

On-Line Optimization

Xueyu Chen and Ralph W. Pike

**Louisiana State University
Baton Rouge, Louisiana USA**

Thomas A. Hertwig

**IMC Agrico Company
Convent, Louisiana USA**

Acknowledgments

Department of Natural Resources

Gulf Coast Hazardous Substance Research Center

Monsanto Enviro-Chem Company

INTRODUCTION

- o Status of on-line optimization
- o Results of a theoretical and numerical evaluation of the best way to conduct on-line optimization
- o An optimal procedure for on-line optimization
- o Application to a Monsanto contact process
- o Interactive Windows program incorporating these methods

Mineral Processing Research Institute
web site
www.leerick.lsu.edu/mpri/

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

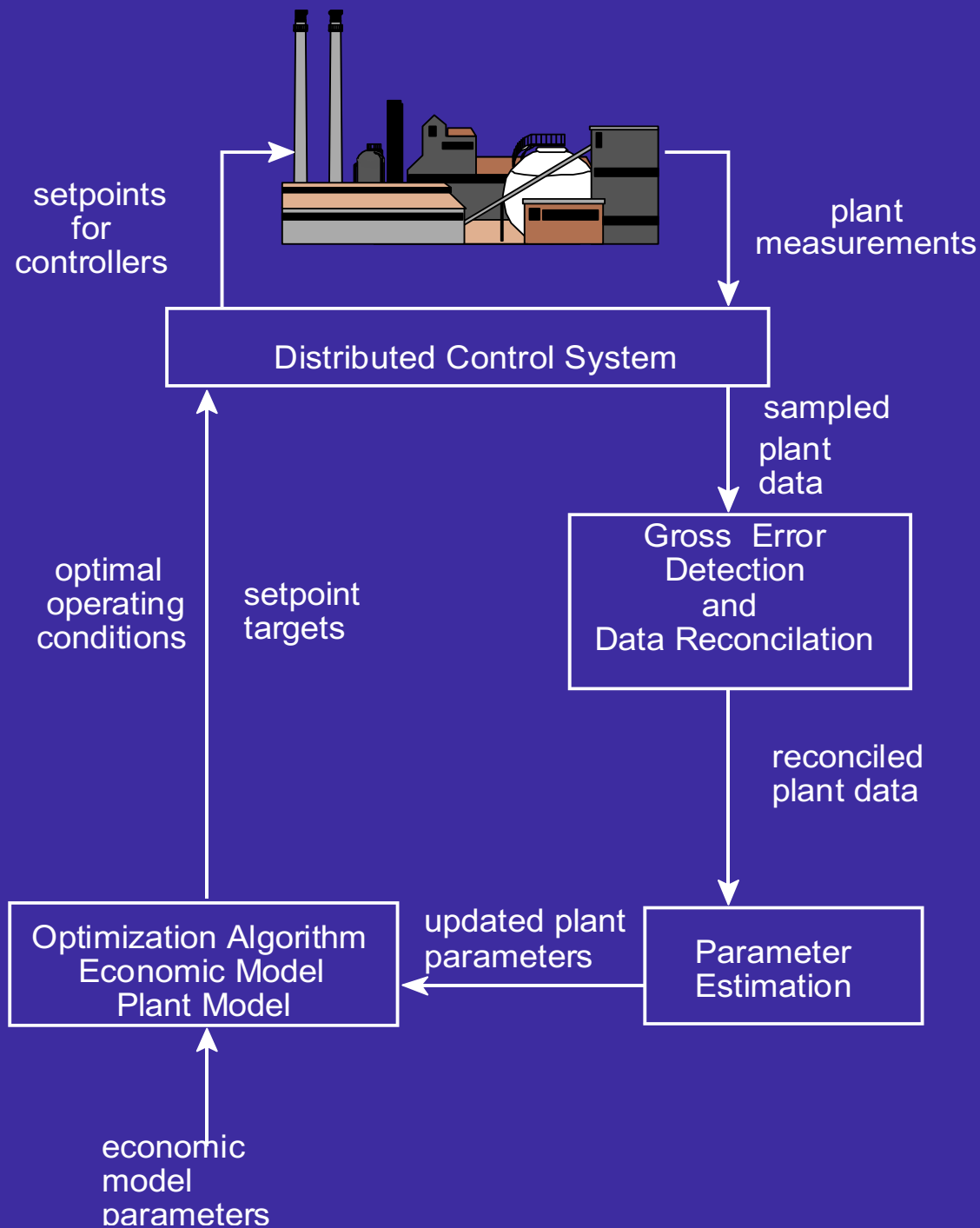
- gross error detection and data reconciliation
- parameter estimation
- economic optimization

BENEFITS

Improves plant profit by 3-5%

Waste generation and energy use are reduced

Increased understanding of plant operations



Some Companies Using On-Line Optimization

United States

Texaco

Amoco

Conoco

Lyondel

Sunoco

Phillips

Marathon

Chevron

Pyrotec/KTI

NOVA Chemicals (Canada)

British Petroleum

Europe

OMV Deutschland

Dow Benelux

Shell

OEMV

Penex

Borealis AB

DSM-Hydrocarbons

Applications

mainly crude units in refineries and ethylene plants

Companies Providing On-Line Optimization

Aspen Technology - RT-OPT

- DMC Corporation
- Setpoint

Simulation Science - ROM

- Shell - Romeo

Profimatics - On-Opt

- Honeywell

Litwin Process Automation - FACS

Hyprotech Ltd.

DOT Products, Inc. - NOVA

Status of Industrial Practice for On-Line Optimization

Steady state detection by time series screening

Gross error detection by time series screening

Data reconciliation by least squares

Parameter estimation by least squares

Economic optimization by standard methods

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

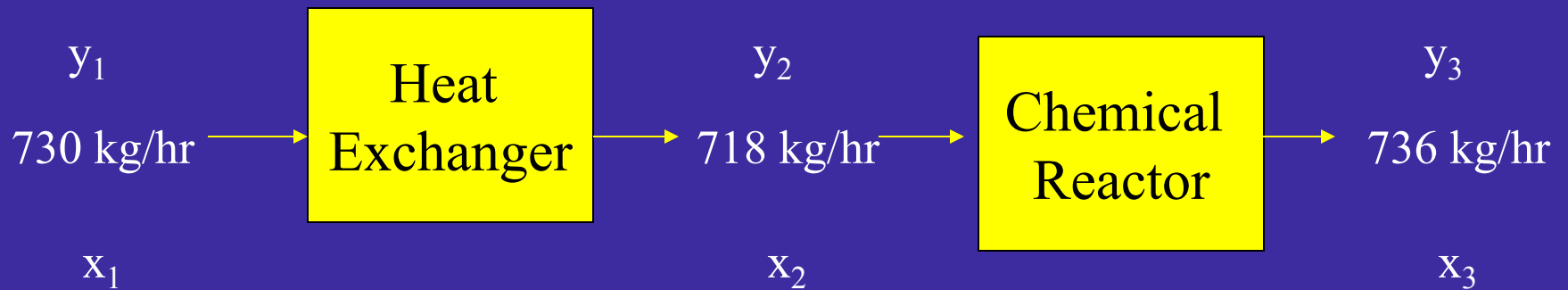
$$e = y - x$$

y = measured process variables

x = true values of the measured variables

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

a - measurement adjustment



Material Balance

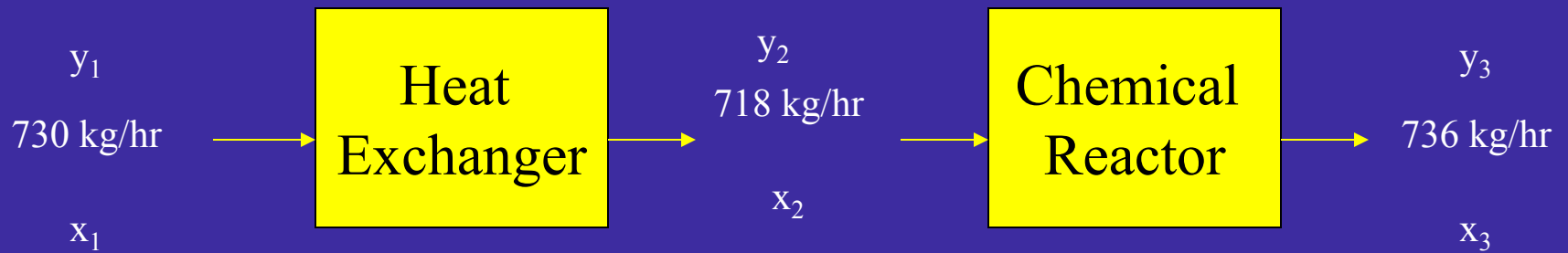
$$x_1 = x_2$$

$$x_1 - x_2 = 0$$

Steady State

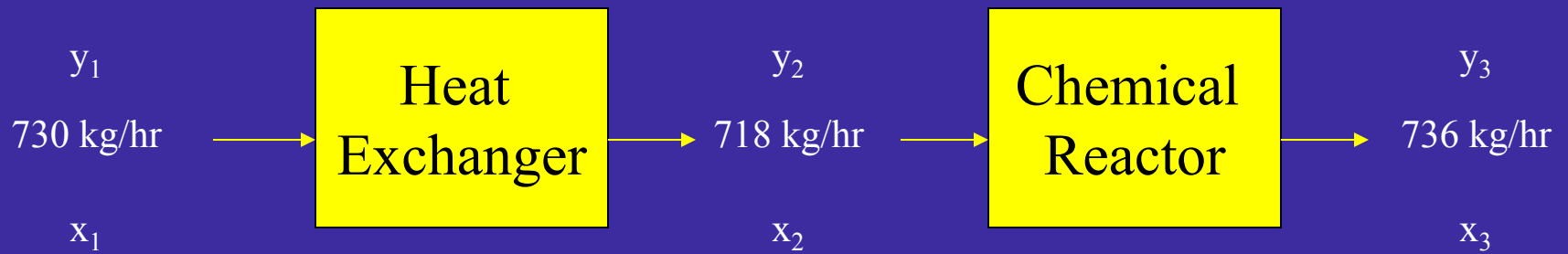
$$x_2 = x_3$$

$$x_2 - x_3 = 0$$



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

$$Ax = 0$$



$$\min_{\mathbf{x}} \sum_{i=1}^3 \left(\frac{y_i - x_i}{\sigma_i} \right)^2$$

$$\mathbf{y} = \begin{bmatrix} 730 \\ 718 \\ 736 \end{bmatrix}$$

Subject to:

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

$$\sigma = \begin{bmatrix} 12 & 0 & 0 \\ 0 & 12 & 0 \\ 0 & 0 & 12 \end{bmatrix}$$

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

Subject to: $\mathbf{Ax} = \mathbf{0}$

Analytical solution using LaGrange Multipliers

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

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

Nonlinear Process Model

Min: $(y - x)^T Q^{-1} (y - x)$

Subject to:

$$f_i(x) = 0$$

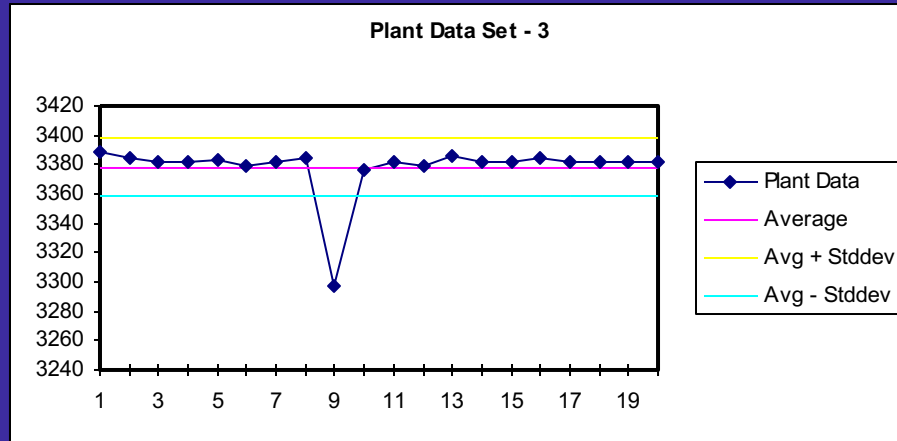
$$f_i(x) \leq 0$$

material and energy balances
capacities of process units
demand for product
availability of raw materials

Requires the solution of a nonlinear programming problem

Gross Error Detection Methods

Time series
screening



Statistical testing

- o many methods
- o can include data reconciliation

Combined Gross Error Detection and Data Reconciliation

Measurement Test Method - least squares

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

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

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

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

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

Test statistic:

if $|e_i| / \sigma_i \geq C$ 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

$$P(y_i \mid x_i) = (1-\eta)P(y_i \mid x_i, R) + \eta P(y_i \mid x_i, G)$$

$P(y_i \mid x_i, R)$ = probability distribution function for the random error

$P(y_i \mid x_i, G)$ = probability distribution function for the gross error.

Gross error occur with probability η

Gross Error Distribution Function

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

Tjao-Biegler Method

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

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

Subject to: $\mathbf{f}(\mathbf{x}) = 0$ plant model
 $\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U$ bounds on the process variables

A NLP, and values are needed for $\mathbf{x}^L$ and $\mathbf{x}^U$

Test for Gross Errors

If $P(y_i - x_i, G) > (1 - \alpha)P(y_i - x_i, R)$, gross error
 probability of a gross error probability of a random error

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

Robust Function Methods

$$\begin{array}{ll}\text{Minimize:} & - \sum_i \rho(y_i, x_i) \\ \text{Subject to:} & \mathbf{f}(\mathbf{x}) = 0 \\ & \mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U\end{array}$$

Lorentzian distribution

$$\rho(\varepsilon_i) = \frac{1}{1 + \frac{1}{2}\varepsilon_i^2}$$

Fair function

$$\rho(\varepsilon_i, c) = c^2 \left[\frac{\varepsilon_i}{c} + \log \left(1 + \frac{\varepsilon_i^2}{c^2} \right) \right]$$

c is a tuning parameter

Test statistic

$$\varepsilon_i = (y_i - x_i) / \sigma_i$$

Parameter Estimation

Error-in-Variables Method

Least squares

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

$\boldsymbol{\theta}$

$$\text{Subject to: } \mathbf{f}(\mathbf{x}, \boldsymbol{\theta}) = 0$$

$\boldsymbol{\theta}$ - plant parameters

Simultaneous data reconciliation and parameter estimation

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

$\mathbf{x}, \boldsymbol{\theta}$

$$\text{Subject to: } \mathbf{f}(\mathbf{x}, \boldsymbol{\theta}) = 0$$

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

Theoretical Evaluation of Algorithms for Data Reconciliation

Determine sensitivity of distribution functions to gross errors

Objective function is the product or sum of distribution functions for individual measurement errors

$$P = \prod p(\varepsilon) \quad \ln P = \sum \ln p(\varepsilon) \quad \rho = \sum \rho(\varepsilon)$$

Three important concepts
in the theoretical evaluation
of the robustness and precision
of an estimator from a distribution function

Influence Function

Robustness of an estimator is unbiasedness (insensitivity) to the presence of gross errors in measurements. The sensitivity of an estimator to the presence of gross errors can be measured by the influence function of the distribution function. For M-estimate, the influence function is defined as a function that is proportional to the derivative of a distribution function with respect to the measured variable, (ρ / x)

Relative Efficiency

The precision of an estimator from a distribution is measured by the relative efficiency of the distribution. The estimator is precise if the variation (dispersion) of its distribution function is small

Breakdown Point

The break-down point can be thought of as giving the limiting fraction of gross errors that can be in a sample of data and a valid estimation of the estimator is still obtained using this data. For repeated samples, the break-down point is the fraction of gross errors in the data that can be tolerated and the estimator gives a meaningful value.

Influence Function

proportional to the derivative of the distribution function, $IF \propto \rho' / x$

represents the sensitivity of reconciled data to the presence of gross errors

Normal Distribution

$$IF_{MF} = \frac{\rho_i}{x_i} \frac{y_i - x_i}{\sigma_i^2} \frac{\varepsilon_i}{\sigma_i}$$

Contaminated Gaussian Distribution

$$IF = \frac{\rho_i}{x_i} \frac{\frac{\varepsilon_i}{\sigma_i} \left\{ (1 - \eta) e^{-\frac{\varepsilon_i^2}{2} \left(1 + \frac{1}{b^2} \right)} - \frac{\eta}{b^3} \right\}}{(1 - \eta) e^{-\frac{\varepsilon_i^2}{2} \left(1 + \frac{1}{b^2} \right)} - \frac{\eta}{b}}$$

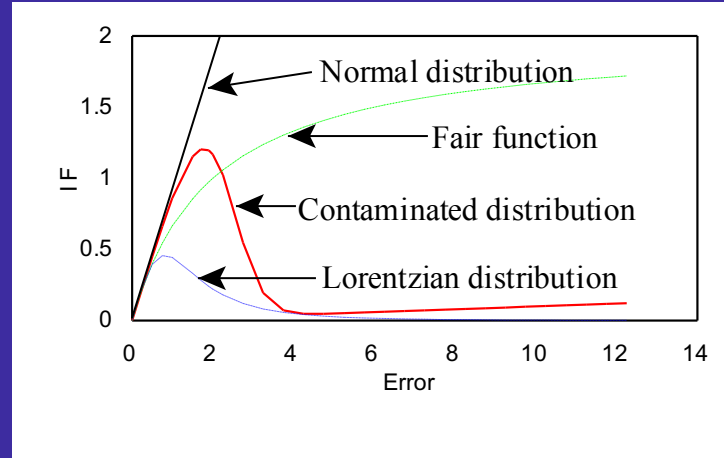
Lorentzian Distribution

$$IF_{Lorentzian} = \frac{\rho_i}{\varepsilon_i} \frac{\varepsilon_i}{\left(1 + \frac{1}{2} \varepsilon_i^2 \right)^2}$$

Fair Function

$$IF_{Fair} = \frac{\rho_i}{\varepsilon_i} c^2 \left(\frac{1}{c} - \frac{\frac{1}{c}}{1 + \frac{\varepsilon_i}{c}} \right) = \frac{1}{\frac{1}{\varepsilon_i} - \frac{1}{c}}$$

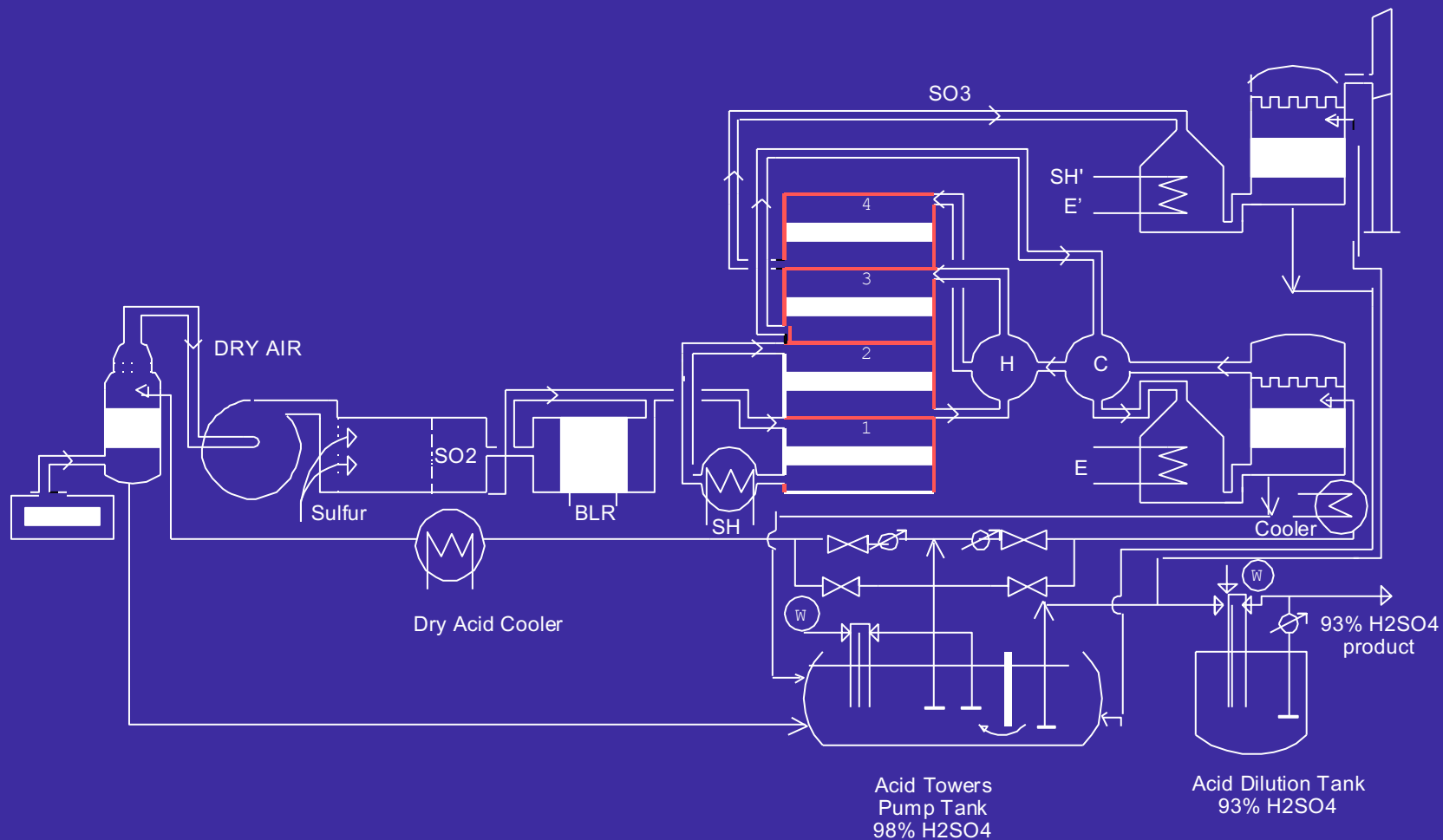
Comparison of Influence Functions



Effect of Gross Errors on Reconciled Data - Least to Most

Lorentzian Contaminated Gaussian Fair Normal

Air Inlet	Air Dryer	Main Compressor	Sulfur Burner	Waste Heat Boiler	Super-Heater	SO ₂ to SO ₃ Converter	Hot & Cold Gas to Gas Heat EX.	Heat Exchangers	Final & Interpass Towers
-----------	-----------	-----------------	---------------	-------------------	--------------	--	--------------------------------	-----------------	--------------------------



Numerical Evaluation of Algorithms

Simulated plant data is constructed by

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

$\mathbf{y}$ - simulated measurement vector for measured variables

$\mathbf{x}$ - true values (plant design data) for measured variables

$\mathbf{e}$ - random errors added to the true values

$\mathbf{a}$ - magnitude of a gross error added to one of measured variables

- a vector with one in one element corresponding to the measured variable with gross error and zero in other elements

Criteria for Numerical Evaluation

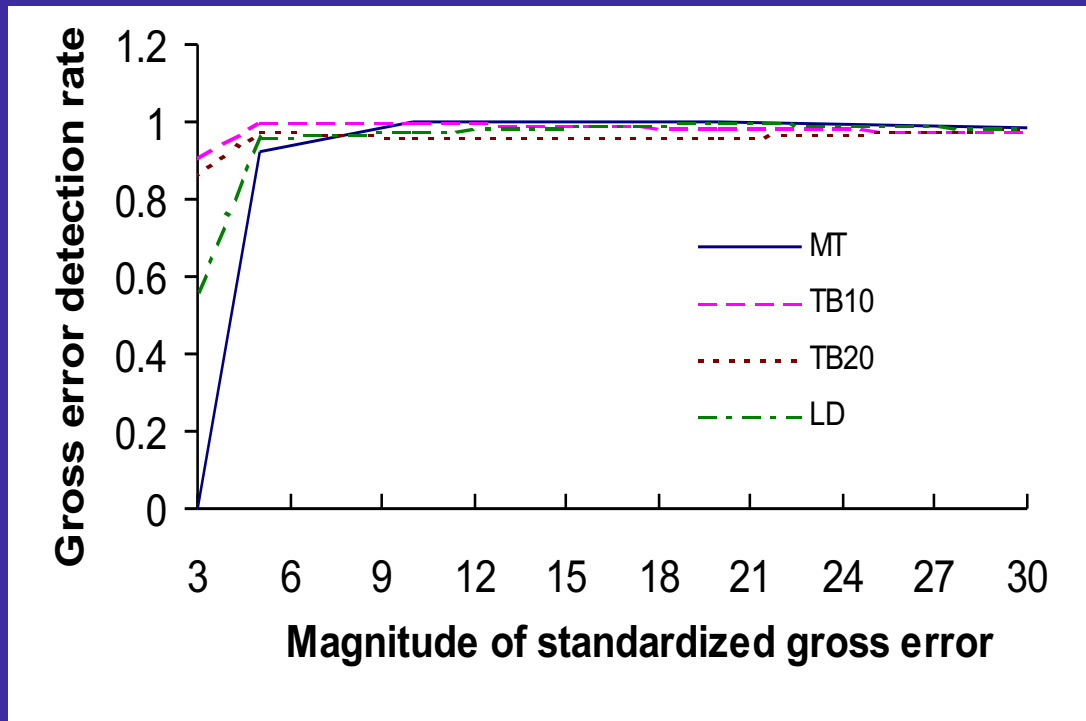
Gross error detection rate - ratio of number of gross errors that are correctly detected to the total number of gross errors in measurements

Number of type I errors - If a measurement does not contain a gross error and the test statistic identifies the measurement as having a gross error, it is called a type I error

Random and gross error reduction - the ratio of the remaining error in the reconciled data to the error in the measurement

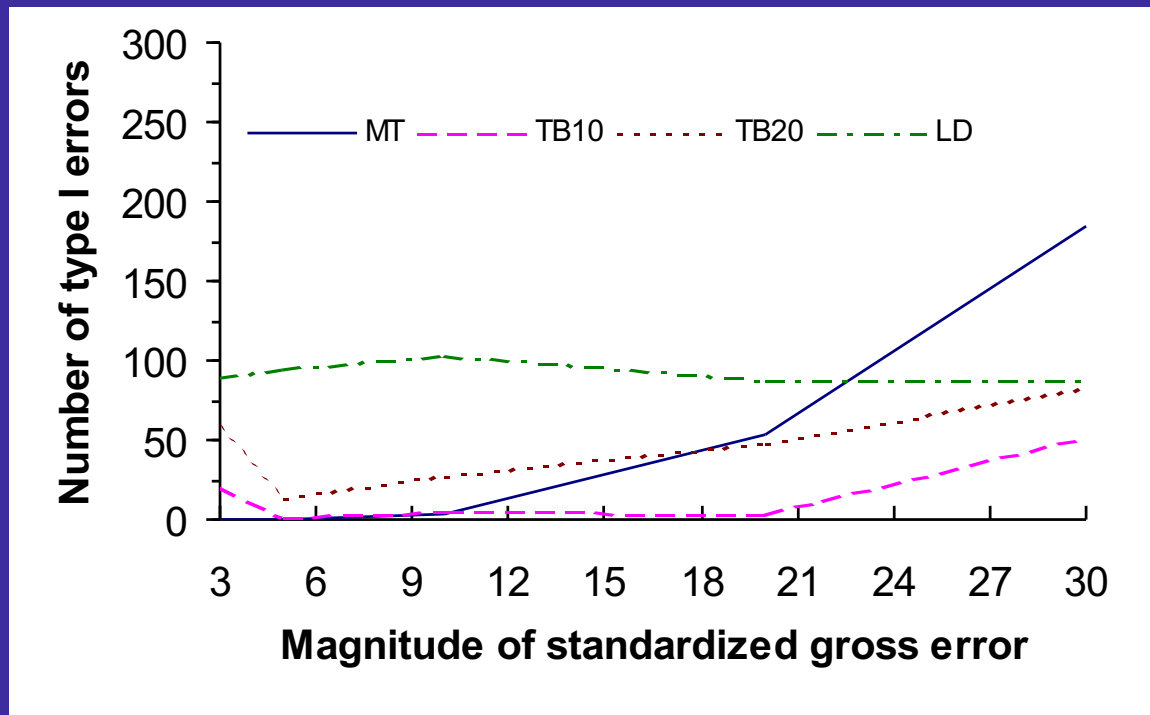
Comparison of Gross Error Detection Rates

390 Runs for Each Algorithm



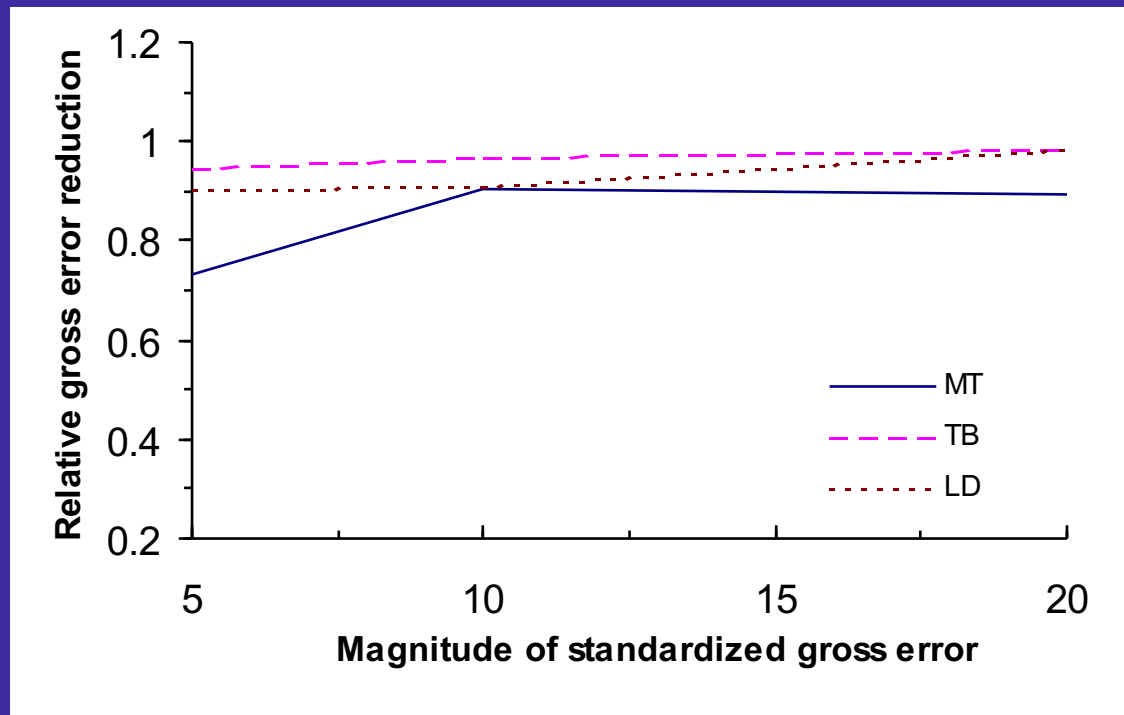
Comparison of Numbers of Type I Errors

390 Runs for Each Algorithm



Comparison of Relative Gross Error Reductions

645 Runs for Each Algorithm



Results of Theoretical and Numerical Evaluations

Tjoa-Biegler's method has the best performance for measurements containing random errors and moderate gross errors (3σ - 30σ)

Robust method using Lorentzian distribution is more effective for measurements with very large gross errors (larger than 30σ)

Measurement test method gives a more accurate estimation for measurements containing only random errors. It gives significantly biased estimation when measurements contain gross errors larger than 10σ

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.

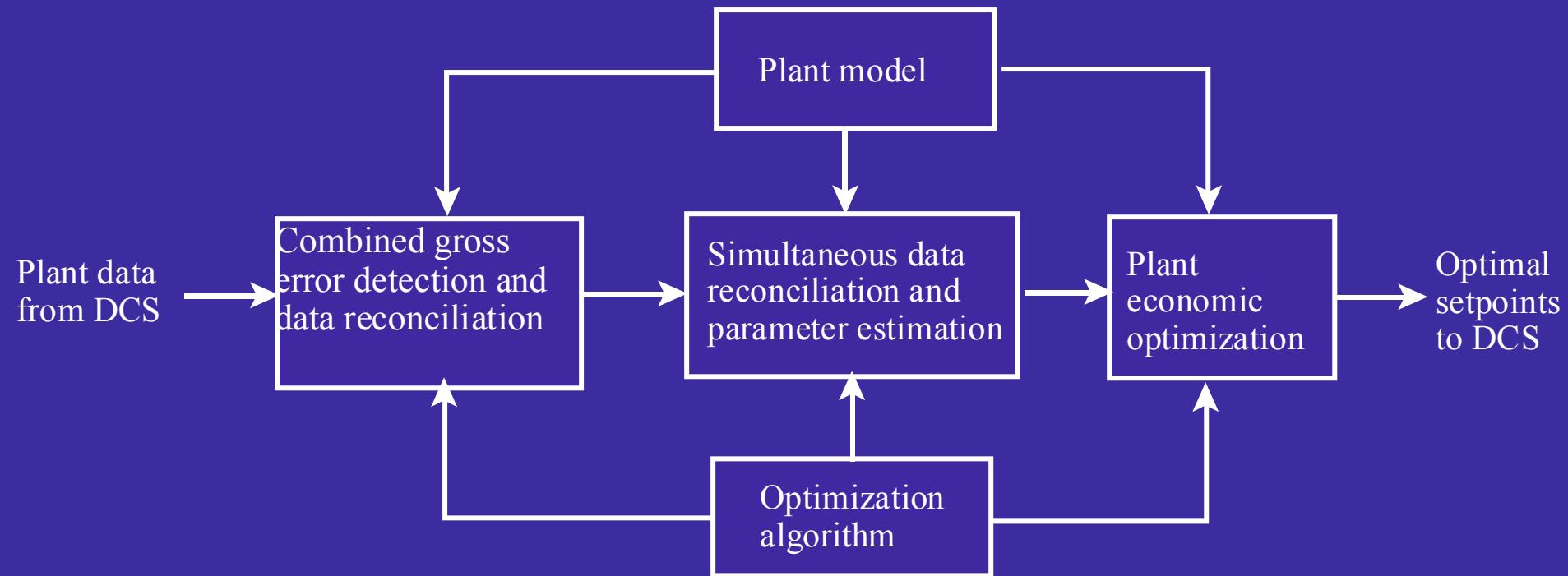
Economic Optimization

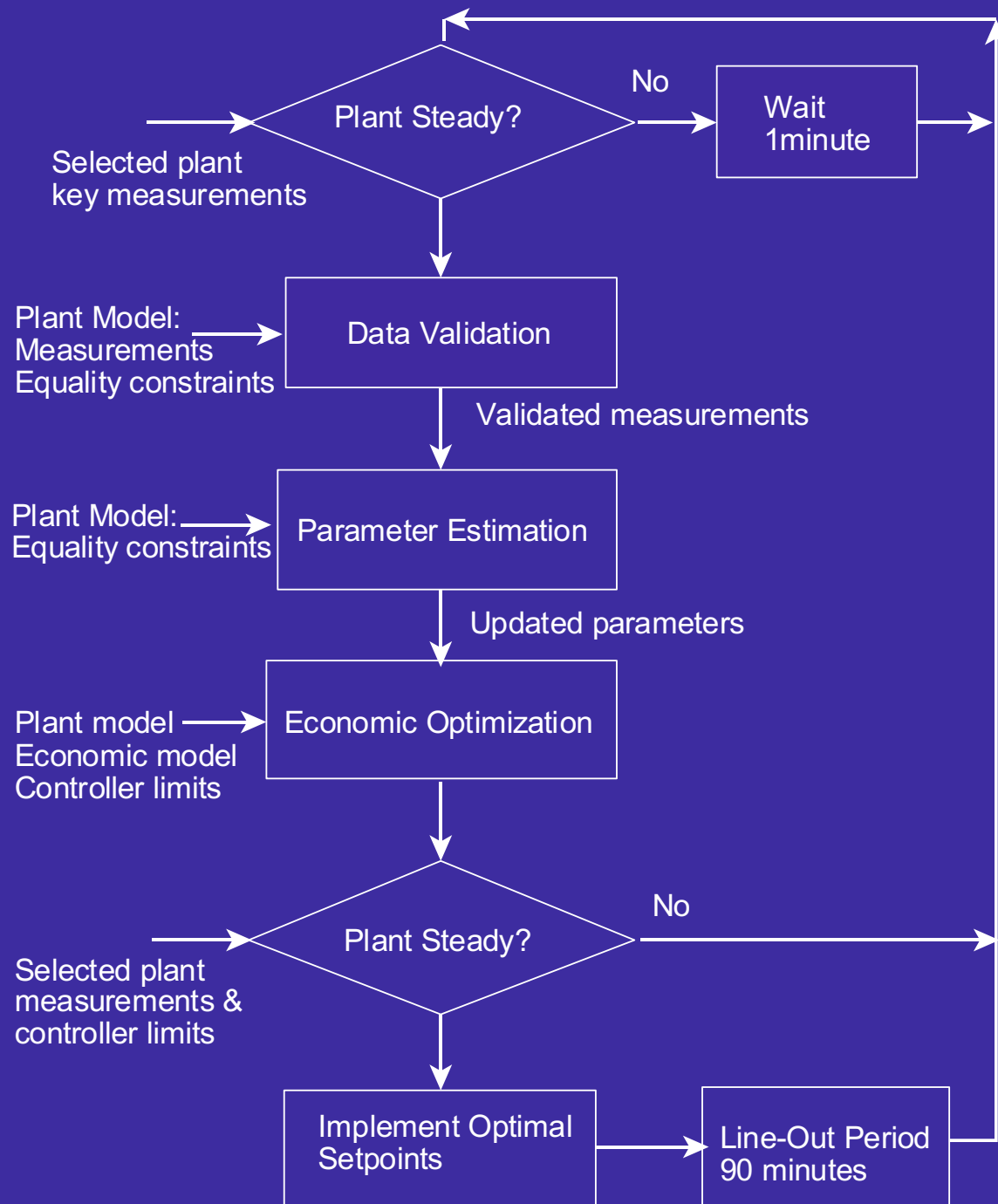
Value Added Profit Function

$$s_{F64}F_{64} + s_{FS8}F_{S8} + s_{FS14}F_{S14} - c_{F50}F_{50} - c_{FS1}F_{S1} - c_{F65}F_{65}$$

On-Line Optimization Results

Date	Current (\$/day)	Profit Optimal (\$/day)	Improvement
6-10-97	37,290	38,146	2.3% \$313,000/yr
6-12-97	36,988	38,111	3.1% \$410,000/yr





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

URL <http://www.leeric.lsu.edu/mpri/>

Some Other Considerations

Redundancy

Observeability

Variance estimation

Closing the loop

Dynamic data reconciliation
and parameter estimation

Summary

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

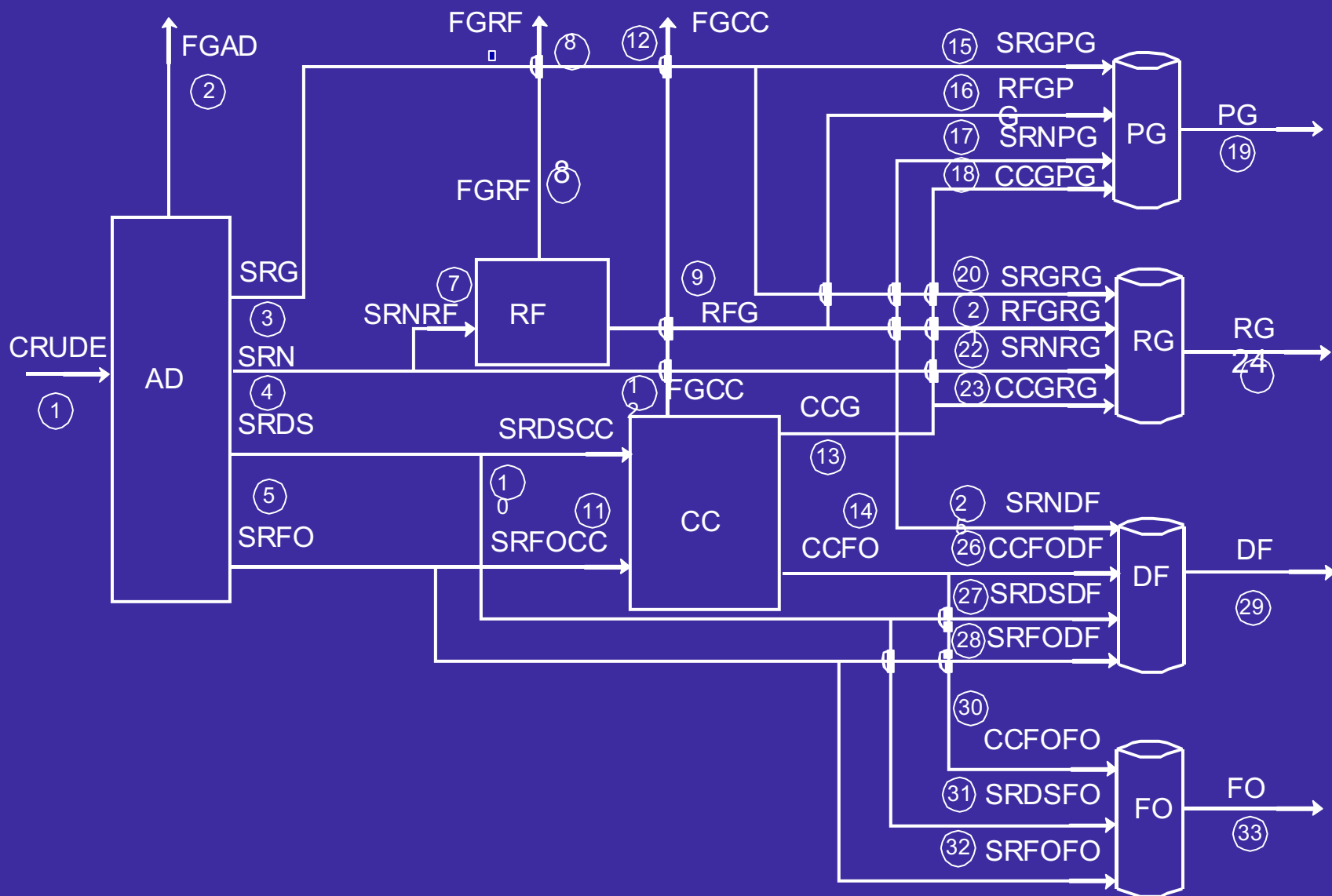


Table 20 Description and Plant Data for Process Variables of the Refinery

	Name	Definition (Flow rates are in barrels per day)	Plant Data	Standard Deviation
Measured Variables	CRUDE	Crude oil flow rate to atmospheric distillation column (AD)	99686.7	1000.0
	FGAD	Fuel gas flow rate from AD	3553606	35420.0
	SRG	Straight run gasoline flow rate from AD	27125.2	270.0
	SRN	Straight run naphtha flow rate from AD	23266.3	237.0
	SRDS	Straight run distillate flow rate from AD	8636.35	87.0
	SRFO	Straight run fuel oil flow rate from AD	36838.6	372.0
	SRNRF	Straight run naphtha feed rate to reformer (RF)	23606.6	237.0
	FGRF	Fuel gas flow rate from the reformer	3796351	37612.0
	RFG	Reformer gasoline flow rate	21826.6	219.9
	SRDSCC	Straight run distillate flow rate to the catalytic cracking unit (CCU)	0.004	10.0
	SRFOCC	Straight run fuel oil flow rate to the CCU	29727.3	300.0
	FGCC	Fuel gas flow rate from the CCU	1.2212E+7	115920.0
	CCG	Gasoline flow rate from CCU	20503.3	206.4
	CCFO	Fuel oil flow rate from CCU	6567.9	66.0
	SRGPG	Straight run gasoline flow rate for premium gasoline (PG) blending	17394.8	170.7
	RFGPG	Reformer gasoline flow rate for PG blending	21835.1	219.9
	SRNPG	Straight run naphtha flow rate for PG blending	12.99	10.0
	CCGPG	CCU gasoline flow rate for PG blending	7935.7	80.5
	PG	Premium gasoline flow rate	47263.8	471.1
	SRGRG	Straight run gasoline flow rate for regular gasoline (RG) blending	10044.6	99.3
	RFGRG	Reformer gasoline flow rate for RG blending	11.532	10.0
	SRNRG	Straight run naphtha flow rate for RG blending	7.100	10.0
	CCGRG	CCU gasoline flow rate for RG blending	12721.8	125.9
	RG	Regular gasoline flow rate	22357.3	225.2
	SRNDF	Straight run naphtha flow rate for diesel fuel (DF) blending	9.994	10.0
	CCFODF	CCU fuel oil flow rate for DF blending	3270.1	32.7
	SRDSDF	Straight run distillate flow rate for DF blending	8613.5	87.0
	SRFODF	Straight run fuel oil flow rate for DF blending	525.34	5.3
	DF	No. 2 diesel fuel flow rate	12582.8	125.0
	CCFOFO	CCU fuel oil flow rate for fuel oil (FO) blending	3382.5	33.3
	SRDSFO	Straight run distillate flow rate for FO blending	22.13	10.0
	SRFOFO	Straight run fuel oil flow rate for FO blending	6628.2	66.7
Unmeasured Variables	FO	No. 6 fuel oil flow rate		

Table 21 Capacities, Operating Costs and Volumetric Yields
for the Refinery Process Units

Unit	Capacity (bbl/day)	Operating Cost (\$/bbl)	Input	Output	Mass Yield of Output Stream	Volumetric Yield of Output Stream
Crude oil Atmospheric Distillation Column	100,000	1.00	CRUDE	FGAD	0.029	35.42
				SRG	0.236	0.270
				SRN	0.223	0.237
				SRDS	0.087	0.087
				SRFO	0.426	0.372
Catalytic Reformer	25,000	2.50	SRNRF	FGRF	0.138	158.7
				RFG	0.862	0.928
Catalytic Cracking Unit	30,000	2.20	SRDSCC	FGCC	0.273	336.9
				CCG	0.536	0.619
				CCFO	0.191	0.189
			SRFOCC	FGCC	0.277	386.4
				CCG	0.527	0.688

Table 22 Names and Definition of Parameters for the Refinery

Units of Parameters	Names of Parameters	Initial Values	Definitions of parameters Volumetric yields (BBL output/BBL input)
Crude Oil Atmospheric Distillation Column	VFGAD	35.42	BBLs of fuel gas per BBL crude
	VSRG	0.27	BBLs of straight-run gasoline per BBL crude
	VSRN	0.237	BBLs of straight-run naphtha per BBL crude
	VSRDS	0.087	BBLs of straight-run distillate per BBL crude
	VSRFO	0.372	BBLs of Straight-run fuel oil per BBL crude
Catalytic Reformer	VSRNFGRF	158.7	BBLs of reformer fuel gas per BBL of straight-run naphtha
	VSRNRFG	0.928	BBLs reformer gasoline per BBL straight-run naphtha
Catalytic Cracking	VSRDSFGCC	336.9	BBLs of fuel gas per BBL straight-run distillate
	VSRDSCCG	0.619	BBLs of gasoline from CC per BBL straight-run distillate
	VSRDSCCFO	0.189	BBLs of fuel oil per BBL of straight-run distillate
	VSRFOFGCC	386.4	BBLs of fuel gas per BBL straight-run fuel oil
	VSRFOCCG	0.688	BBLs of gasoline from CC per BBL of straight-run fuel oil
	VSRFOCCFO	0.220	BBLs of fuel oil per BBL straight-run fuel oil

Table 23 Quality Specifications and Physical Properties for Products and Intermediate Streams for the Refinery

Stream	Motor Octane Number	Vapor pressure (mmHg)	Density (lb/bbl)	Sulfur Content (lb/bbl)
Premium Gasoline	93.0	12.7	-	-
Regular Gasoline	87.0	12.7	-	-
Diesel Fuel	-	-	306.0	0.5
Fuel Oil	-	-	352.0	3.0
SRG	78.5	18.4	-	-
RFG	104.0	2.57	-	-
SRN	65.0	6.54	272.0	0.283
CCG	93.7	6.90	-	-
CCFO	-	-	294.4	0.353
SRDS	-	-	292.0	0.526
SRFO	-	-	295.0	0.980

Table 24 Crude Oil Cost and Product Sales Prices for the Refinery

	Prices
Gulf Cost Crude	\$32.00/bbl
Premium Gasoline	\$45.36/bbl
Regular Gasoline	\$43.68/bbl Names
No.2 Diesel Fuel	\$40.32/bbl
No.6 Fuel Oil	\$13.14/bbl
Fuel Gas	\$0.01965/bbl

Table 25 Refinery Objective Function and Constraint Equations

[illegible]

Table 25 Refinery Objective Function and Constraint Equations (continued)

Objective Function	Catalytic Cracker		CCG	CCFO	SRGPG	Premium Gasoline Blending			PG
	SRDSCC	SRFOCC FGCC				RFGPG	SRNPG	CCGPG	
Crude Availability	-2.20	-2.20	-0.01965						45.36
Products									
Premium Gasoline									
Min. PG Prod.									1.0
PG Blending						1.0	1.0	1.0	1.0
-1.0									
PG Octane Rating					78.5	104.0	65.0	93.7	-93.0
PG Vapor Press.					18.4	2.57	6.54	6.90	-12.7
Regular Gasoline									
Min. RG Prod.									
RG Blending									
RG Octane Rating									
RG Vapor Press.									
Diesel Fuel									
Min. DF Prod.									
DF Blending									
DF Density Spec.									
DF Sulfur Spec.									
Fuel Oil									
Min. FO Prod.									
FO Blending									
FO Density Spec.									
FO Sulfur Spec.									
Process Units									
Atm. Distillation									
AD Capacity									
FGAD Yield									
SRG Yield									
SRN Yield									
SRDS Yield									
SRFO Yield									
Reformer									
RF Capacity									
FGRF Yield									
RFG Yield									
Catalytic Cracker									
CC Capacity		1.0	1.0						
FGCC Yield		336.9	386.4	-1.0					
CCG Yield		0.619	0.688		-1.0				
CCFO Yield		0.189	0.220			-1.0			
Stream Splits									
SRG					-1.0				
SRN							-1.0		
SRDS	-1.0								
SRFO		-1.0							
RFG						-1.0			
CCG				1.0				-1.0	
CCFO					1.0				

Table 25 Refinery Objective Function and Constraint Equations (continued)

SRGRG	Regular Gasoline Blending			RG 43.68	SRNDF	CCFODF	Diesel Fuel Blending			DF 40.32	Fuel Oil Blending			FO 13.14	= Maximum OBJ	
	RFGRG	SRNRG	CCGRG				SRDSDF	SRFODF	CCFOFO		SRDSFO	SRFOFO	$\leq 110,000$		CRDAVAIL	
															$\geq 10,000$	PGMIN
															$= 0$	PGBLEND
															≥ 0	PGOCTANE
															≤ 0	PGVAPP
				1.0											$\geq 10,000$	RGMIN
1.0	1.0	1.0	1.0	-1.0											$= 0$	RGBLEND
78.5	104.0	65.0	93.7	-87.0											≥ 0	RGOCTANE
18.4	2.57	6.54	6.90	-12.7											≤ 0	RGVAPP
									1.0						$\geq 10,000$	DFMIN
					1.0	1.0	1.0	1.0	-1.0						$= 0$	DFBLEND
					272.0	294.4	292.0	295.0	-306.0						≤ 0	DFDENS
					0.283	0.353	0.526	0.980	-0.50						≤ 0	DFSULFUR
														1.0	$\geq 10,000$	FOMIN
										1.0	1.0	1.0	-1.0		$= 0$	FOBLEND
										294.4	292.0	295.0	-352.0		≤ 0	FODENS
										0.353	0.526	0.980	-3.0		≤ 0	FOSULFUR
															$\geq 100,000$	ADCAP
															$= 0$	ADFGYLD
															$= 0$	ADSRGYLD
															$= 0$	ADNYLD
															$= 0$	ADDSYLD
															$= 0$	ADFOYLD
															$\geq 25,000$	RFCAP
															$= 0$	RFFGYLD
															$= 0$	RFRFGYLD
															$\geq 30,000$	CCCAP
															$= 0$	CCFGYLD
															$= 0$	CCGYLD
															$= 0$	CCFOYLD
-1.0															$= 0$	SRGSPLIT
	-1.0				-1.0										$= 0$	SRNSPLIT
							-1.0					-1.0			$= 0$	SRDSSPLIT
								-1.0					-1.0		$= 0$	SRFOPLIT
	-1.0														$= 0$	RFGSPLIT
			-1.0												$= 0$	CCGSPLIT
						-1.0				-1.0					$= 0$	CCFOSPLIT

Table 26 Quantity and Quality Constraints of the Refinery Products

Premium Gasoline						
	<u>SRGPG</u>	<u>RFGPG</u>	<u>SRNPG</u>	<u>CCGPG</u>	<u>PG</u>	<u>RHS</u>
Min. P.G. Production					1.0	$\geq 10,000$
PG Blending	1.0	1.0	1.0	1.0	-1.0	$= 0$
PG Octane Rating	78.5	104.0	65.0	93.7	-93.0	≥ 0
PG Vapor Pressure	18.4	2.57	6.54	6.90	-12.7	≤ 0
Regular Gasoline						
	<u>SRGRG</u>	<u>RFGRG</u>	<u>SRNRG</u>	<u>CCGRG</u>	<u>RG</u>	<u>RHS</u>
Min R.G. Production					1.0	$\geq 10,000$
RG Blending	1.0	1.0	1.0	1.0	-1.0	$= 0$
RG Octane Rating	78.5	104.0	65.0	93.7	-87.0	≥ 0
RG Vapor Pressure	18.4	2.57	6.54	6.90	-12.7	≤ 0
Diesel Fuel						
	<u>SRNDF</u>	<u>CCFODF</u>	<u>SRDSDF</u>	<u>SRFODF</u>	<u>DF</u>	<u>RHS</u>
Min D.F. Production					1.0	$> 10,000$
DF Blending	1.0	1.0	1.0	1.0	-1.0	$= 0$
DF Density Spec.	272.0	294.4	292.0	295.0	-306.0	≤ 0
DF Sulfur Spec.	0.283	0.353	0.526	0.980	-0.50	≤ 0
Fuel Oil						
	<u>CCFOFO</u>	<u>SRDSFO</u>	<u>SRFOFO</u>	<u>FO</u>	<u>RHS</u>	
Min. FO Production				1.0	$\geq 10,000$	
FO Blending	1.0	1.0	1.0	-1.0	$= 0$	
FO Density Spec.	294.4	292.0	295.0	-352.0	≤ 0	
FO Sulfur Spec.	0.353	0.526	0.980	-3.0	≤ 0	

Table 27 Process Unit Material Balances Using Volumetric Yields

Crude Oil Atmospheric Distillation Column:

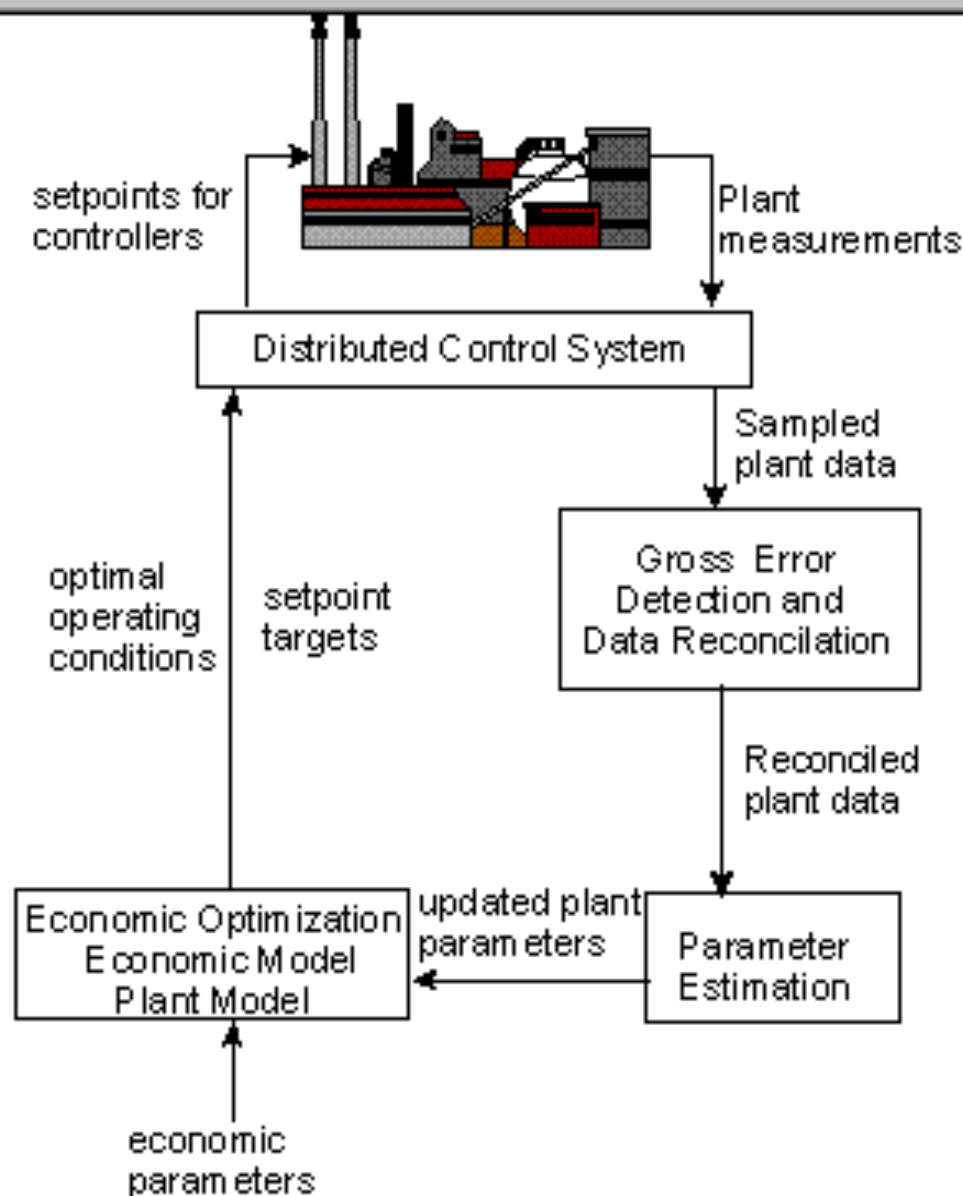
	<u>CRUDE</u>	<u>FGAD</u>	<u>SRG</u>	<u>SRN</u>	<u>SRDS</u>	<u>SRFO</u>	<u>RHS</u>
AD Capacity	1.0						$\leq 100,000$
FGAD Yield	35.42	-1.0					$= 0$
SRG Yield	0.270		-1.0				$= 0$
SRN Yield	0.237			-1.0			$= 0$
SRDS Yield	0.087				-1.0		$= 0$
SRFO Yield	0.372					-1.0	$= 0$

Catalytic Reformer:

	<u>SRNRF</u>	<u>FGRF</u>	<u>RFG</u>	<u>RHS</u>
RF Capacity	1.0			$\leq 25,000$
FGRF Yield	158.7	-1.0		$= 0$
RFG Yield	0.928		-1.0	$= 0$

Catalytic Cracking Unit:

	<u>SRDSCC</u>	<u>SRFOCC</u>	<u>FGCC</u>	<u>CCG</u>	<u>CCFO</u>	<u>RHS</u>
CC Capacity	1.0	1.0				$\leq 30,000$
FGCC Yield	336.9	386.4	-1.0			$= 0$
CCG Yield	0.619	0.688		-1.0		$= 0$
CCFO Yield	0.189	0.220			-1.0	$= 0$



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**

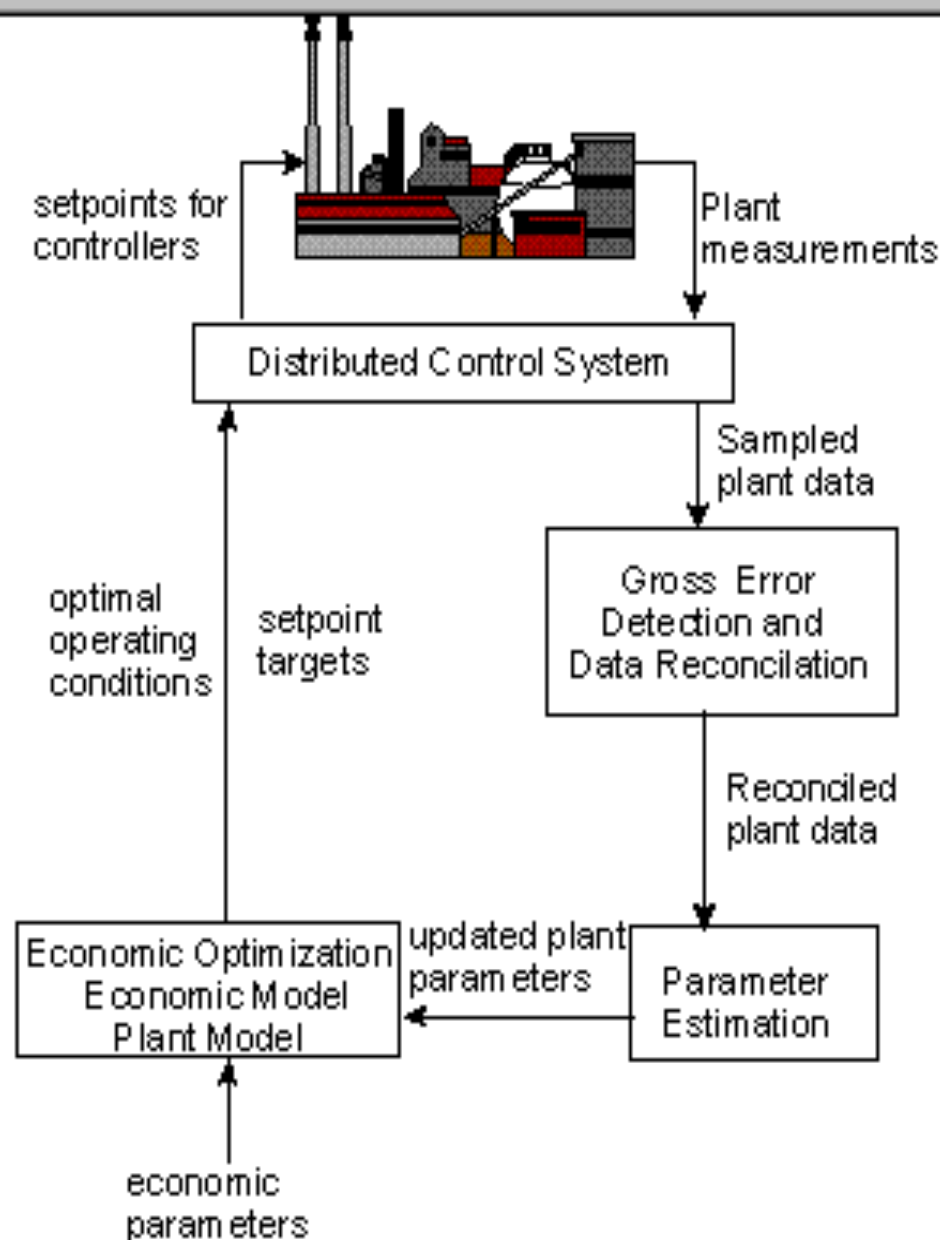
Revise Plant Information

OK

Cancel

Help

☐ Do not display this window next time



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

Open



Look in:



loo



Backup



Examples



Gams225



Temp

File name:

Files of type:



Open

Cancel



Open as read-only

Open



Look in:



loo



Backup

Examples

Gams225

Temp

File name:

Files of type:

loo files *.loo



Open

Cancel

☐ Open as read-only

Open



Look in:



Examples



refinery.ioo

File name:

Files of type:

ioo files *.ioo



Open

Cancel



Open as read-only

Open



Look in:



Examples



refinery.ioo

File name:

refinery.ioo

Files of type:

IoO files *.IoO



Open

Cancel



Open as read-only

Interactive On-line Optimization - E:\lcoo\Examples\refinery.ioo

File View Help



Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Model Name:

Refinery

Process Description:

Simple Refinery

Optimization Objective:

On-Line Optimization

ModelType:

Linear

Interactive On-line Optimization - C:\loo\Examples\refinery.loo

File View Help



Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Measured Variables

	Name	Plant Data	Standard Deviation Plant Data	Initial Point	Scaling Fac
▶	ccfo	6567.914	66	6567.914	
	ccfodi	3270.056	32.699	3270.056	
	ccfofo	3382.46	33.301	3382.46	
	ccg	20503.298	206.4	20503.298	
	ccgpg	7935.679	80.464	7935.679	
	ccgrg	12721.761	125.936	12721.761	
	crude	99686.657	1000	99686.657	10
	df	12582.842	125	12582.842	
	fgad	3553606.242	35420	3553606.242	3
	fgcc	12211460	115920	12211460	10
	fgf	3796351.148	37612	3796351.148	4
	pg	47263.811	471.132	47263.811	
	rfg	21826.603	219.936	21826.603	
	rfgpg	21835.077	219.936	21835.077	
	rfgrg	11.532	10	11.532	
	rg	22357.336	225.204	22357.336	
	srds	8636.35	87	8636.35	

☒ Include SCALING OPTION for variables

Interactive On-line Optimization - C:\loo\Examples\refinery.loo

File View Help

New Ctrl+N

Open... Ctrl+O

Close

Save

Save As...

Export

Import Plant Data

Import Standard Deviation

Execute... Ctrl+E

Exit

1. C:\loo\Examples\refinery.loo

2. S:\D-Train Sulfuric Model\Dsulfuric.loo

fgrf 3796351.148

pg 47263.811

rfg 21826.603

rfgpg 21835.077

rfgrg 11.532

rg 22357.336

srds 8636.35



☐ Include SCALING OPTION for variables

Optimization Algorithms

Constant Properties

Variables

Unmeasured Variables

Plant Parameters

Measured Variables

Std Deviation	Plant Data	Initial Point	Scaling Fac
66		6567.914	
32.699		3270.056	
33.301		3382.46	
206.4		20503.298	
80.464		7935.679	
105.000		10701.704	

Open

Look in: loo

Backup
Examples
Gams225
Temp

File name:

Open

Files of type:

Excel files *.xls

Cancel

☐ Open as read-only

File View Help



Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Unmeasured Variables

	Unmeasured Variables	Initial Point	Scaling Factor	Lower Bound	Upper Bound	Stream number	Process UnitID	Units of Process Variable
▶	fo	9978.183		0		s33		
*								

☐ Include SCALING OPTION for variables

File View Help



Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Plant Parameters

	Plant Parameter	Initial Point	Lower Bound	Upper Bound	Process UnitID	Unit of parameter
	vfgad	35.42	10	100	AD	BBL/BBL
	vsrds	0.087	0	1	AD	
	vsrdsccfo	0.188	0.15	0.2	CC	
	vsrdsccg	0.619	0	0.7	CC	
	vsrdsfgcc	336.9	300	400	CC	
	vsrfo	0.372	0	3	AD	
	vsrfccfo	0.22	0	5	CC	
	vsrfccg	0.688	0	5	CC	
	vsrfolgcc	386.4	100	1000	CC	
	vsrg	0.27	0	5	AD	
	vsrn	0.237	0	5	AD	
▶	vsrnfgf	158.17	0	1000	RF	
	vsrnfg	0.928	0	10	RF	
*						

File View Help



Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Equality Constraints

Equality Constraints	Scaling Factor	Process UnitID	Stream Number	
$SRGPG + RFGPG + SRNPG + CCGPG - PG = E = 0$		PG		
$SRGRG + RFGRG + SRNRG + CCGRG - RG = E = 0$		RG		
$SRNDF + CCFODF + SRDSDF + SRFODF - DF = E = 0$		DF		
$CCFOFO + SRDSFO + SRFOFO - FO = E = 0$		FO		
$VFGAD * CRUDE - FGAD = E = 0$	300	AD		
$VSRG * CRUDE - SRG = E = 0$	100	AD		
$VSRN * CRUDE - SRN = E = 0$	100	AD		
$VSRDS * CRUDE - SRDS = E = 0$	100	AD		
$VSRFO * CRUDE - SRFO = E = 0$	100	AD		
$VSRNFGRF * SRNRF - FGRF = E = 0$		RF		
$VSRNRFG * SRNRF - RFG = E = 0$		RF		
$VSRDSFGCC * SRDSCC + VSRFOFGCC * SRFOCC - FGCC = E = 0$		CC		
$VSRDSCCG * SRDSCC + VSRFOCCG * SRFOCC - CCG = E = 0$		CC		
$VSRDSCCFO * SRDSCC + VSRFOCCFO * SRFOCC - CCFO = E = 0$		CC		
$SRG - SRGPG - SRGRG = E = 0$		Split2		
$SRN - SRNRF - SRNPG - SRNRG - SRNDF = E = 0$		Split1		
$SRDS - SRDSCC - SRDSDF - SRDSFO = E = 0$		Split4		

☐ Include SCALING OPTION for equations

File View Help



Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Inequality Constraints

Inequality Constraints	Scaling Factor
▶ CRUDE=L=100000	
CRUDE=L=110000	
$78.5 \cdot \text{SRGPG} + 104 \cdot \text{RFGPG} + 65 \cdot \text{SRNPG} + 93.7 \cdot \text{CCGPG} - 93 \cdot \text{PG} = \text{G} = 0$	
$18.4 \cdot \text{SRGPG} + 2.57 \cdot \text{RFGPG} + 6.54 \cdot \text{SRNPG} + 6.9 \cdot \text{CCGPG} - 12.7 \cdot \text{PG} = \text{L} = 0$	
$78.5 \cdot \text{SRGRG} + 104 \cdot \text{RFGRG} + 65 \cdot \text{SRNRG} + 93.7 \cdot \text{CCGRG} - 87 \cdot \text{RG} = \text{G} = 0$	
$18.4 \cdot \text{SRGRG} + 2.57 \cdot \text{RFGRG} + 6.54 \cdot \text{SRNRG} + 6.9 \cdot \text{CCGRG} - 12.7 \cdot \text{RG} = \text{L} = 0$	
$272 \cdot \text{SRNDF} + 294.4 \cdot \text{CCFODF} + 292 \cdot \text{SRDSDF} + 295 \cdot \text{SRFODF} - 306 \cdot \text{DF} = \text{L} = 0$	
$0.283 \cdot \text{SRNDF} + 0.353 \cdot \text{CCFODF} + 0.526 \cdot \text{SRDSDF} + 0.98 \cdot \text{SRFODF} - 0.5 \cdot \text{DF} = \text{L} = 0$	
$294.4 \cdot \text{CCFOFO} + 292 \cdot \text{SRDSFO} + 295 \cdot \text{SRFOFO} - 352 \cdot \text{FO} = \text{L} = 0$	
$0.353 \cdot \text{CCFOFO} + 0.526 \cdot \text{SRDSFO} + 0.98 \cdot \text{SRFOFO} - 3 \cdot \text{FO} = \text{L} = 0$	
$\text{SRDSCC} + \text{SRFOCC} = \text{L} = 30000$	
$\text{pg} = \text{g} = 10000$	
$\text{rg} = \text{g} = 10000$	
$\text{df} = \text{g} = 10000$	
$\text{fo} = \text{g} = 10000$	
*	

☒ Include SCALING OPTION for equations

File View Help



Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Data Validation Algorithm:

Tjoa-Biegler Method (moderate gross errors)

Parameters Estimation Algorithm:

Least Squares Method (small gross errors)

Economic Optimization Objective Function:

$$-33 \times \text{crude} + 0.01965 \times \text{fgad} - 2.5 \times \text{smrf} + 0.01965 \times \text{fgrf} - 2.2 \times \text{srdscc} - 2.2 \times \text{srfocc} + 0.01965 \times \text{fgcc} +$$

Optimization Direction:

Maximizing

Economic Model Type:

Linear



Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Data Validation Algorithm:

Tjoo-Biegler Method (moderate gross errors)

Parameters Estimation Algorithm:

Least Squares Method (small gross errors)

Tjoo-Biegler Method (moderate gross errors)

Robust Function (large gross errors)

Economic Optimization Objective Function:

$$-33 \times \text{crude} + 0.01965 \times \text{fgad} - 2.5 \times \text{smrf} + 0.01965 \times \text{grf} - 2.2 \times \text{srdscc} - 2.2 \times \text{srfocc} + 0.01965 \times \text{fgcc} +$$

Optimization Direction:

Maximizing

Economic Model Type:

Linear



Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Data Validation Algorithm:

Tjoa-Biegler Method (moderate gross errors)

Parameters Estimation Algorithm:

Least Squares Method (small gross errors)

Economic Optimization Objective:

Least Squares Method (small gross errors)
Tjoa-Biegler Method (moderate gross errors)
Robust Function (large gross errors)

 $-33 \cdot \text{crude} + 0.01965 \cdot \text{fgad} - 2.5 \cdot \text{smr}$

Optimization Direction:

Maximizing

Economic Model Type:

Linear



Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Data Validation Algorithm:

Tjoa-Biegler Method (moderate gross errors)

Parameters Estimation Algorithm:

Least Squares Method (small gross errors)

Economic Optimization Objective Function:

$$-33 \cdot \text{crude} + 0.01965 \cdot \text{fgad} - 2.5 \cdot \text{srnrf} + 0.01965 \cdot \text{fgrf} - 2.2 \cdot \text{srdsc} - 2.2 \cdot \text{srfoc} + 0.01965 \cdot \text{fgcc} +$$

Optimization Direction:

Maximizing

Economic Model Type:

Maximizing
Minimizing



Model Description

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Data Validation Algorithm: Tjoo-Biegler Method (moderate gross errors)

Parameters Estimation Algorithm: Least Squares Method (small gross errors)

Economic Optimization Objective Function:

$$-33 \cdot \text{crude} + 0.01965 \cdot \text{fgad} - 2.5 \cdot \text{smrf} + 0.01965 \cdot \text{fgrf} - 2.2 \cdot \text{srdsc} - 2.2 \cdot \text{srfoc} + 0.01965 \cdot \text{fgcc} +$$

Optimization Direction: Maximizing

Economic Model Type:

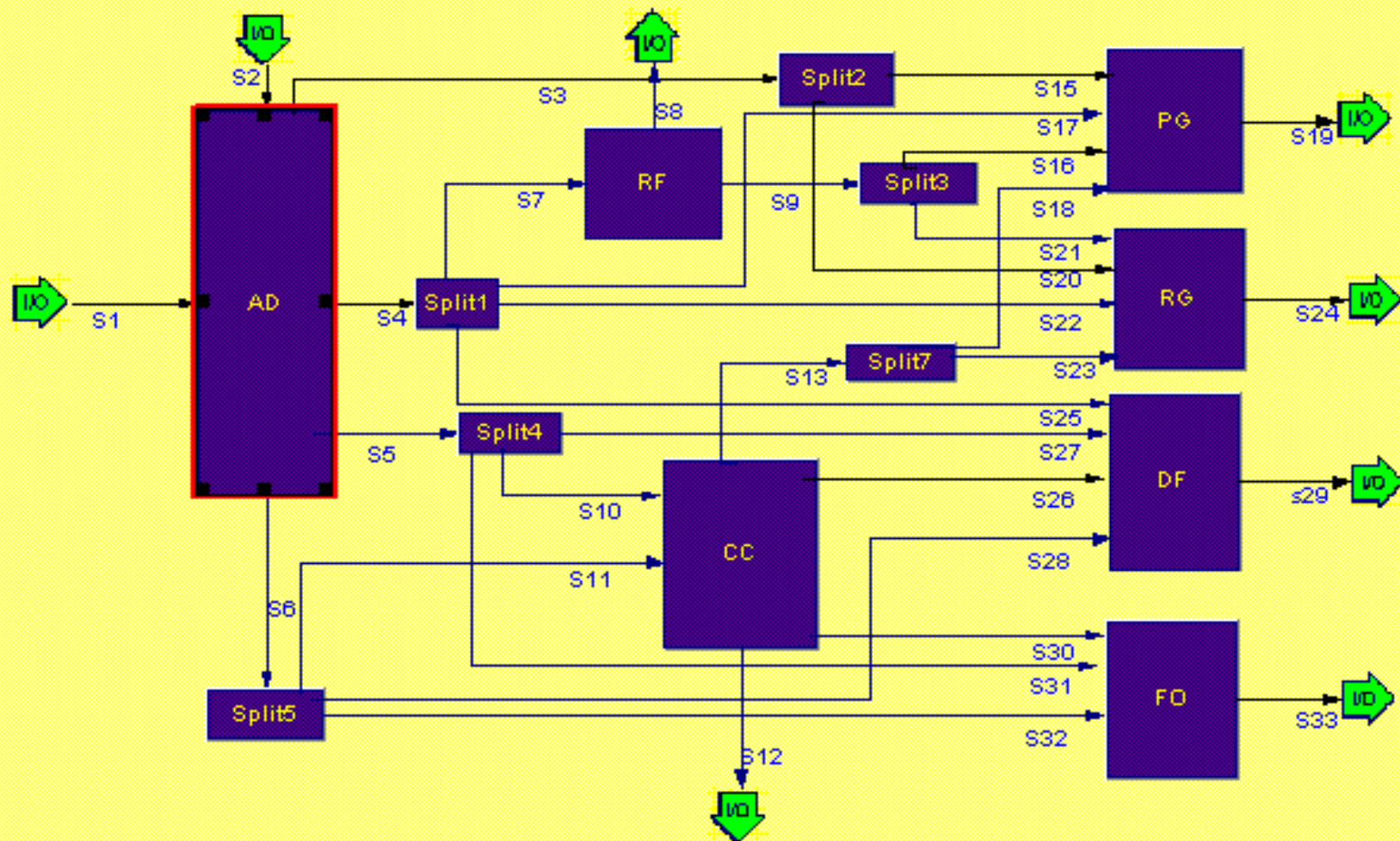
Linear

Linear

Nonlinear

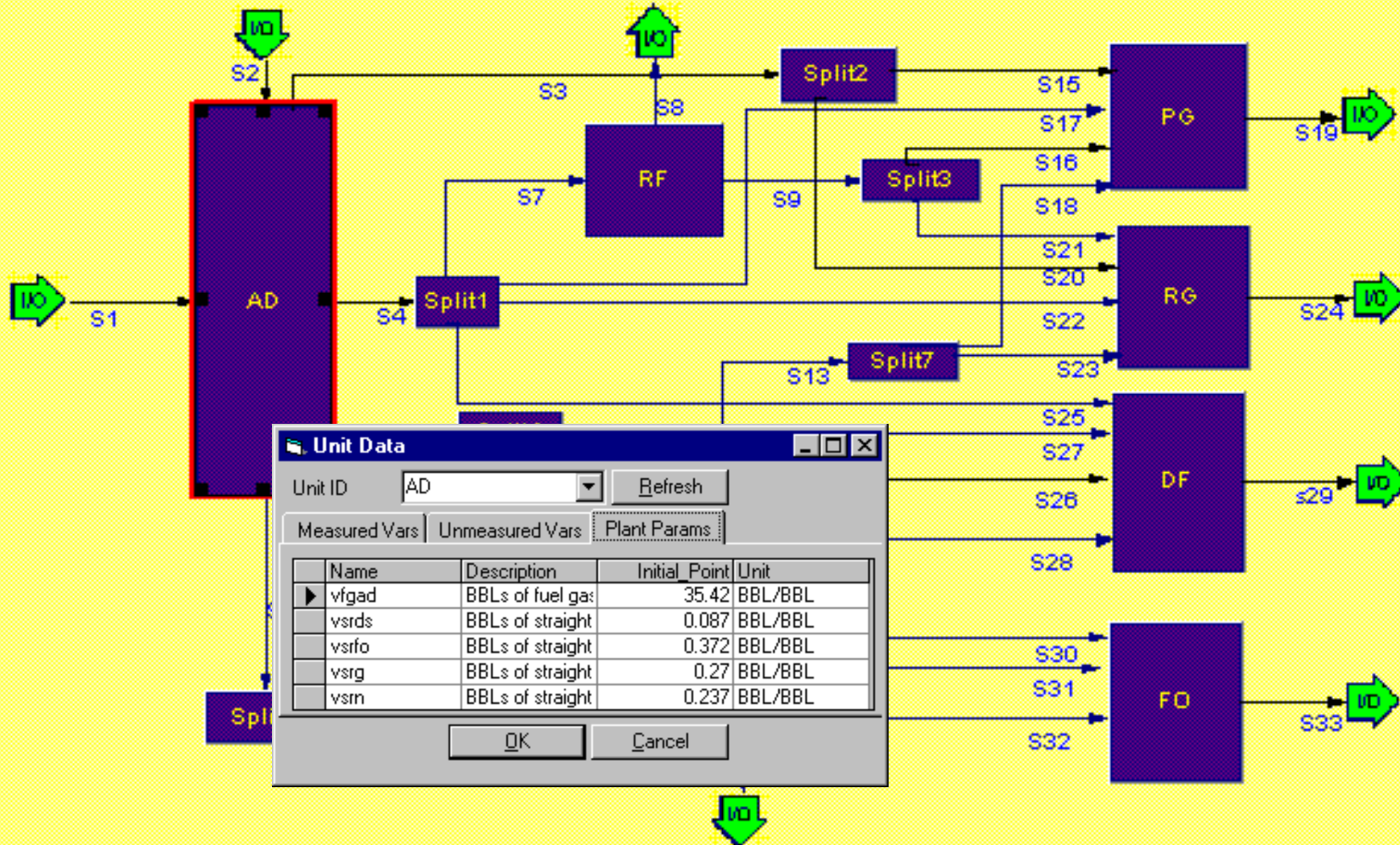
Flow Diagram

File Edit Options



Flow Diagram

File Edit Options



Unit Data							
Unit ID		AD		Refresh			
Measured Vars		Unmeasured Vars		Plant Params			
	Name	Description	Initial Point	Unit			
	vfgad	BBLs of fuel gas	35.42	BBL/BBL			
	vsrds	BBLs of straight	0.087	BBL/BBL			
	vsrfo	BBLs of straight	0.372	BBL/BBL			
	vsrg	BBLs of straight	0.27	BBL/BBL			
	vsrn	BBLs of straight	0.237	BBL/BBL			
OK		Cancel					

Interactive On-line Optimization - D:\Ioo\Examples\refinery.ioo

File View Help



Model Description

Execute

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Equality Constraints

Inequality Constraints

Optimization Algorithms

Constant Properties

Data Validation Algorithm:

Tjoa-Biegler Method (moderate gross errors)

Parameters Estimation Algorithm:

Least Squares Method (small gross errors)

Economic Optimization Objective Function:

$$-33 \cdot \text{crude} + 0.01965 \cdot \text{fgad} - 2.5 \cdot \text{smrf} + 0.01965 \cdot \text{fgrf} - 2.2 \cdot \text{srdsc} - 2.2 \cdot \text{srfo} + 0.01965 \cdot \text{fgcc} + 45.36 \cdot \text{pg} + 43.68 \cdot \text{rg} + 40.32 \cdot \text{df} + 13.14 \cdot \text{fo}$$

Optimization Direction:

Maximizing

Economic Model Type:

Linear

Model Summary & Execute

Summary of Refinery

Plant model: Linear

Economic model: Linear, Maximizing

Parameter estimation algorithm: Least Squares Method

Data validation algorithm: Tjoa-Biegler Method (no

Description: Simple Refinery

Conduct D.V., P.E., E.O. in sequence

Measured variables: 32

Unmeasured variables: 1

Plant parameters: 13

Tables: 0

Equality constraints: 21

Inequality constraints: 15

Page length: 80

Do not include column list

Do not include equation list

☒ Data Validation

☒ Parameter Estimation

☒ Economic Optimization

Execute

Close

Previous Result...

```
MS gamscmex
T 7 x 14
E:\OFFICE\PRWIN\FILES\Ioo\Examples>cd E:\OFFICE\PRWIN\FILES\Ioo\Gams225

E:\OFFICE\PRWIN\FILES\Ioo\Gams225>gams.exe do_data save=put_data pagesize= 80
GAMS 2.25.089 Copyright (C) 1988-1996 GAMS Development. All rights reserved
Licensee: Prof. Ralph Pike C970207:1424AF-WAT
Louisiana State University, Chem. Engin.
--- Starting compilation
--- DO_DATA(131)
--- Starting execution
--- DO_DATA(129)
--- Generating model REFINERY
--- DO_DATA(130)
--- 22 rows, 34 columns, and 100 non-zeroes.
--
```



Economic Objective = 700734.61975

9/28/98 3:48:00 PM

	Name	Gross_Error
▶	ccfo	
	ccfodf	
	ccfofo	
	ccg	
	ccgpg	
	ccgrg	
	crude	
	df	
	fgad	
	fgcc	-5.33387149396135
	fgrf	
	pg	
	rfg	
	rfgpg	
	rfgrg	
	rg	
	srds	
	srdscc	
	srdsdf	
	srdsfo	

Output

File View



Values of Measured Variables

9/28/98 3:48:00 PM

	Name	Optimal Set Point	Data From Parameter Estimation	Reconciled Data From Data Validation	
▶	ccfo	6606.3	6634.94762	6600.65902	
	ccfodf	3442.80193	3270.056	3249.28602	
	ccfofo	3163.49807	3364.89162	3351.37301	
	ccg	20640.3	20730.22104	20642.06169	
	ccgpg	10491.06299	7935.679	7956.28167	
	ccgrg	10149.23701	12794.54204	12685.78001	
	crude	100000	100188.95139	99908.29873	
	df	12516.3	12495.89361	12455.40653	
	fgad	3542000	3548692.68012	3538751.94089	
	fgcc	11592000	11642423.34337	11593157.61642	
	fgrf	3731546.64	3733862.09383	3740432.58444	
	pg	46724.06523	47238.72121	46996.68208	
	rfg	21893.14008	21906.75821	21945.51077	
	rfgpg	20315.08974	21895.22621	21934.31875	
	rfrg	1578.05034	11.532	11.19202	
	rg	22883.37485	22543.89309	22585.6082	
	srds	8696	8712.64461	8692.02199	
	srdscc	0	0.004	0.02644	
	srdsdf	8673.867	8690.50761	8669.90103	

Output

File

View

Export...

Print

Close

Measured Variables

10/4/98 9:22:00 PM

	Name	Optimal Set Point	Reconciled Data From Parameter Estimation	Reconciled Data From [
▶	ccfo	6606.3	6634.94762	
	ccfodf	3820.3	3270.056	
	ccfofo	2786	3364.89162	
	ccg	20640.3	20730.22104	
	ccgpg	7843.6759		
	ccgrg	12796.6241		
	crude	100000		
	df	12516.3		
	fgad	3542000		
	fgcc	11592000		
	fgrf	3731546.64		
	pg	46724.06523		
	rfg	21893.14008		
	rfgpg	21893.14008		
	rfgrg	0		
	rg	22883.37485		
	srds	8696		
	srdsc	0		

Save As

Save in:

Examples

File name:

Save as type:

Excel files *.xls

☐ Open as read-only

Save

Cancel

Output

File View



Values of Unmeasured Variables

9/28/98 3:48:00 PM

	Unmeasured Variables	Value From Data Validation	Value From Parameter Estimation	Value From Economic Op
▶	fo	10010.77225	10015.20862	

Output

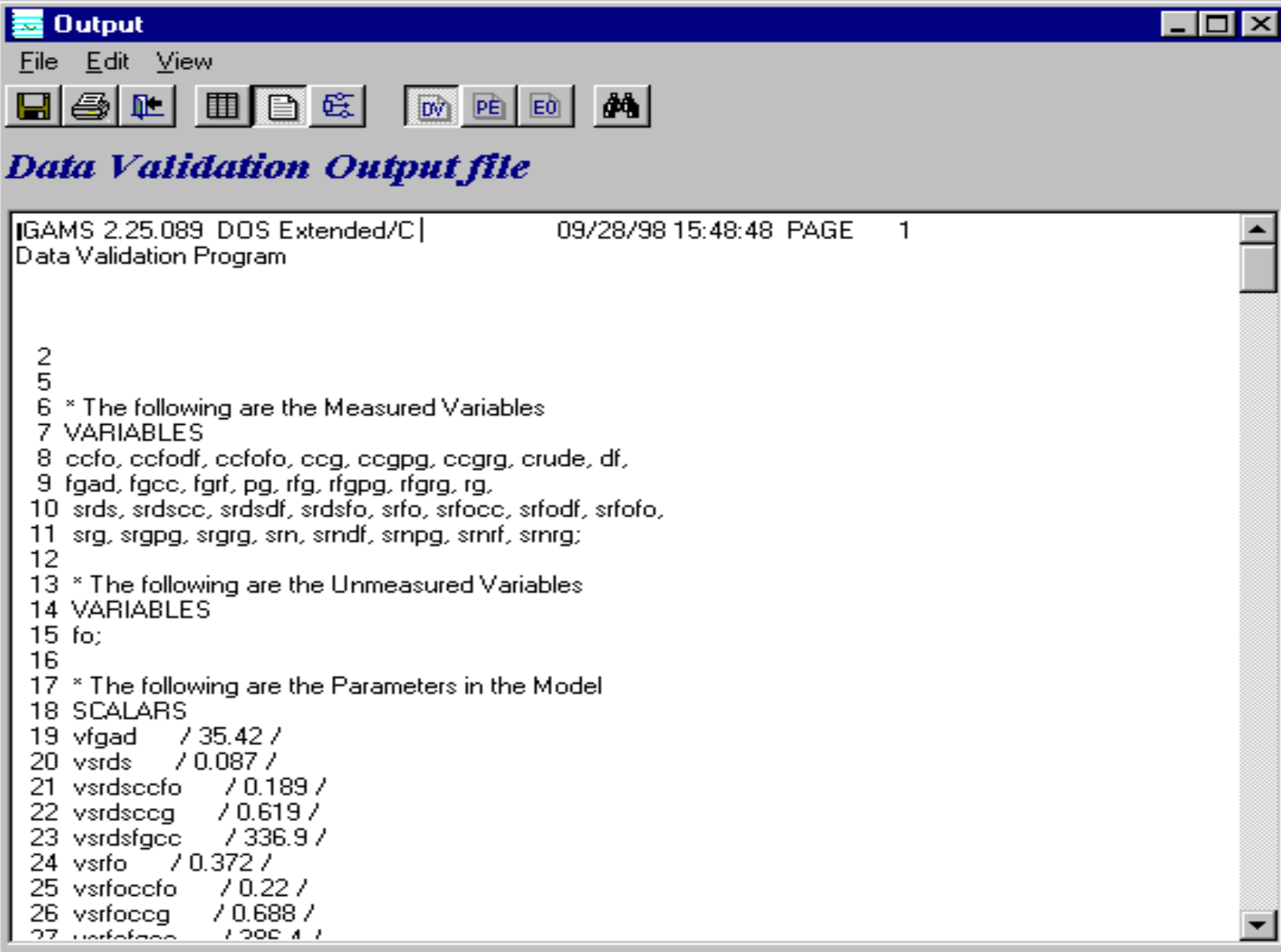
File View



Values of Plant Parameters

9/28/98 3:

	Plant_Parameter	Initial_Point	Estimated_Value	Process_UnitID	Unit_of_Parameter
▶	vfgad	35.42	35.42	AD	BBL/BBL
	vsrds	0.087	0.08696	AD	BBL/BBL
	vsrdsccfo	0.189	0.189	CC	BBL/BBL
	vsrdsccg	0.619	0.619	CC	BBL/BBL
	vsrdsfgcc	336.9	336.9	CC	BBL/BBL
	vsrfo	0.372	0.37214	AD	BBL/BBL
	vsrfocfo	0.22	0.22021	CC	BBL/BBL
	vsrfoccg	0.688	0.68801	CC	BBL/BBL
	vsrfofgcc	386.4	386.4	CC	BBL/BBL
	vsrg	0.27	0.27074	AD	BBL/BBL
	vsrn	0.237	0.23592	AD	BBL/BBL
	vsrngrf	158.17	158.17	RF	BBL/BBL
	vsrnrg	0.928	0.92799	RF	BBL/BBL





Parameter Estimation Output file

IGAMS 2.25.089 DOS Extended/C

09/28/98 15:48:50 PAGE 1

Parameter Estimation Program

2

5

6 * The following are the Measured Variables

7 VARIABLES

8 ccfo, ccfof, ccfofo, ccg, ccgpg, ccgrg, crude, df,

9 fgad, fgcc, fgrf, pg, rfg, rfgpg, rfgrg, rg,

10 slds, sldsc, sldsdf, sldsfo, srfo, srfocc, srfof, srfofo,

11 srg, srgpg, srgrg, sm, smdf, smpg, smrf, smrg;

12

13 * The following are the Unmeasured Variables

14 VARIABLES

15 fo;

16

17 VARIABLE ObjVar Objective function using ' ' algorithm

18 vfgad, vslds, vsldscfo, vsldscg, vsldsfcc, vsrfo, vsrfof, vsrfofo,

19 vsrfof, vsrg, vsrn, vsrnfg, vsrnfg;

20

21 EQUATIONS

22 * The Constraints

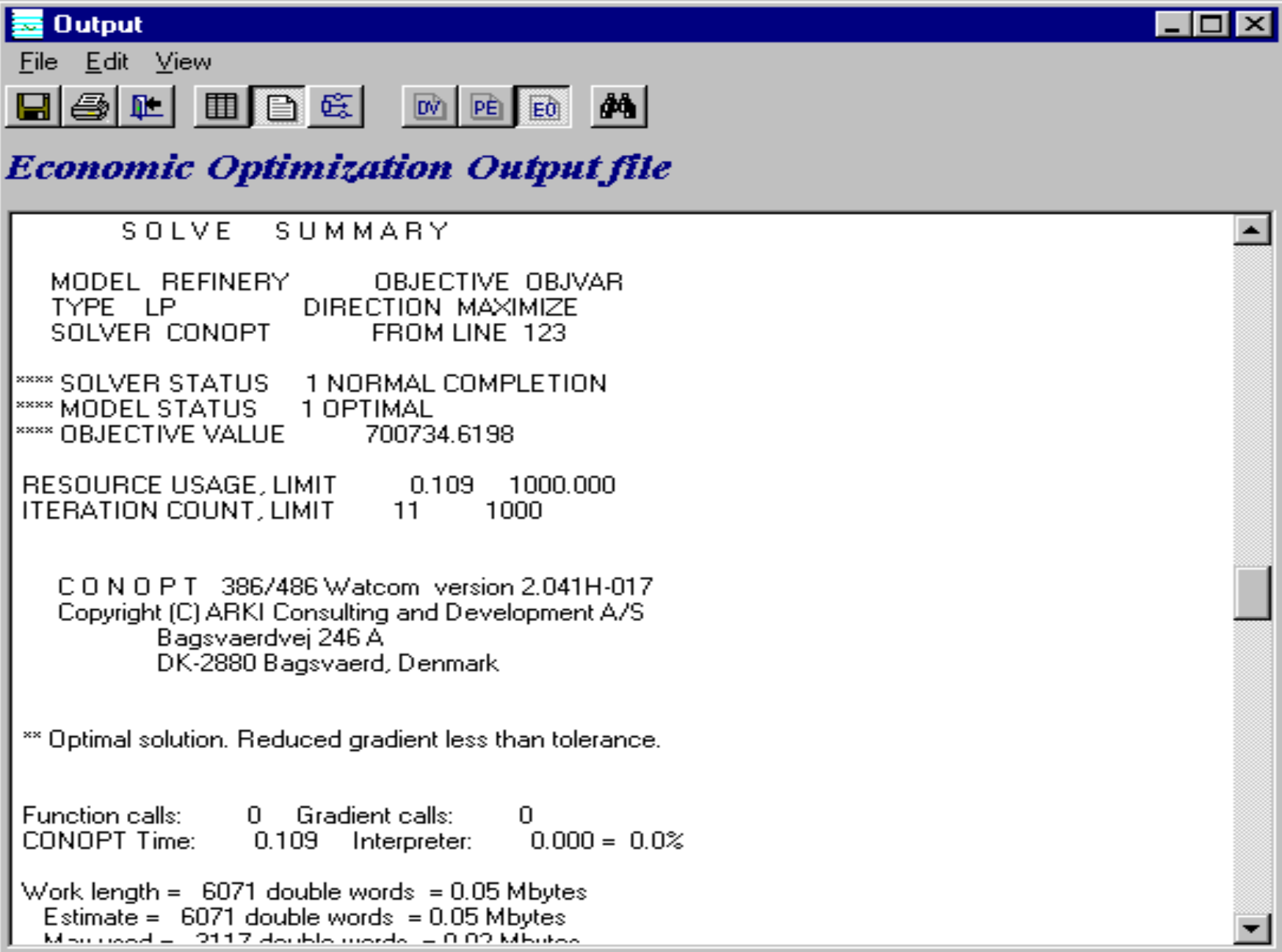
23 EQU1, EQU2, EQU3, EQU4, EQU5, EQU6,

24 EQU7, EQU8, EQU9, EQU10, EQU11, EQU12,

25 EQU13, EQU14, EQU15, EQU16, EQU17, EQU18,

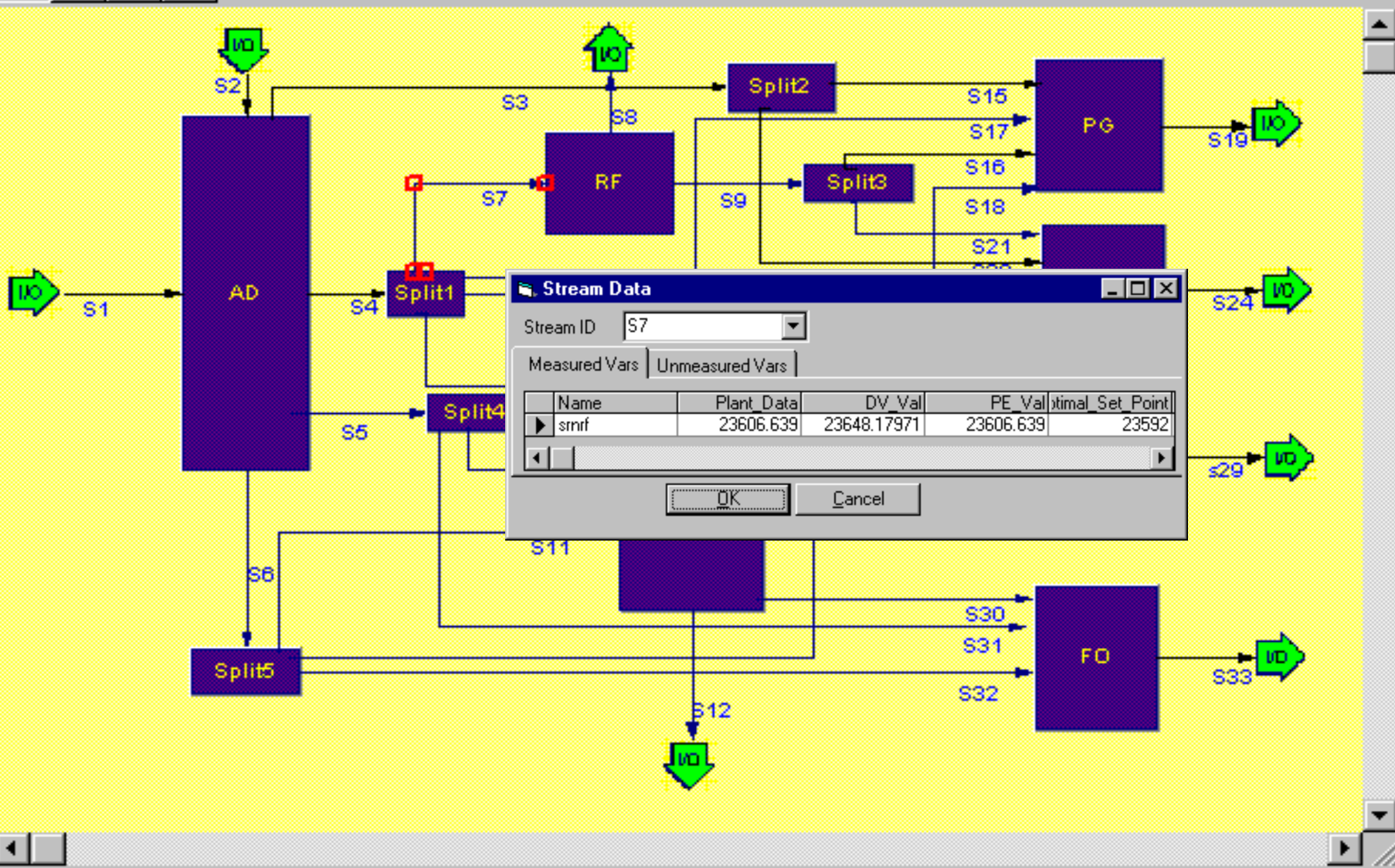
26 EQU19, EQU20, EQU21, ObjName;

