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Data reconciliation and optimal operation

With applications to refinery processes

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Introduction

- Data reconciliation and optimal operation
- Started December 1998
- Funded by Statoil
- Ph.D advisor professor Ph.D.Sigurd Skogestad
- Statoil advisor Ph.D. Stig Strand

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Thesis

1. Introduction
2. **Steady state models for effective on-line applications**
3. Data reconciliation
4. **Data reconciliation and optimal operation of a catalytic naphtha reformer**
5. On-line optimization of a crude unit heat exchanger network
6. Implementation issues for real time optimization of a crude unit heat exchanger network.
7. Conclusions and further work

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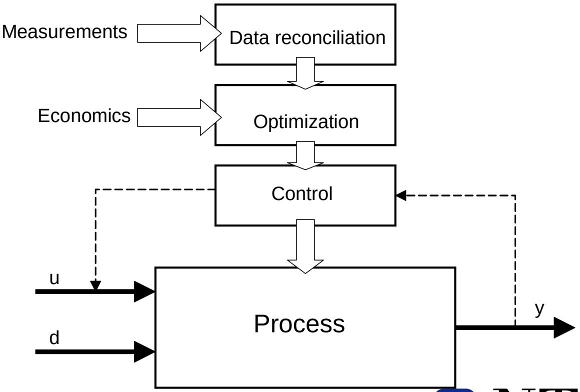
Data reconciliation and optimal operation



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Models for effective on-line applications

Preferred properties

- Open-equation formulation, $f(z) = 0$
- Equations written as unit models
- Standardization of equations
- Scaling
- Analytical first order derivatives
- Automatic generation of initial values
- Reuse of models

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Data reconciliation

$$\min_{z} \; J_r(z)$$

$$\text{s.t.} \quad f(z) = 0$$
$$A_r z = b_r$$
$$z_{r\,\min} \leq z \leq z_{r\,\max}$$

where $J_r(z) = (Uz - y_m)^{\mathrm{T}} \Sigma^{-1} (Uz - y_m)$

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Optimization

$$\min_{z} \quad J_{opt}(z)$$

$$\text{s.t.} \qquad f(z) = 0$$

$$A_{opt} z = b_{opt}$$

$$z_{opt\,\text{min}} \leq z \leq z_{opt\,\text{max}}$$

where $J_{opt}(z) = -p^{\mathrm{T}} z$ and $b_{opt} = A_{opt} z_r$

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Simulation

$$\min_{z} \; J_s(z)$$

$$\text{s.t.} \quad f(z) = 0$$

$$A_s z = b_s$$

where $J_s(z) = 0$

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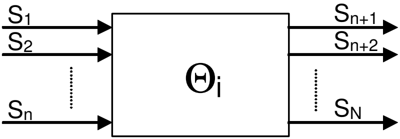
Unit model



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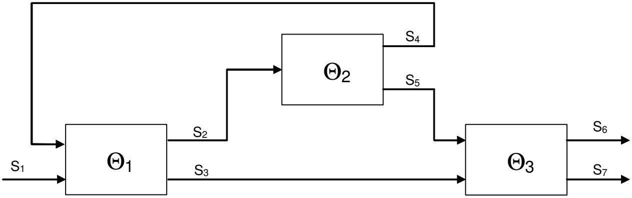
Process model



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Variables and equations

$$z = \begin{bmatrix} S_1 \\ S_2 \\ \vdots \\ S_7 \\ \Theta_1 \\ \Theta_2 \\ \Theta_3 \end{bmatrix}$$

$$r_i = f_i(z)$$

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Variables and equations

$$r = f(z) = \begin{bmatrix} f_1(z) \\ f_2(z) \\ f_3(z) \end{bmatrix}$$

$$\frac{\partial f(z)}{\partial z} = \begin{bmatrix} \frac{\partial f_1(z)}{\partial z} \\ \frac{\partial f_2(z)}{\partial z} \\ \frac{\partial f_3(z)}{\partial z} \end{bmatrix}$$

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The scaled process model

$$\tilde{f}(\tilde{z}) = 0$$
$$\widetilde{A}_s\tilde{z} = \tilde{b}$$

where $\tilde{z} = S_v^{-1}z$.

$$\tilde{f}(\tilde{z}) = S_f f(S_v\tilde{z})$$
$$\widetilde{A}_s = S_l A_s$$
$$\widetilde{J}(\tilde{z}) = S_o J(S_v\tilde{z})$$

where $\tilde{b} = S_l b_s$. S_l, S_f and S_v are fixed diagonal scaling matrices and S_o is a fixed factor.

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Scaling

1. Make a pairing of equations and variables.
2. