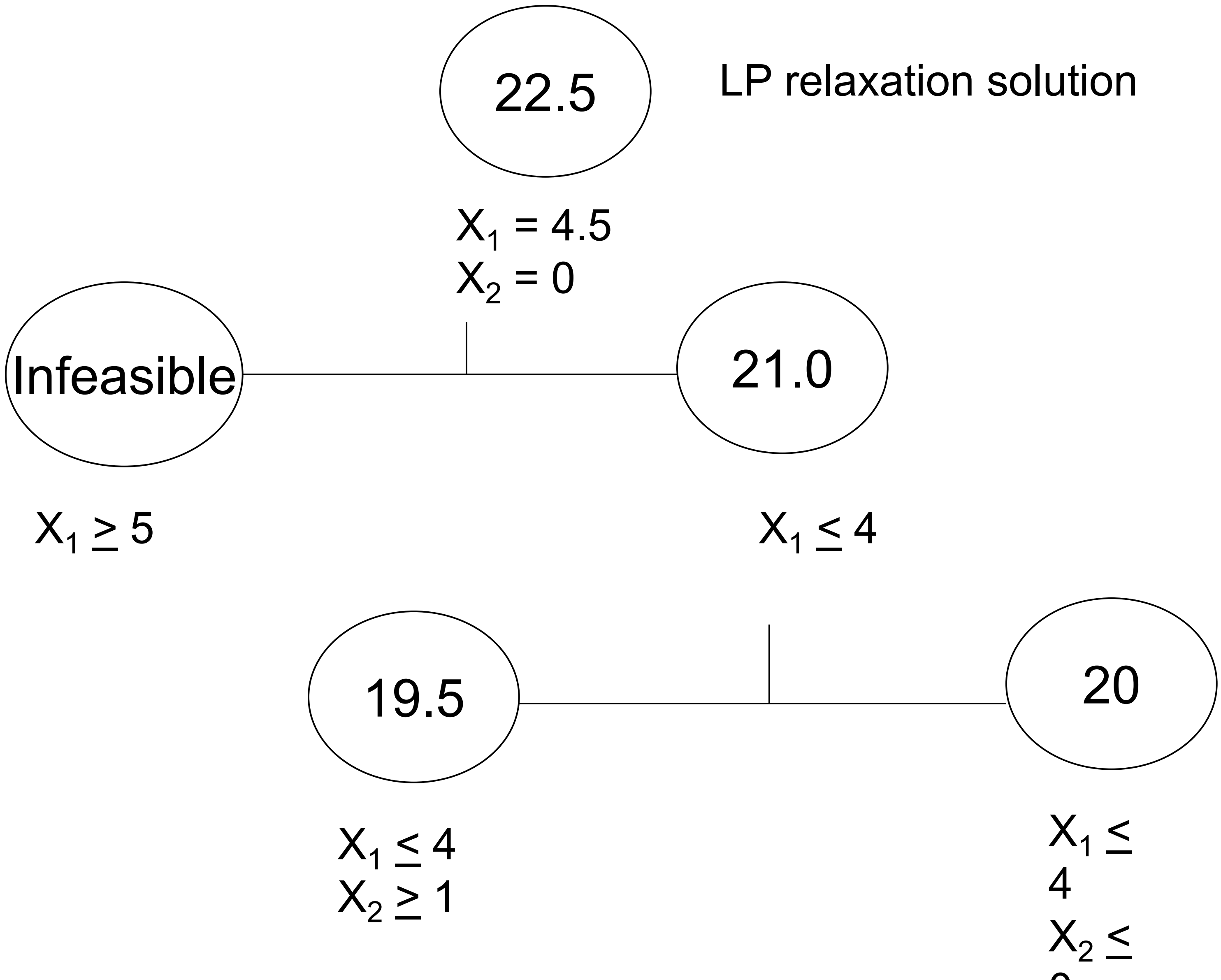
Max: $5x_1 + 2x_2 = P$
Subject to:
$x_1 + x_2 \leq 4.5$
$-x_1 + 2x_2 \leq 6.0$
$x_1 \leq 4$
$x_2 \geq 1$

$P = 19.5$
$x_1 = 3.5$
$x_2 = 1$

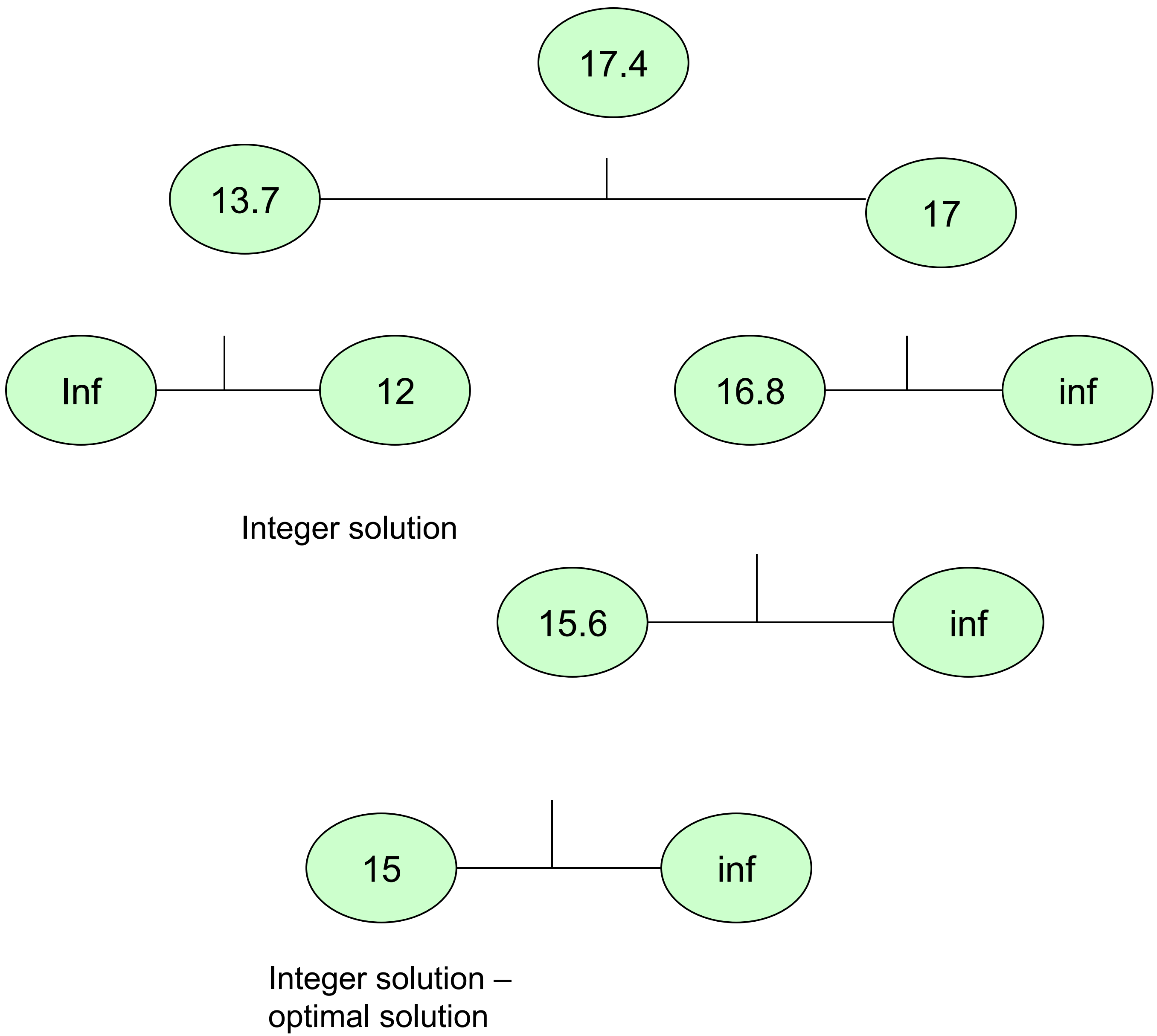
Max: $5x_1 + 2x_2 = P$
Subject to:
$x_1 + x_2 \leq 4.5$
$-x_1 + 2x_2 \leq 6.0$
$x_1 \leq 4$
$x_2 \leq 0$

$P = 20$
$x_1 = 4$
$x_2 = 0$
optimal solution

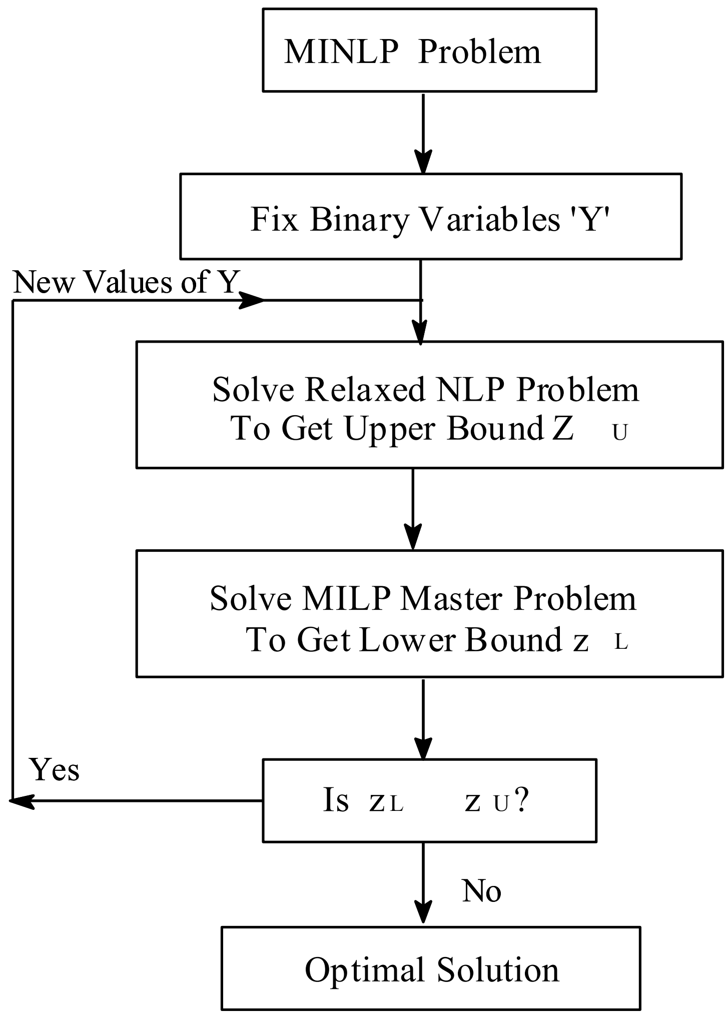
Branch and Bound Algorithm



Branch and Bound Algorithm



Mixed Integer Nonlinear Programming



Flow Chart of GBD Algorithm to Solve MINPL Problems,
Duran and Grossmann, 1986, Mathematical Programming, Vol. 36, p. 307-339

Triple Bottom Line

Triple Bottom Line =

Product Sales

- Manufacturing Costs (raw materials, energy costs, others)
- Environmental Costs (compliance with environmental regulations)
- Sustainable Costs (repair damage from emissions within regulations)

Triple Bottom Line =

Profit (sales – manufacturing costs)

- Environmental Costs

+ Sustainable (Credits – Costs) (credits from reducing emissions)

Sustainable costs are costs to society from damage to the environment caused by emissions within regulations, e.g., sulfur dioxide 4.0 lb per ton of sulfuric acid produced.

Sustainable development: Concept that development should meet the needs of the present without sacrificing the ability of the future to meet its needs

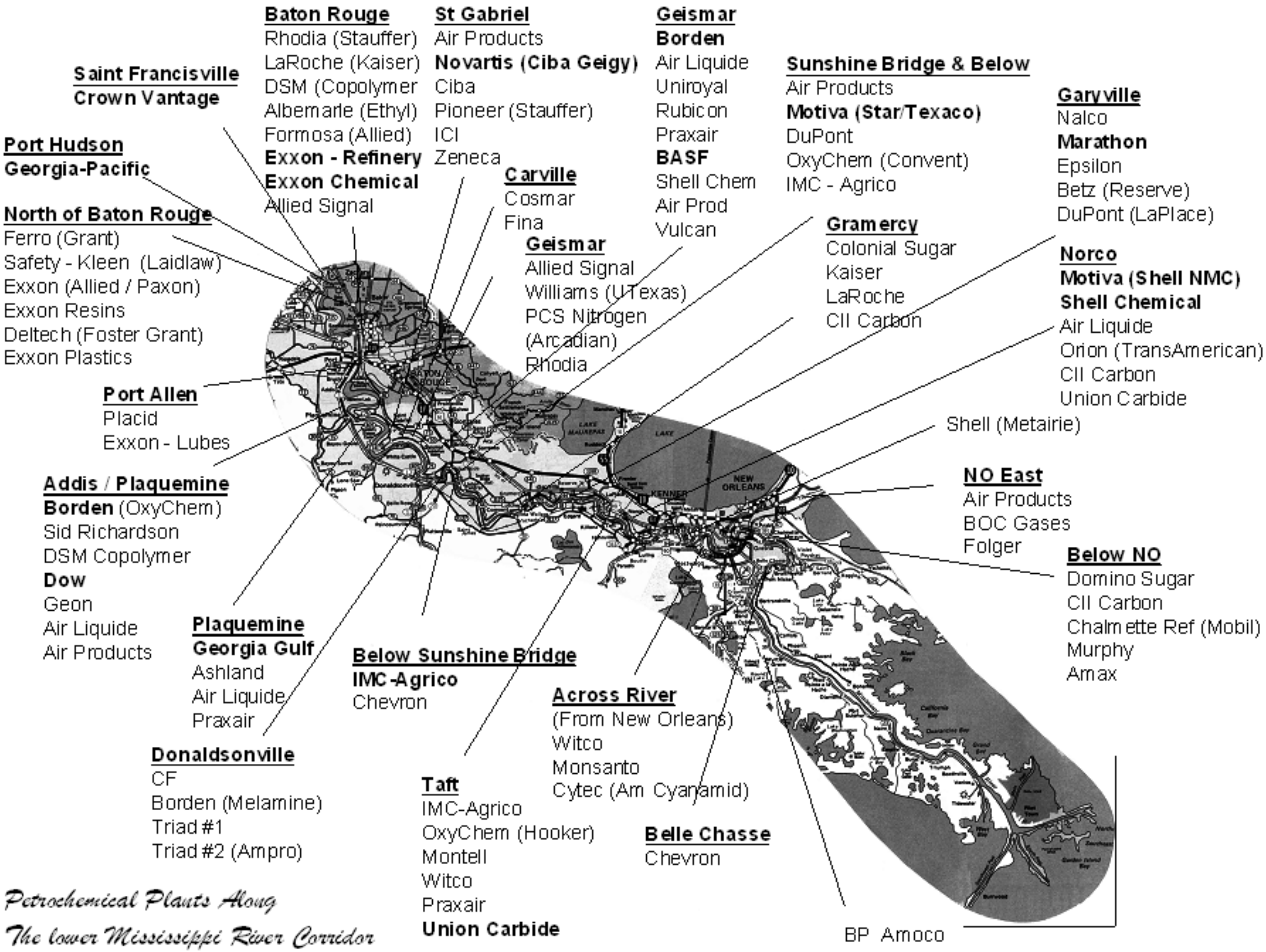
Optimization of Chemical Production Complexes

- Opportunity
  - New processes for conversion of surplus carbon dioxide to valuable products

- Methodology
  - Chemical Complex Analysis System

  - Application to chemical production complex in the lower Mississippi River corridor

Plants in the lower Mississippi River Corridor

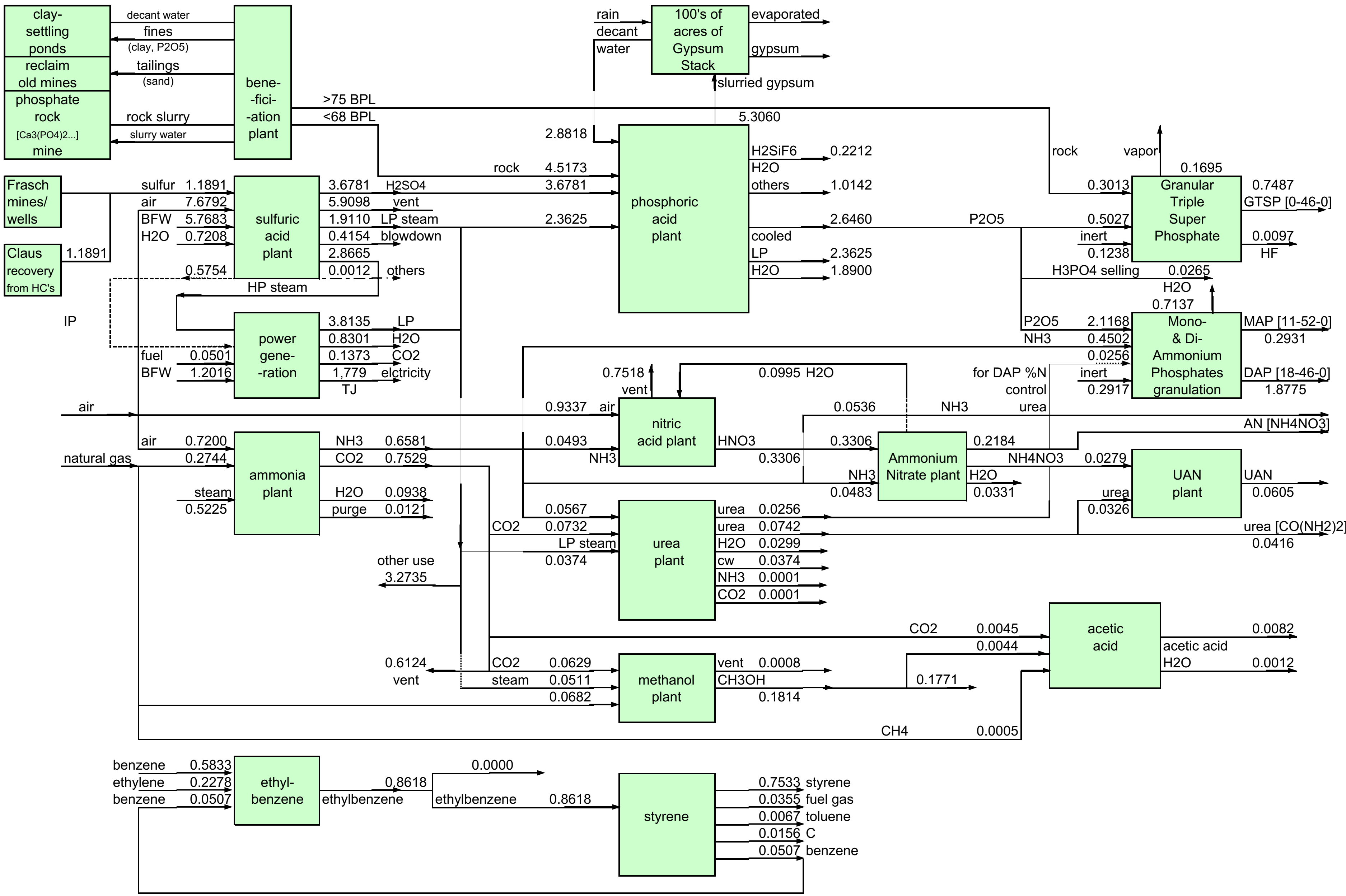


Source: Peterson, R.W., 2000

Some Chemical Complexes in the World

- North America
  - Gulf coast petrochemical complex in Houston area
  - Chemical complex in the Lower Mississippi River Corridor
- South America
  - Petrochemical district of Camacari-Bahia (Brazil)
  - Petrochemical complex in Bahia Blanca (Argentina)
- Europe
  - Antwerp port area (Belgium)
  - BASF in Ludwigshafen (Germany)
- Oceania
  - Petrochemical complex at Altona (Australia)
  - Petrochemical complex at Botany (Australia)

Plants in the lower Mississippi River Corridor, Base Case. Flow Rates in Million Tons Per Year



Commercial Uses of CO_2

Chemical synthesis in the U. S. consumes 110 million m tons per year of CO_2

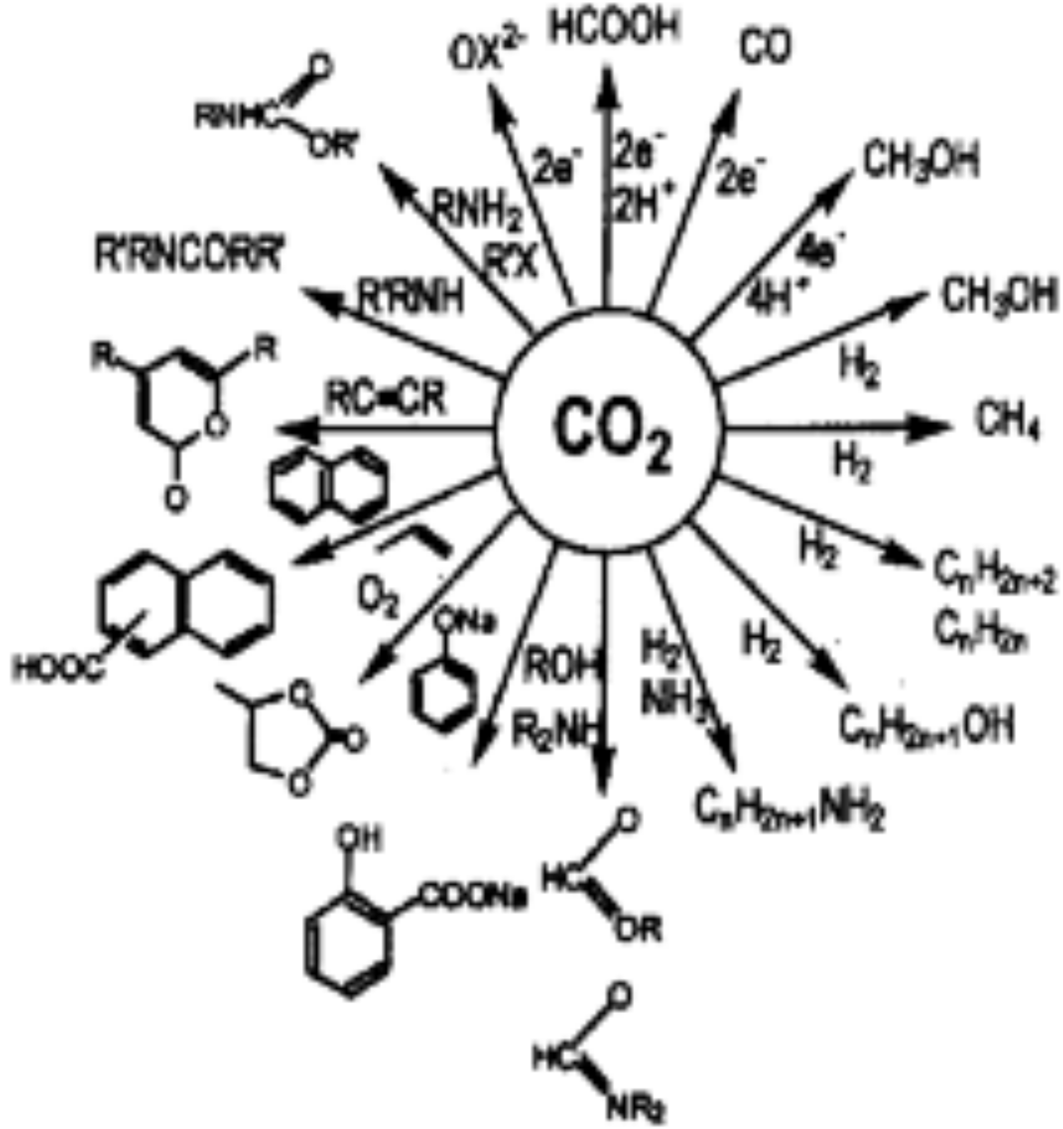
- Urea (90 million tons per year)
- Methanol (1.7 million tons per year)
- Polycarbonates
- Cyclic carbonates
- Salicylic acid
- Metal carbonates

Surplus Carbon Dioxide

- Ammonia plants produce 0.75 million tons per year in lower Mississippi River corridor.
- Methanol and urea plants consume 0.14 million tons per year.
- Surplus high-purity carbon dioxide 0.61 million tons per year vented to atmosphere.
- Plants are connected by CO_2 pipelines.

Greenhouse Gases as Raw Material

- Intermediate of fine chemicals for the chemical industry
  - -C(O)O-: Acids, esters, lactones
  - -O-C(O)O-:Carbonates
  - -NC(O)OR-: Carbamic esters
  - -NCO: Isocyanates
  - -N-C(O)-N: Ureas
- Use as a solvent
- Energy rich products
  CO, CH_3OH



From Creutz and Fujita, 2000

Some Catalytic Reactions of CO_2

Hydrogenation

$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$ methanol

$2CO_2 + 6H_2 \rightarrow C_2H_5OH + 3H_2O$ ethanol

$CO_2 + H_2 \rightarrow CH_3\text{-O-}CH_3$ dimethyl ether

Hydrolysis and Photocatalytic Reduction

$CO_2 + 2H_2O \rightarrow CH_3OH + O_2$

$CO_2 + H_2O \rightarrow HC\text{=O-OH} + 1/2O_2$

$CO_2 + 2H_2O \rightarrow CH_4 + 2O_2$

Hydrocarbon Synthesis

$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$ methane and higher HC

$2CO_2 + 6H_2 \rightarrow C_2H_4 + 4H_2O$ ethylene and higher olefins

Carboxylic Acid Synthesis

$CO_2 + H_2 \rightarrow HC\text{=O-OH}$ formic acid

$CO_2 + CH_4 \rightarrow CH_3\text{-C=O-OH}$ acetic acid

Other Reactions

CO_2 + ethylbenzene $\rightarrow$ styrene

$CO_2 + C_3H_8 \rightarrow C_3H_6 + H_2 + CO$
dehydrogenation of propane

$CO_2 + CH_4 \rightarrow 2CO + H_2$ reforming

Graphite Synthesis

$CO_2 + H_2 \rightarrow C + H_2O$

$CH_4 \rightarrow C + H_2$
$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$

Amine Synthesis

$CO_2 + 3H_2 + NH_3 \rightarrow CH_3\text{-}NH_2 + 2H_2O$ methyl amine and higher amines

Methodology for Chemical Complex Optimization with New Carbon Dioxide Processes

- Identify potentially new processes
- Simulate with HYSYS
- Estimate utilities required
- Evaluate value added economic analysis
- Select best processes based on value added economics
- Integrate new processes with existing ones to form a superstructure for optimization

Twenty Processes Selected for HYSYS Design

Chemical	Synthesis Route	Reference
Methanol	CO_2 hydrogenation	Nerlov and Chorkendorff, 1999
	CO_2 hydrogenation	Toyir, et al., 1998
	CO_2 hydrogenation	Ushikoshi, et al., 1998
	CO_2 hydrogenation	Jun, et al., 1998
	CO_2 hydrogenation	Bonivardi, et al., 1998
Ethanol	CO_2 hydrogenation	Inui, 2002
	CO_2 hydrogenation	Higuchi, et al., 1998
Dimethyl Ether	CO_2 hydrogenation	Jun, et al., 2002
Formic Acid	CO_2 hydrogenation	Dinjus, 1998
Acetic Acid	From methane and CO_2	Taniguchi, et al., 1998
Styrene	Ethylbenzene dehydrogenation	Sakurai, et al., 2000
	Ethylbenzene dehydrogenation	Mimura, et al., 1998
Methylamines	From CO_2, H_2, and NH_3	Arakawa, 1998
Graphite	Reduction of CO_2	Nishiguchi, et al., 1998
Hydrogen/	Methane reforming	Song, et al., 2002
Synthesis Gas	Methane reforming	Shamsi, 2002
	Methane reforming	Wei, et al., 2002
	Methane reforming	Tomishige, et al., 1998
Propylene	Propane dehydrogenation	Takahara, et al., 1998
	Propane dehydrogenation	C & EN, 2003

Integration into Superstructure

- Twenty processes simulated
- Fourteen processes selected based on value added economic model
- Integrated into the superstructure for optimization with the System

New Processes Included in Chemical Production Complex

Product	Synthesis Route	Value Added Profit (cents/kg)
Methanol	CO_2 hydrogenation	2.8
Methanol	CO_2 hydrogenation	3.3
Methanol	CO_2 hydrogenation	7.6
Methanol	CO_2 hydrogenation	5.9
Ethanol	CO_2 hydrogenation	33.1
Dimethyl Ether	CO_2 hydrogenation	69.6
Formic Acid	CO_2 hydrogenation	64.9
Acetic Acid	From CH_4 and CO_2	97.9
Styrene	Ethylbenzene dehydrogenation	10.9
Methylamines	From CO_2, H_2, and NH_3	124
Graphite	Reduction of CO_2	65.6
Synthesis Gas	Methane reforming	17.2
Propylene	Propane dehydrogenation	4.3
Propylene	Propane dehydrogenation with CO_2	2.5

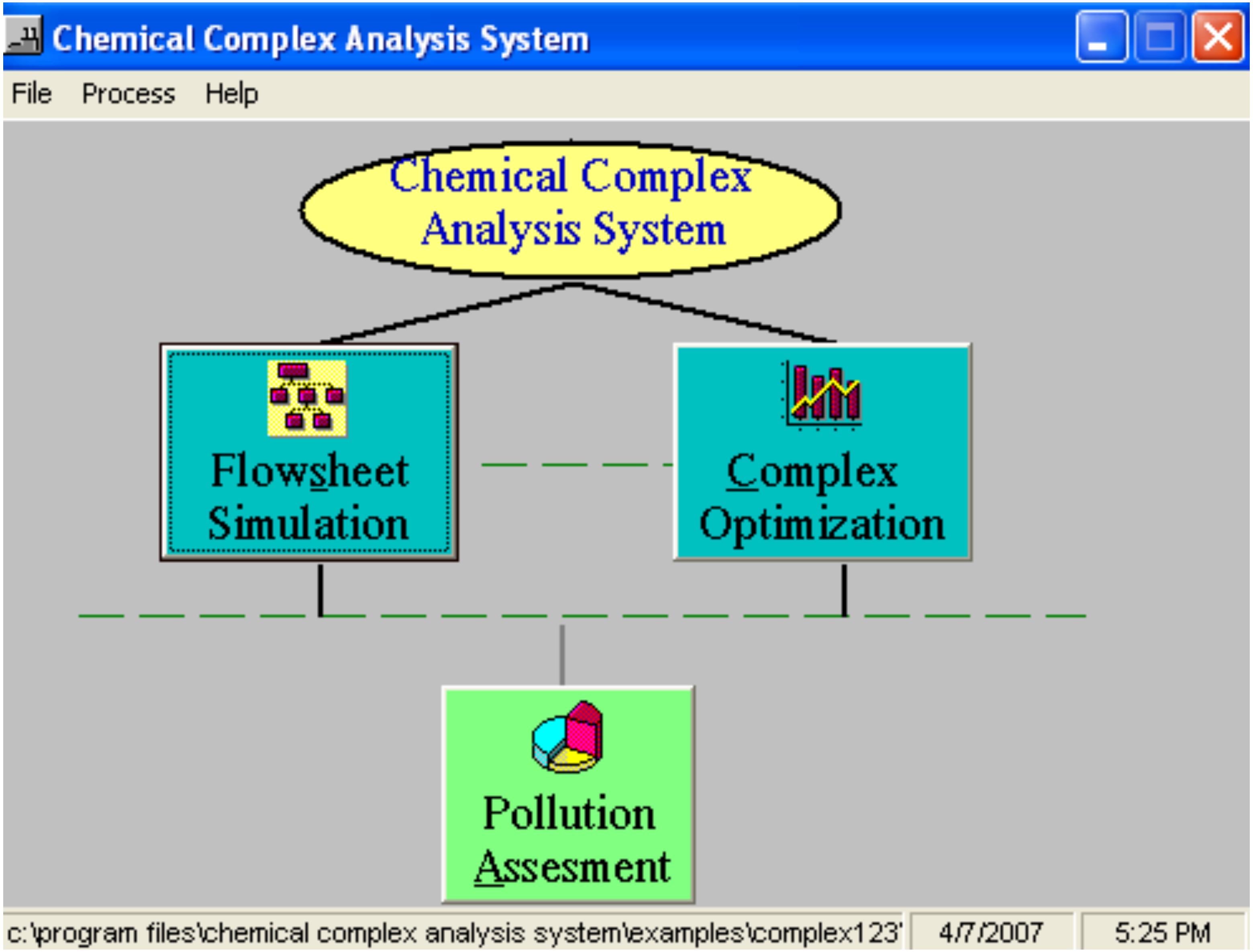
Application of the Chemical Complex Analysis System to Chemical Complex in the Lower Mississippi River Corridor

- Base case – existing plants

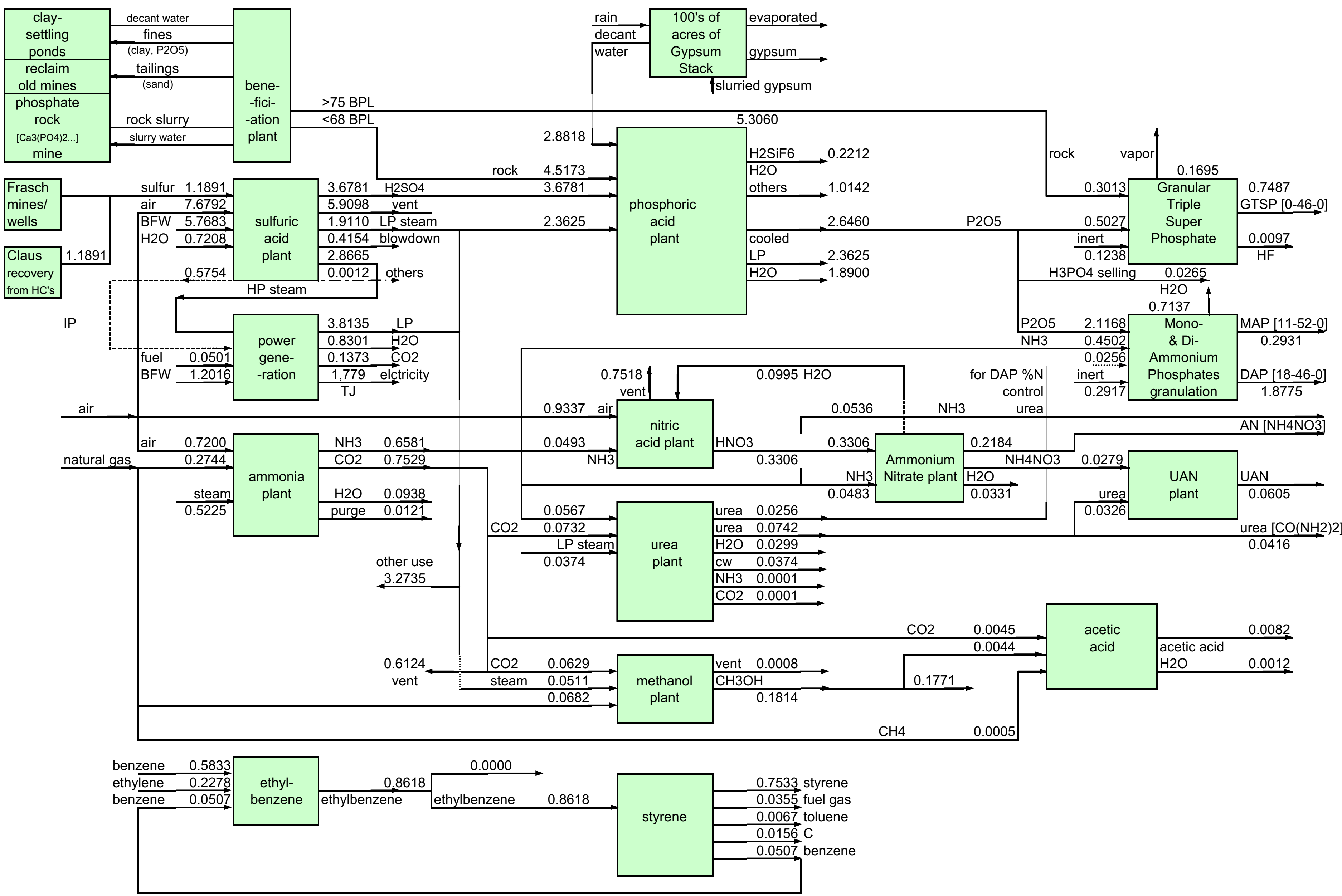
- Superstructure – existing and proposed new plants

- Optimal structure – optimal configuration from existing and new plants

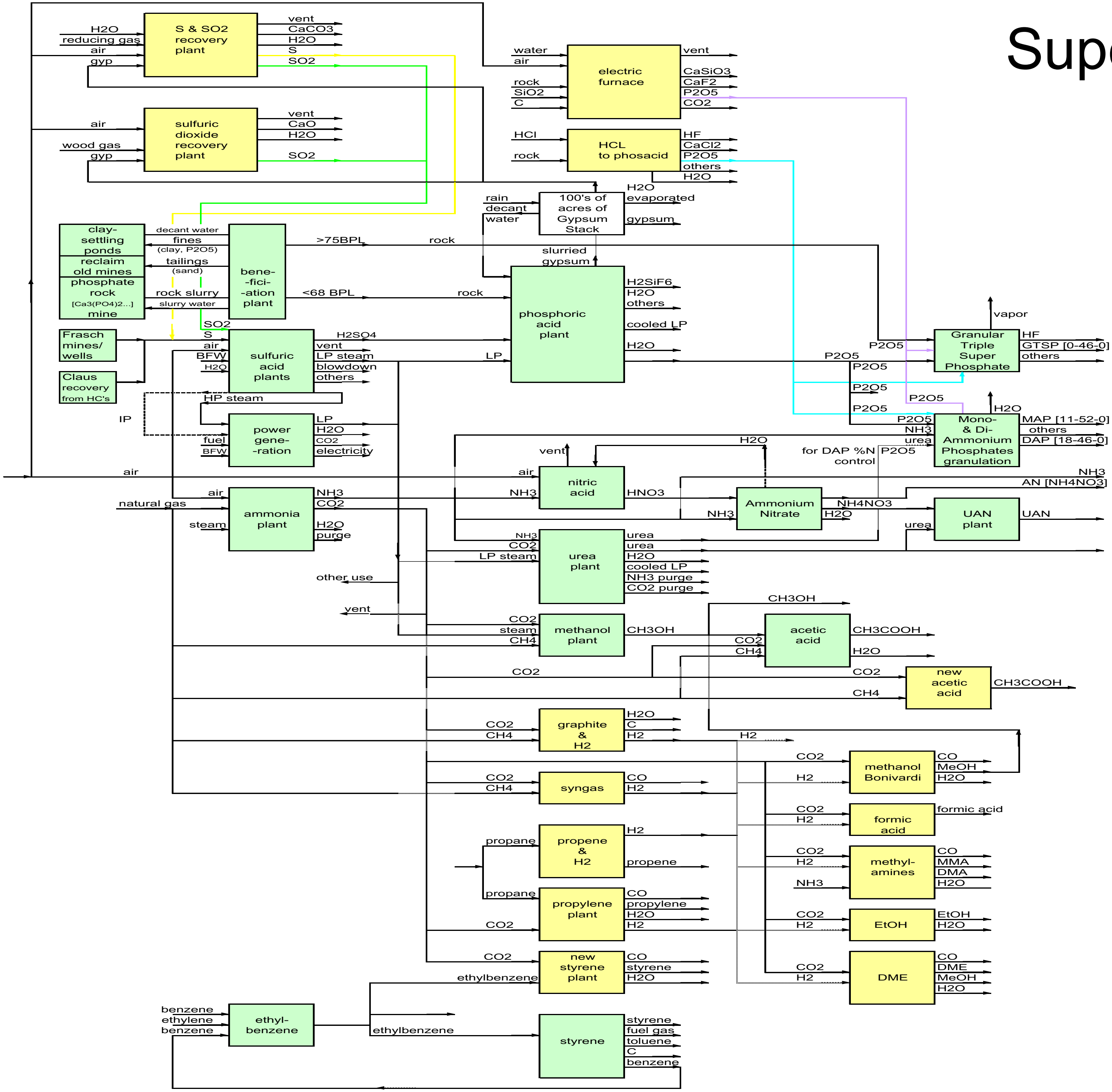
Chemical Complex Analysis System



Plants in the lower Mississippi River Corridor, Base Case. Flow Rates in Million Tons Per Year



Superstructure



Plants in the Superstructure

Plants in the Base Case

- Ammonia
- Nitric acid
- Ammonium nitrate
- Urea
- UAN
- Methanol
- Granular triple super phosphate
- MAP and DAP
- Sulfuric acid
- Phosphoric acid
- Acetic acid
- Ethylbenzene
- Styrene

Plants Added to form the Superstructure

- Acetic acid from CO_2 and CH_4
- Graphite and H_2
- Syngas from CO_2 and CH_4
- Propane dehydrogenation
- Propylene from propane and CO_2
- Styrene from ethylbenzene and CO_2
- Methanol from CO_2 and H_2 (4)
- Formic acid
- Methylamines
- Ethanol
- Dimethyl ether
- Electric furnace phosphoric acid
- HCl process for phosphoric acid
- SO_2 recovery from gypsum
- S and SO_2 recovery from gypsum

Superstructure Characteristics

Options

- Three options for producing phosphoric acid
- Two options for producing acetic acid
- Two options for recovering sulfur and sulfur dioxide
- Two options for producing styrene
- Two options for producing propylene
- Two options for producing methanol

Mixed Integer Nonlinear Program

843 continuous variables

23 integer variables

777 equality constraint equations for material and energy balances

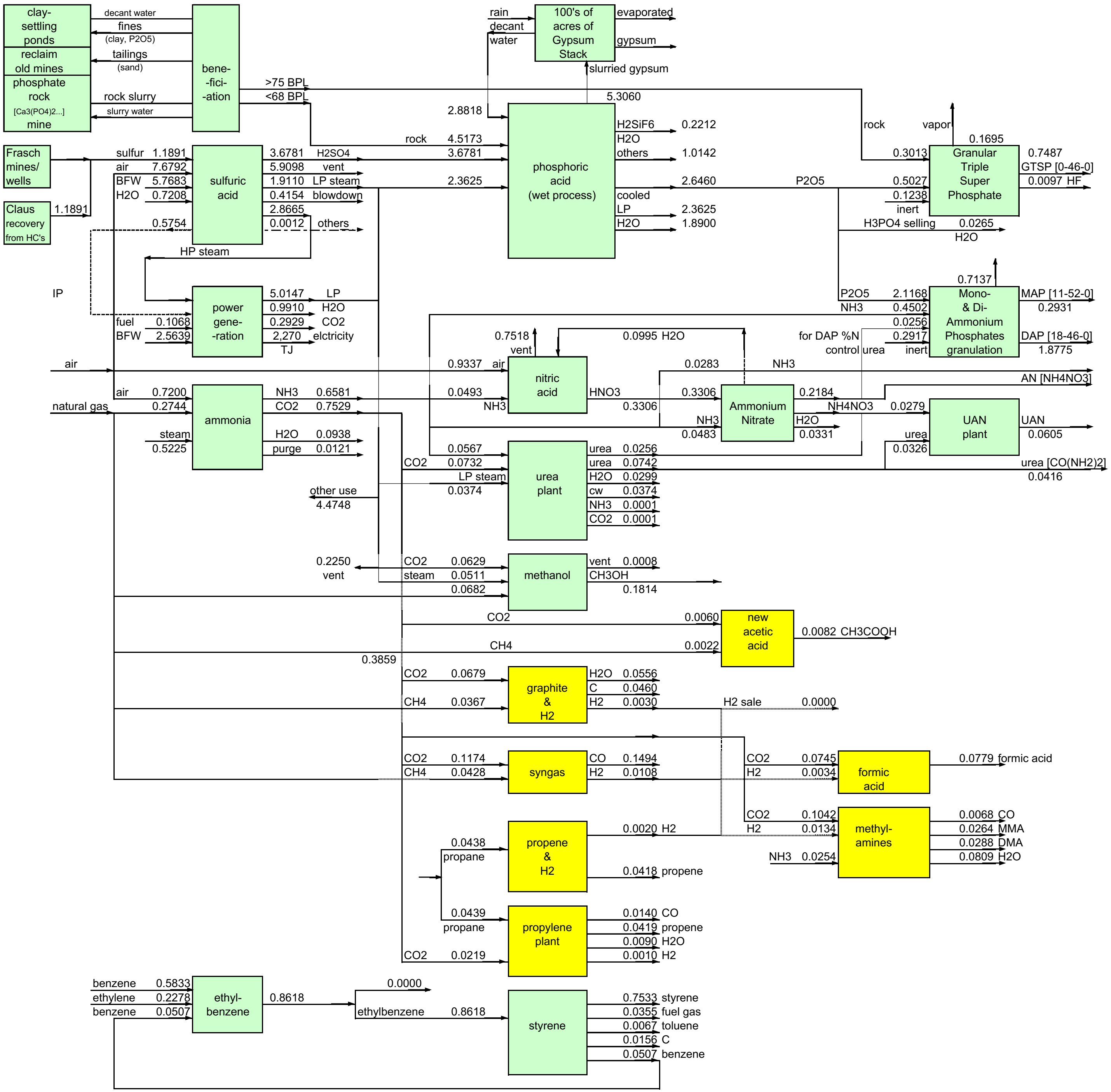
64 inequality constraints for availability of raw materials
demand for product, capacities of the plants in the complex

Some of the Raw Material Costs, Product Prices and Sustainability Cost and Credits

Raw Materials	Cost ($/mt)	Sustainable Cost and Credits	Cost/Credit ($/mt)	Products	Price ($/mt)
Natural gas	235	Credit for CO_2 consumption	6.50	Ammonia	224
Phosphate rock		Debit for CO_2 production	3.25	Methanol	271
Wet process	27	Credit for HP Steam	11	Acetic acid	1,032
Electro-furnace	34	Credit for IP Steam	7	GTSP	132
Haifa process	34	Credit for gypsum consumption	5.0	MAP	166
GTSP process	32	Debit for gypsum production	2.5	DAP	179
HCl	95	Debit for NOx production	1,025	NH_4NO_3	146
Sulfur		Debit for SO_2 production	192	Urea	179
Frasch	53			UAN	120
Claus	21			Phosphoric	496

Sources: Chemical Market Reporter and others for prices and costs,
and AIChE/CWRT report for sustainable costs.

Optimal Structure



Plants in the Optimal Structure from the Superstructure

Existing Plants in the Optimal Structure	New Plants in the Optimal Structure
Ammonia	Formic acid
Nitric acid	Acetic acid – new process
Ammonium nitrate	Methylamines
Urea	Graphite
UAN	Hydrogen/Synthesis gas
Methanol	Propylene from CO_2
Granular triple super phosphate (GTSP)	Propylene from propane dehydrogenation
MAP & DAP	
Power generation	New Plants Not in the Optimal Structure
Contact process for Sulfuric acid	Electric furnace process for phosphoric acid
Wet process for phosphoric acid	HCl process for phosphoric acid
Ethylbenzene	SO_2 recovery from gypsum process
Styrene	S & SO_2 recovery from gypsum process
	Methanol - Bonivardi, et al., 1998
Existing Plants Not in the Optimal	Methanol – Jun, et al., 1998
Structure	Methanol – Ushikoshi, et al., 1998
Acetic acid	Methanol – Nerlov and Chorkendorff, 1999
	Ethanol
	Dimethyl ether
	Styrene - new process

Comparison of the Triple Bottom Line for the Base Case and Optimal Structure

	Base Case million dollars/year	Optimal Structure million dollars/year
Income from Sales	1,316	1,544
Economic Costs (Raw Materials and Utilities)	560	606
Raw Material Costs	548	582
Utility Costs	12	24
Environmental Cost (67% of Raw Material Cost)	365	388
Sustainable Credits (+)/Costs (-)	21	24
Triple Bottom Line	412	574