27



Flow Diagram

File Edit Options



Stream Data

Stream ID: S7

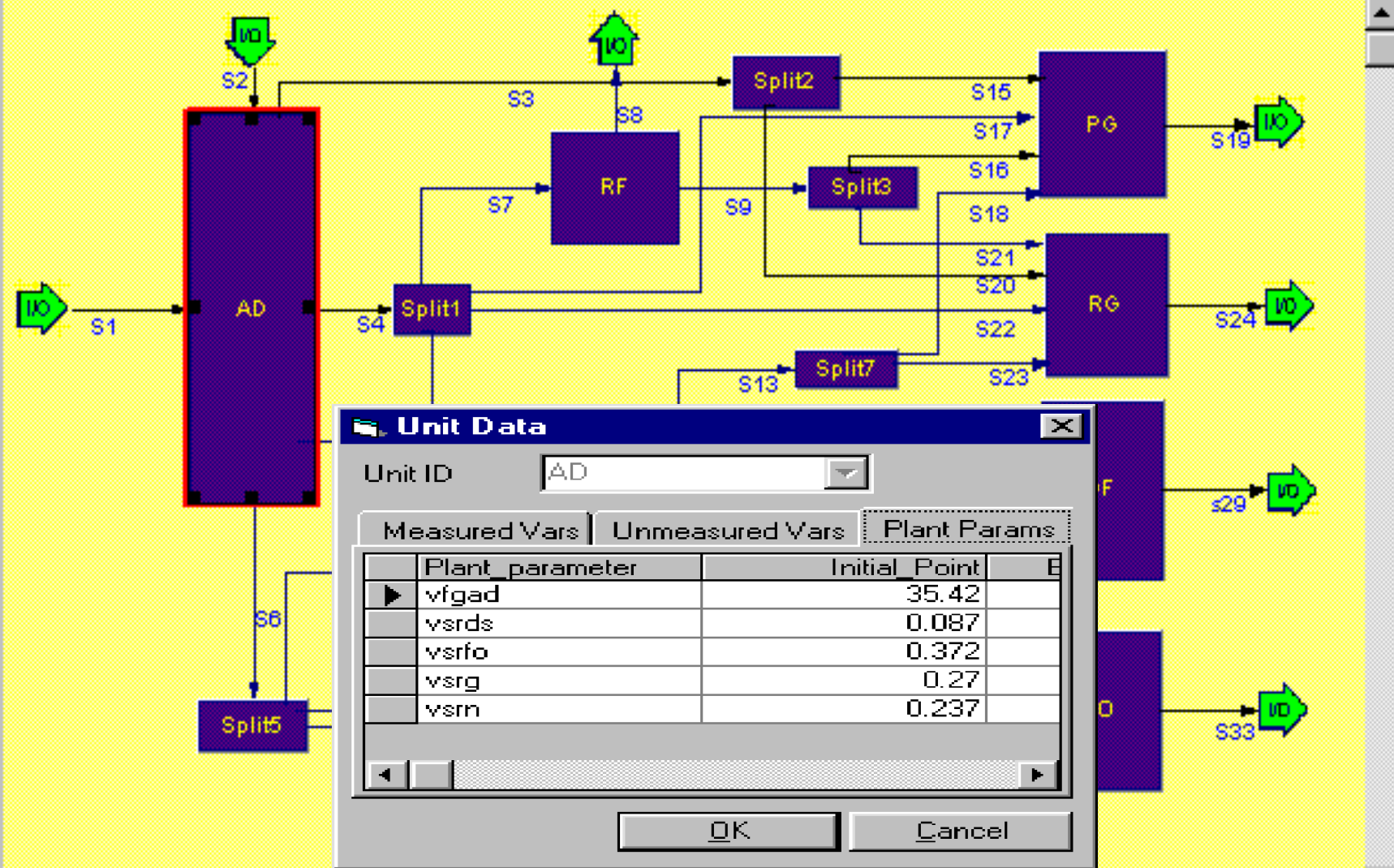
Measured Vars | Unmeasured Vars

Name	Plant Data	DV_Val	PE_Val	Optimal Set Point
snrf	23606.639	23648.17971	23606.639	23592

OK Cancel

Flow Diagram

File Edit Options



Unit Data

Unit ID

AD

Measured Vars

Unmeasured Vars

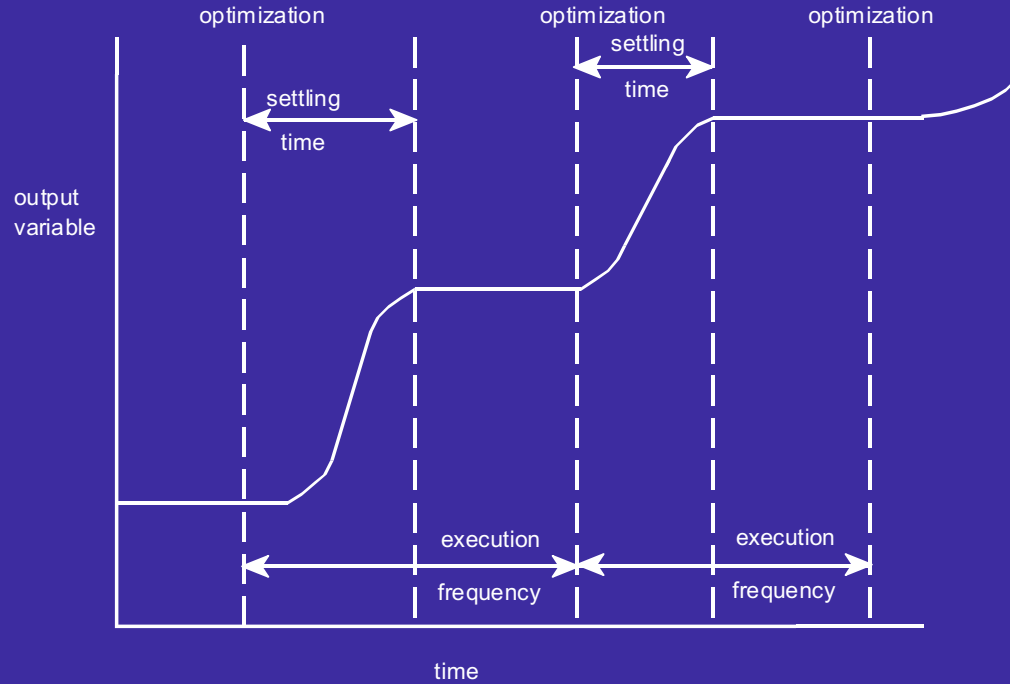
Plant Params

	Plant_parameter	Initial_Point	E
▶	vfgad	35.42	
	vsrds	0.087	
	vsrfo	0.372	
	vsrg	0.27	
	vsrn	0.237	

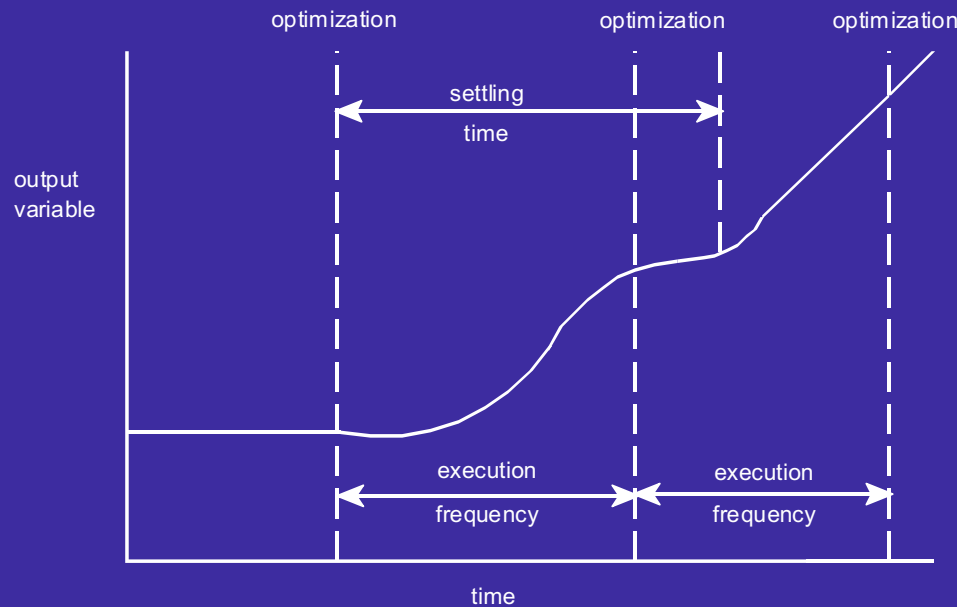
OK

Cancel

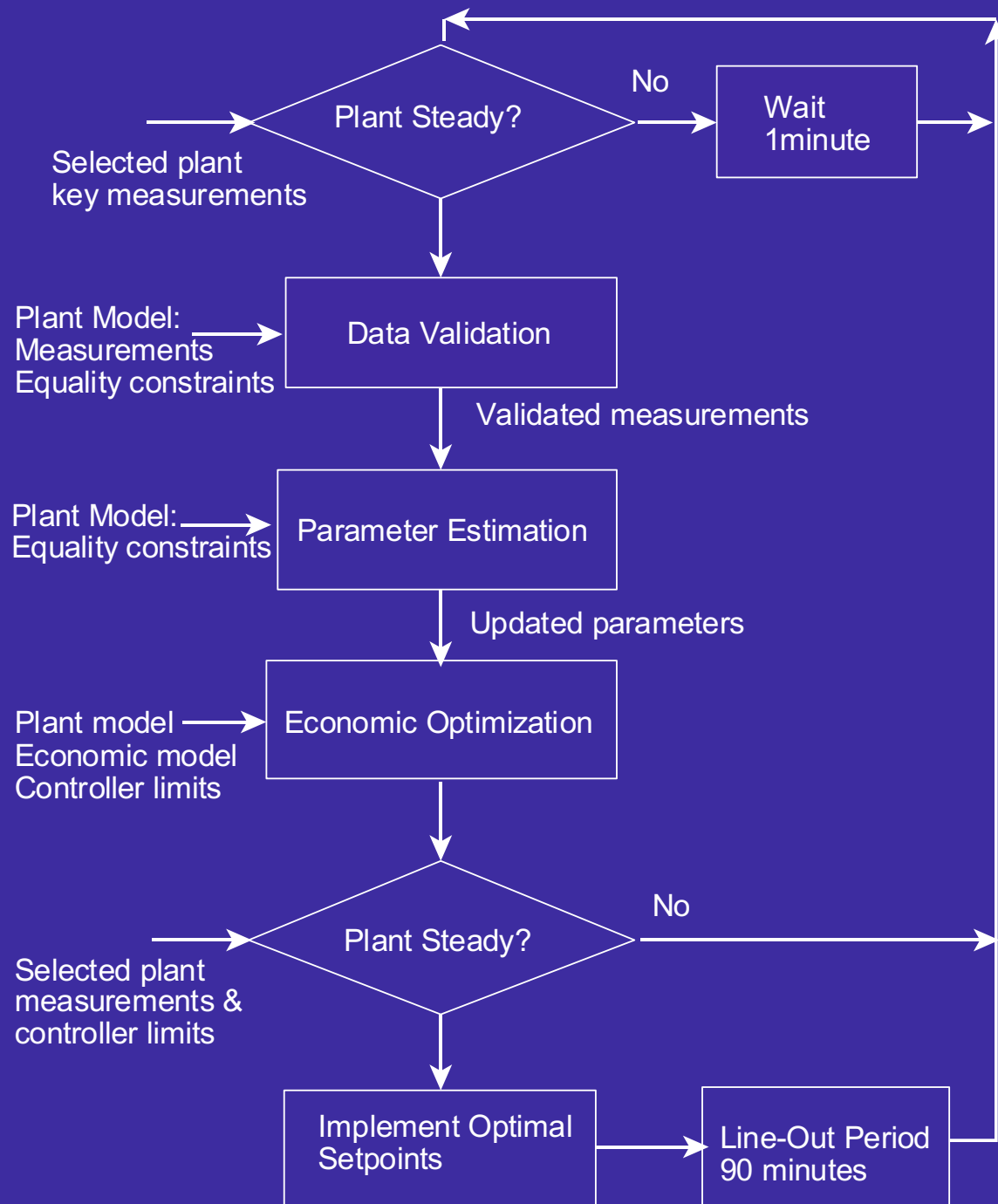
Output				
File View				
<i>Values of Measured Variables</i>			Stream Number	9/28/98 3:
	Name	Optimal Set Point	Reconciled Data From Parameter Estimation	Reconciled
▶	ccfc	6606.3	6634.94762	
	ccfodf	3442.80193	3270.056	
	ccfofo	3163.49807	3364.89162	
	ccg	20640.3	20730.22104	
	ccgpg	10491.06299	7935.679	
	ccgrg	10149.23701	12794.54204	
	crude	100000	100188.95139	
	df	12516.3	12495.89361	
	fgad	3542000	3548692.68012	
	fgcc	11592000	11642423.34337	
	fgrf	3731546.64	3733862.09383	
	pg	46724.06523	47238.72121	
	rfg	21893.14008	21906.75821	
	rfgpg	20315.08974	21895.22621	
	rfgrg	1578.05034	11.532	
	rg	22883.37485	22543.89309	
	srds	8696	8712.64461	
	srdscc	0	0.004	
	srdsdf	8673.867	8690.50761	
	srdsfo	22.133	22.133	
	srfo	37214	37284.01171	
	srfocc	30000	30130.49171	
	srfodf	399.63107	525.336	
	srfofo	3014.20000	3020.104	