Carbon Dioxide Consumption in Bases Case and Optimal Structure

	Base Case million metric tons/year	Optimal Structure million metric tons/year
CO_2 produced by NH_3 plant	0.75	0.75
CO_2 consumed by methanol, urea and other plants	0.14	0.51
CO_2 vented to atmosphere	0.61	0.24

All of the carbon dioxide was not consumed in the optimal structure to maximize the triple bottom line

Other cases were evaluated that forced use of all of the carbon dioxide, but with a reduced triple bottom line

Multi-Criteria or Multi-Objective Optimization

$$opt \begin{bmatrix} y_1(x) \\ y_2(x) \\ \bullet \\ \bullet \\ y_p(x) \end{bmatrix}$$

min: cost

max: reliability

min: waste generation

max: yield

max: selectivity

Subject to: $f_i(x) = 0$

Multi-Criteria Optimization - Weighting Objectives Method

$$opt\left\lfloor w_1 y_1(x) + w_2 y_2(x) + \bullet\bullet + w_p y_p(x) \right\rfloor$$

Subject to: $f_i(x) = 0$

with $\sum w_i = 1$

Optimization with a set of weights generates efficient or Pareto optimal solutions for the $y_i(x)$.

Efficient or Pareto Optimal Solutions
Optimal points where attempting to improving the value of one objective would cause another objective to decrease.

There are other methods for multi-criteria optimization, e.g., goal programming, but this method is the most widely used one

Multicriteria Optimization

$$\max: \begin{pmatrix} P = \Sigma \text{ Product Sales} - \Sigma \text{ Manufacturing Costs} - \Sigma \text{ Environmental Costs} \\ S = \Sigma \text{ Sustainable (Credits – Costs)} \end{pmatrix}$$

subject to: Multi-plant material and energy balances
Product demand, raw material availability, plant capacities

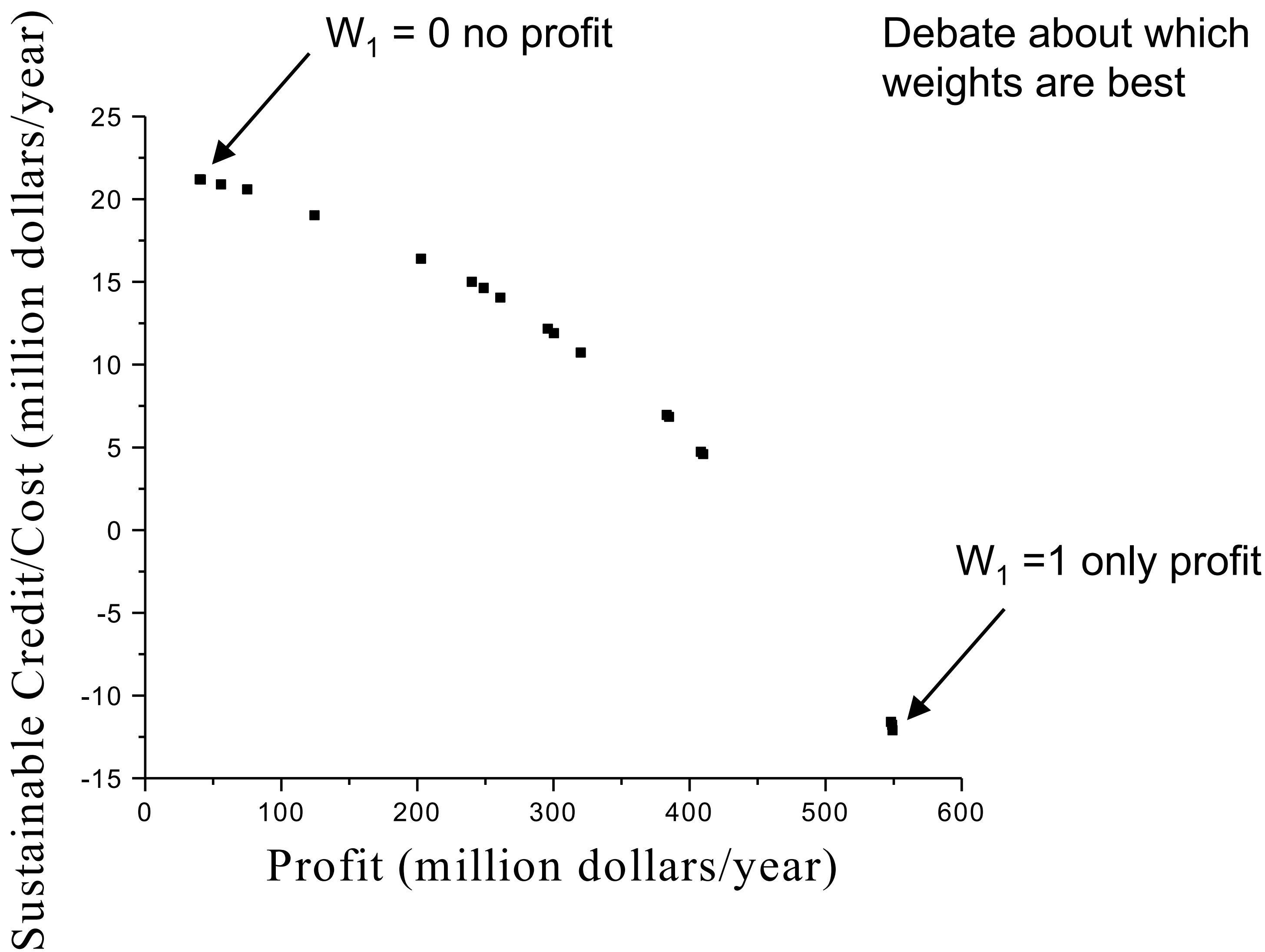
Multicriteria Optimization

Convert to a single criterion optimization problem

max: $w_1 P + w_2 S$

subject to: Multi-plant material and energy balances
Product demand, raw material availability,
plant capacities

Multicriteria Optimization



Monte Carlo Simulation

- Used to determine the sensitivity of the optimal solution to the costs and prices used in the chemical production complex economic model.

- Mean value and standard deviation of prices and cost are used.

- The result is the cumulative probability distribution, a curve of the probability as a function of the triple bottom line.

- A value of the cumulative probability for a given value of the triple bottom line is the probability that the triple bottom line will be equal to or less that value.