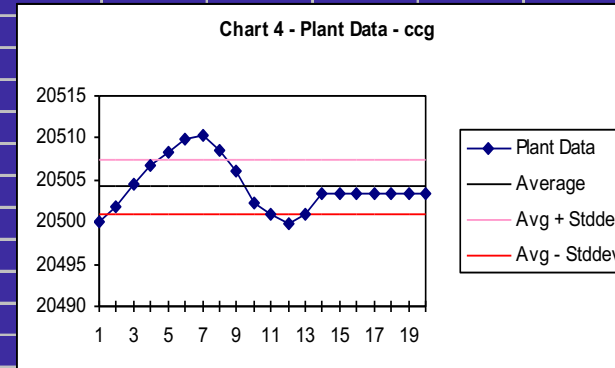
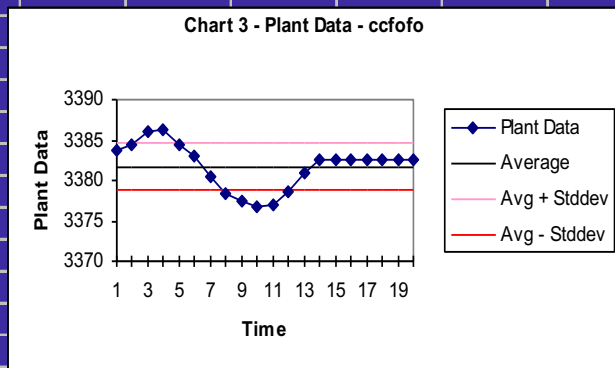
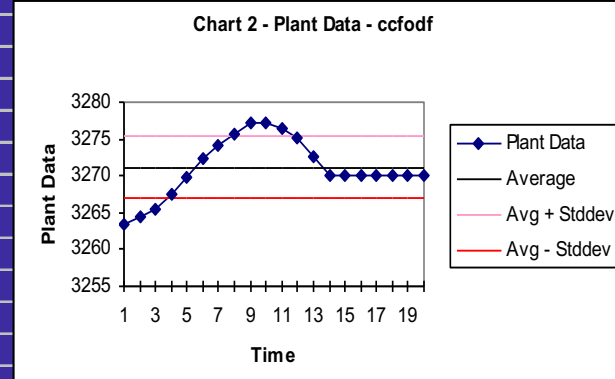
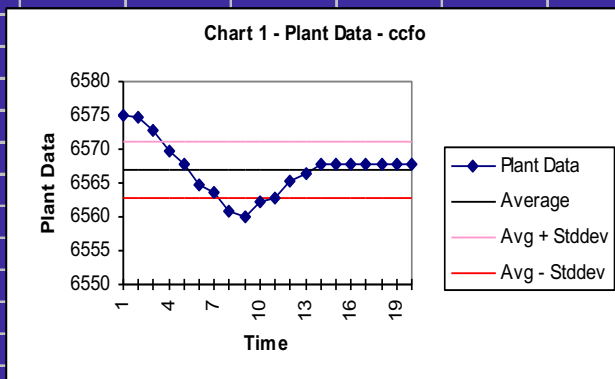


a. Time between optimizations is longer than settling time



b. Time between optimizations is less than settling time





ccfo

Choose Chart

Chart 1	Chart 2
Chart 3	Chart 4

Plot Graph

Save Steady State Data

6567.914
3270.056
3382.46
20503.3
7935.679
12721.76
99686.66
12582.84
3553606
12211460
3796351
47263.81
21826.6
21835.08
11.532
22357.34
8636.35
0.004
8613.47
22.133
36838.57
29727.33
525.336
6628.184
27125.16
17394.83
10044.59
23266.3
9.994
12.99
23606.64
7.1

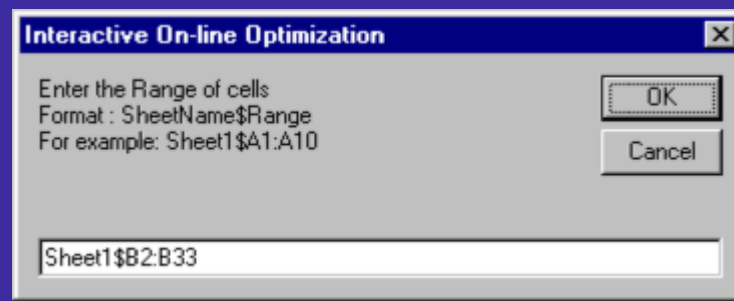
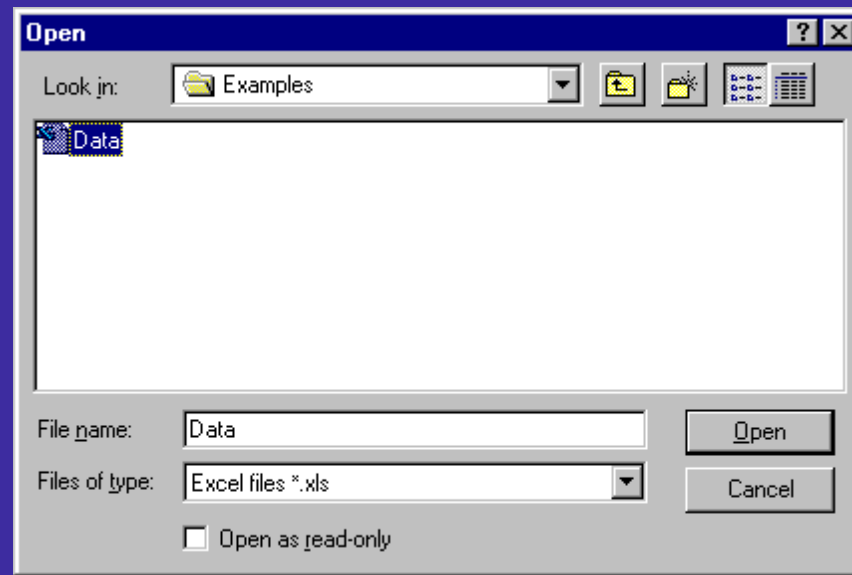


Figure 37 The Screen to Enters the Excel Sheet Name and Range

Data from Contact Process DCS

Plant Data	1	2	3	4	5	6	7	8	9	10	11	12	13	14
F06	1.72	1.74	1.72	1.72	1.72	1.68	1.68	1.72	1.74	1.76	1.66	1.76	1.72	1.74
f50	0.245	0.245	0.248	0.245	0.248	0.245	0.24	0.245	0.249	0.245	0.245	0.245	0.25	0.245
fsbfw	1.93	1.93	1.965	1.93	1.93	1.93	1.965	1.89	1.93	1.958	1.93	1.93	1.93	1.93
O2percent	6	6.03	6.01	6	5.9	6	6.01	6.06	5.7	5.9	6.1	5.97	6	6.07
Pshp1	614.7	610	614.7	614.7	614.7	612	614.7	614.7	610	614.7	614.7	608	614.7	614.7
Pshp2	614.7	610	614.7	614.7	614.7	608	614.7	614.7	610	614.7	614.7	608	614.7	614.7
Pss2	709.7	708.8	709.7	709.7	709.7	709.7	709.7	709.7	709.7	709.7	709.7	709.7	712	709.7
SO2ppm	349	355	359	355	355	357	360	355	355	360	355	355	351	355
T06	359.67	359.67	361.89	362.44	362.44	362.44	360.78	359.67	360.22	359.00	359.67	360.22	362.44	363.00
T07	1321.5	1323.2	1321.5	1321.5	1324.2	1319.4	1321.5	1318.9	1321.5	1321.5	1320	1321.5	1321.5	1321.5
T09	646.5	646.2	646.5	646.5	646.5	645.8	646.5	646.5	646.8	646.5	645.5	646.5	646.5	646.5
T10	708	708.5	708	708.3	708	707.6	708	708	708.1	708	708	707.9	708	708
T11	893.56	894.11	893.56	893.00	892.44	893.56	894.11	894.67	893.56	893.00	892.44	893.00	893.56	893.56
T12	689.3	689.3	689.1	689.3	689.3	690.1	689.3	689.3	689	689.3	689.5	689.3	689.2	689.3
T13	785.7	785.9	785.9	785.8	785.9	786.1	785.9	785.9	786.3	785.9	786	785.9	785.9	785.6
T15	501.5	501.2	501.5	501.5	501.6	501.5	501.4	502	501.5	501.5	501.1	501.5	501	501.5
T16	349.8	349.8	349.5	349.7	349.8	349.8	349.9	350	349.8	349.8	349.6	349.8	350	349.8
T19	549.3	549.1	549.3	549.3	549.6	549.3	549.2	549.3	549.4	549.3	549.3	549.6	549.3	549.3
T20	690.9	691	690.9	691.1	690.9	690.8	690.9	690.8	690.7	690.6	690.9	691	690.9	690.9
T21	737	737.2	737	737.3	737	736.9	737	737.1	737	737	737.2	737	737.1	737
T22	683.5	683.5	683.3	683.5	683.5	683.6	683.5	683.5	683.6	683.6	683.5	683.5	683.4	683.5
T23	692.6	692.6	692.7	692.6	692.5	692.6	692.6	692.4	692.6	692.6	692.7	692.6	692.7	692.6
T235	673.2	673.2	673.3	673.2	673.1	673.2	673.2	673.3	673.2	673.4	673.2	673.3	673.2	673.2
T24	504.8	504.6	504.8	504.8	504.7	504.8	504.8	504.9	504.8	504.7	504.8	504.8	504.8	504.8
T25	350.4	350.6	350.4	350.4	350.2	350.4	350.4	350.5	350.4	350.5	350.4	350.4	350.6	350.4
TSBFW	225	225	225.1	225	225.2	225	224.9	225	225	225.1	225.2	225	225	225
TSHP1	665	664.8	665	665.2	665	665	664.9	665	665.1	665	665.1	665	665	665
TSHP2	650	650.2	650	649.7	650	650.2	650	650.1	650	649.8	650	650.3	650	650
TSW1	340	339.6	340	340	340.4	340	340.1	340	339.9	340	340	340.6	340	340

Chart 1 - Plant Data - F06

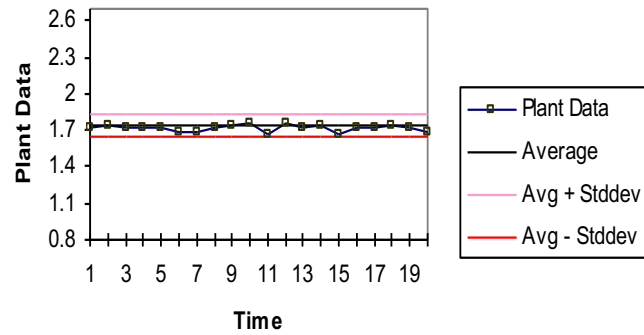


Chart 2 - Plant Data - O2percent

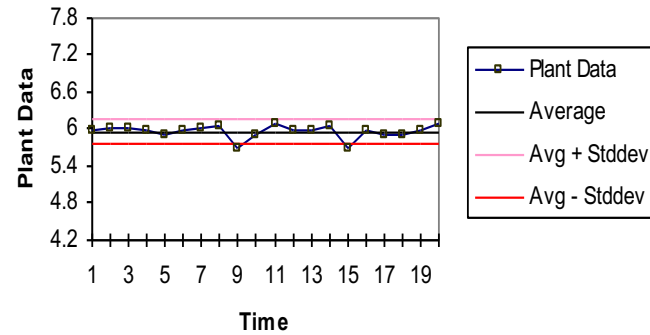


Chart 3 - Plant Data - T06

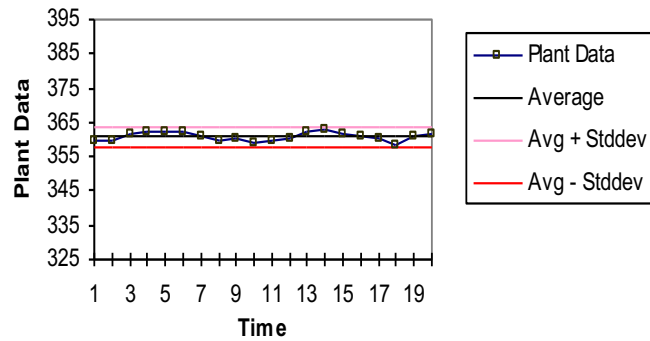
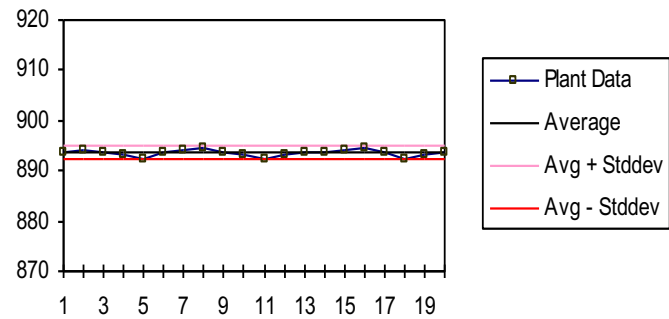


Chart 4 - Plant Data - T11



Choose

Chart 1

Chart 2

Chart 3

Chart 4

Plot Graph

Save Steady State Data

6567.234
3271.247
3384.938
20542.59
7940.337
12711.45
99673.84
12572.05
3548524
12235392
3791338
47302.53
21818.31
21838.05
12.78068
22350.21
8640.12
0.00429
8624.112
21.24542
36835.25
29725.27
525.4783
6630.703
27123.65
17412.39
10062.55
23275.79

DATA RECONCILIATION

measurements having only random errors - least squares

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

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

Σ = variance matrix = $\{\sigma^2_{ij}\}$.

σ_i = standard deviation of e_i .

$\mathbf{f}(\mathbf{x})$ - process model
- linear or nonlinear

DATA RECONCILIATION

Linear Constraint Equations - material balances only

$$\mathbf{f}(\mathbf{x}) = \mathbf{Ax} = 0$$

analytical solution - $\tilde{\mathbf{x}} = \mathbf{y} - \mathbf{\Sigma A}^T(\mathbf{A}\mathbf{\Sigma A}^T)^{-1}\mathbf{Ay}$

Nonlinear Constraint Equations

$\mathbf{f}(\mathbf{x})$ includes material and energy balances, chemical reaction rate equations, thermodynamic relations

nonlinear programming problem

GAMS and a solver, e.g. MINOS



Values of Measured Variables

9/28/98 3:

	Name	Optimal_Set_Point	Reconciled_Data_From_Parameter_Estimation	Reconciled
▶	ccfo	6606.3	6634.94762	
	ccfodf	3442.80193	3270.056	
	ccfofo	3163.49807		
	ccg	20640.3		
	ccgpg	10491.06299		
	ccgrg	10149.23701		
	crude	100000		
	df	12516.3		
	fgad	3542000		
	fgcc	11592000	11642423.34337	
	fgrf	3731546.64	3733862.09383	
	pg	46724.06523	47238.72121	
	rfg	21893.14008	21906.75821	
	rfgpg	20315.08974	21895.22621	
	rfgrg	1578.05		
	rg	22883.37		
	srds	8		
	srdscc			
	srdsdf	8673		
	srdsfo	22		
	srfo	37		
	srfocc	30000	30130.49171	
	srfodf	399.63107	525.336	
	srfofo	6014.20000	6620.104	

Stream Number

Please type in your request:

OK

Cancel

s15

Output

File

View

Data Validation results based on Stream No. = s15

Measured Variable	value	Units of Process Variables
▶ rrgpg	17093.12614	barrels/day



ective = 700734.61975

	Name	Gross_Error
▶	ccfo	
	ccfodf	
	ccfofo	
	ccg	
	ccgpg	
	ccgrg	
	crude	
	df	
	fgad	
	fgcc	-5.33387149396135
	fgrf	
	pg	
	rfg	
	rfgpg	
	rfgrg	
	rg	
	srds	
	srdscc	
	srdsdf	
	srdsfo	
	srfo	
	srfocc	
	srfodf	
	srfofo	
	srgr	
	srpgpg	
	srgrg	

Model Summary & Execute

Summary of Refinery

Plant model: Linear

Economic model: Linear, Maximizing

Parameter estimation algorithm: Least Squares Method

Data validation algorithm: Tjoa-Biegler Method (m)

Description: Simple Refinery

Conduct D.V., P.E., E.O. in sequence

Measured variables: 32

Unmeasured variables: 1

Plant parameters: 13

Tables: 0

Equality constraints: 21

Inequality constraints: 15

Page length: 80

Do not include column list

Do not include equation list

☒ Data Validation

☒ Parameter Estimation

☒ Economic Optimization

Execute

Close

Previous Result...

Interactive On-line Optimization - C:\loo\Examples\refinery.loo

File View Help

New Ctrl+N

Open... Ctrl+O

Close

Save

Save As...

Export

Import Plant Data

Import Standard Deviation

Execute... Ctrl+E

Exit

1. C:\loo\Examples\refinery.loo

2. C:\kedar\Data Validation\sulfuric42.loo

Measured Variables | Plant Parameters | Equality Constraints | Inequality Constr

Measured Variables

Plant_Data Initial_Point Scaling_Factor Lower_Bound Upper_Bound

66	6567.914		0	
32.699	3270.056		0	
33.301	3382.46		0	
206.4	20503.298	1	0	
80.464	7935.679		0	
125.936	12721.761	1	0	
1000	99686.657	1000	0	
125	12582.842	1	0	
35420	3553606.242	300	0	
fgcc	12211460	115920	12211460	1000
fgrf	3796351.148	37612	3796351.148	400
pg	47263.811	471.132	47263.811	1
rfg	21826.603	219.936	21826.603	1
rfgpg	21835.077	219.936	21835.077	1
rfgrg	11.532	10	11.532	
rg	22357.336	225.204	22357.336	1
srds	8636.35	87	8636.35	1

File View Help

New Ctrl+N

Open... Ctrl+O

Close

Save

Save As...

Export

Execute... Ctrl+E

Exit Ctrl+X



Inequality Constraints

Optimization Algorithms

Constant Properties

Tables

Measured Variables

Unmeasured Variables

Plant Parameters

Model Name: Refinery

Process Description: Simple Refinery

Optimization Objective: On-Line Optimization ▼

Model Type: Linear ▼