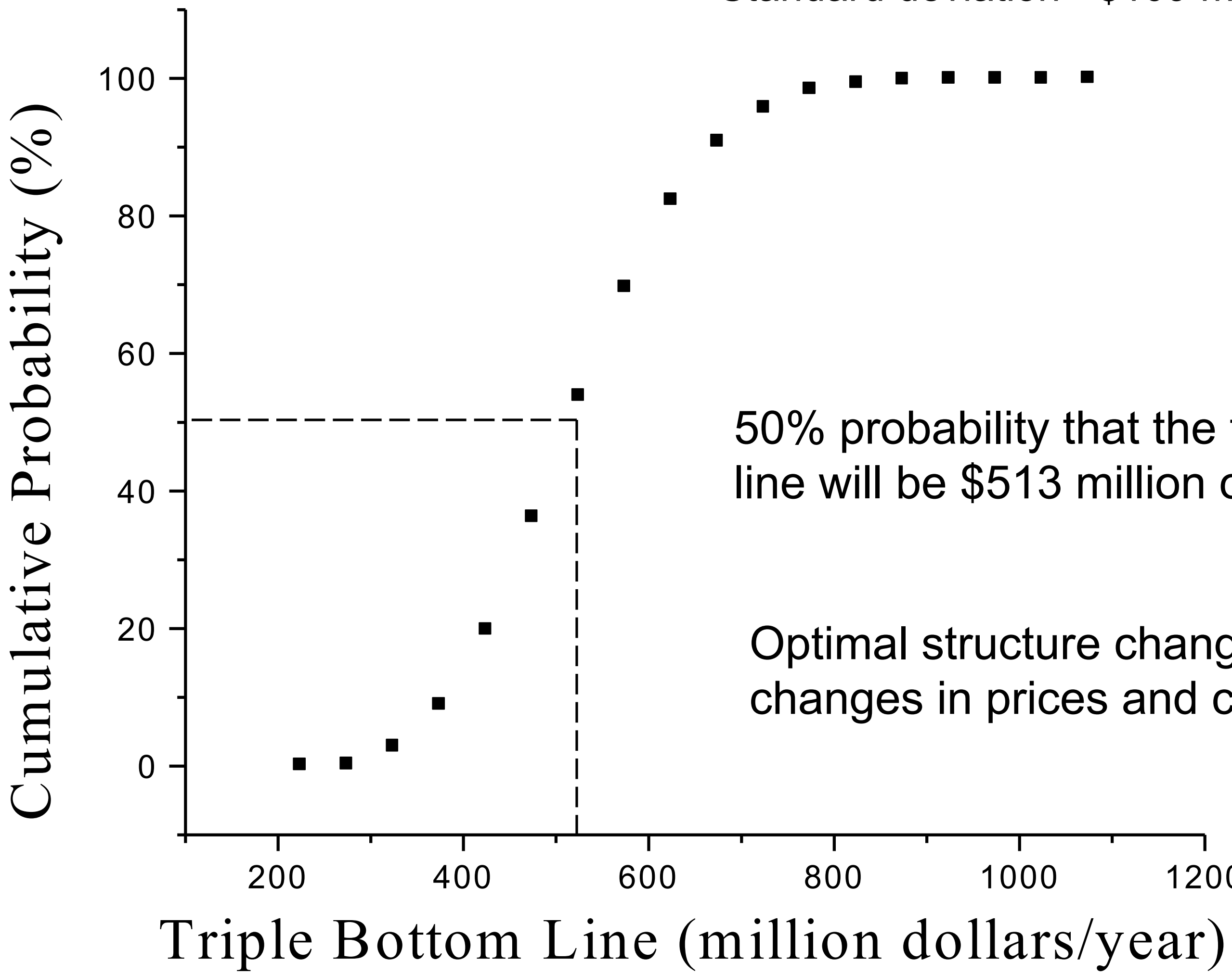
- This curve is used to determine upside and downside risks

Monte Carlo Simulation

Triple Bottom Line

Mean $513million per year

Standard deviation - $109 million per year



50% probability that the triple bottom line will be $513 million or less

Optimal structure changes with changes in prices and costs

Conclusions

- The optimum configuration of plants in a chemical production complex was determined based on the triple bottom line including economic, environmental and sustainable costs using the Chemical Complex Analysis System.

- Multcriteria optimization determines optimum configuration of plants in a chemical production complex to maximize corporate profits and maximize sustainable credits/costs.

- Monte Carlo simulation provides a statistical basis for sensitivity analysis of prices and costs in MINLP problems.

- Additional information is available at www.mpri.lsu.edu

Transition from Fossil Raw Materials to Renewables

Introduction of ethanol into the ethylene product chain.
Ethanol can be a valuable commodity for the manufacture of plastics, detergents, fibers, films and pharmaceuticals.

Introduction of glycerin into the propylene product chain.
Cost effective routes for converting glycerin to value-added products need to be developed.

Generation of synthesis gas for chemicals by hydrothermal gasification of biomaterials.

The continuous, sustainable production of carbon nanotubes to displace carbon fibers in the market. Such plants can be integrated into the local chemical production complex.

Energy Management Solutions: Cogeneration for combined electricity and steam production (CHP) can substantially increase energy efficiency and reduce greenhouse gas emissions.

Global Optimization

Locate the global optimum of a mixed integer nonlinear programming problem directly.

Branch and bound separates the original problem into sub-problems that can be eliminated showing the sub-problems that can not lead to better points

Bound constraint approximation rewrites the constraints in a linear approximate form so a MILP solver can be used to give an approximate solution to the original problem. Penalty and barrier functions are used for constraints that can not be linearized.

Branch on local optima to proceed to the global optimum using a sequence of feasible sets (boxes).

Box reduction uses constraint propagation, interval analysis convex relations and duality arguments involving Lagrange multipliers.

Interval analysis attempts to reduce the interval on the independent variables that contains the global optimum

Leading Global Optimization Solver is BARON, Branch and Reduce Optimization Navigator, developed by Professor Nikolaos V. Sahinidis and colleagues at the University of Illinois is a GAMS solver.

Global optimization solvers are currently in the code-testing phase of development which occurred 20 years ago for NLP solvers.

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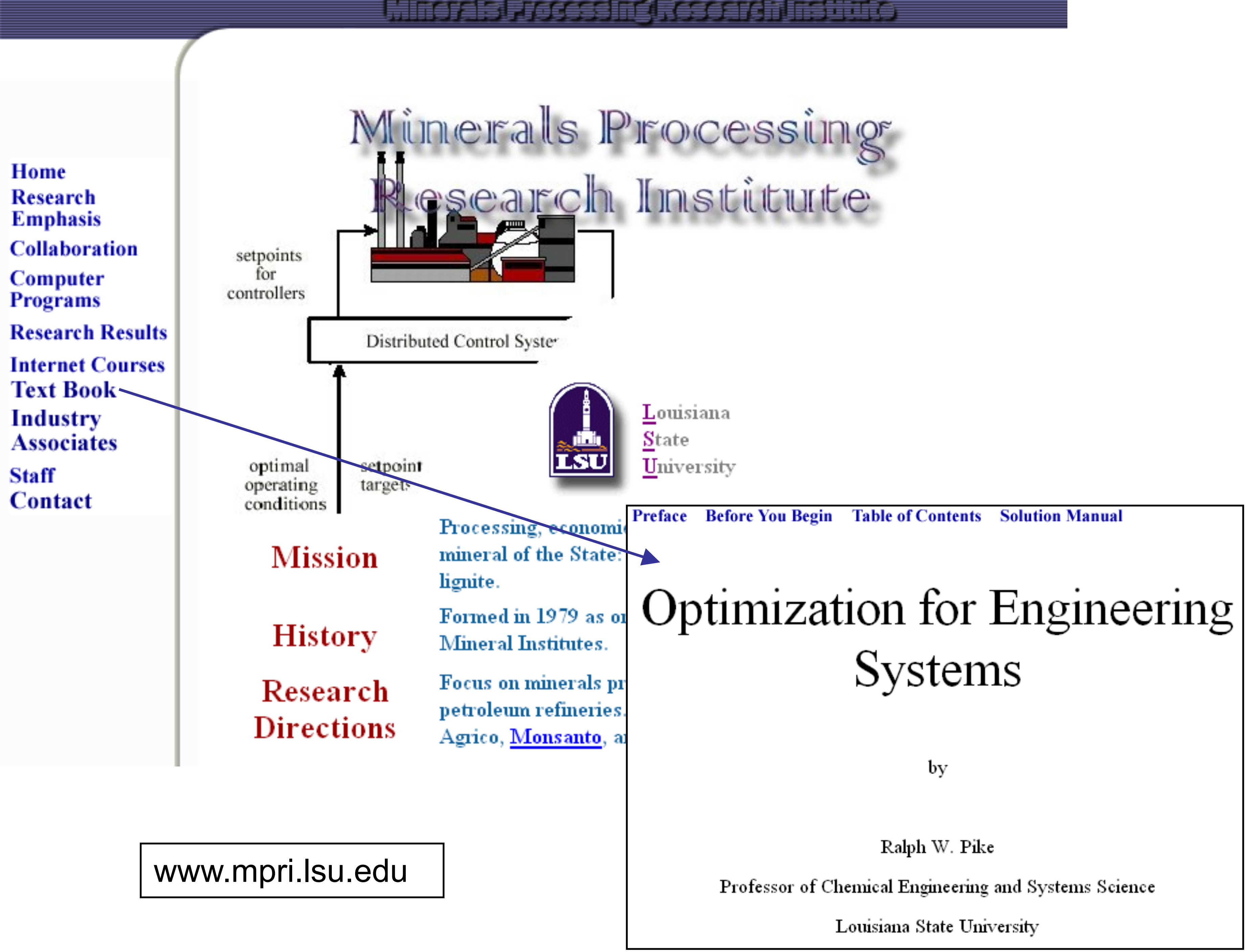
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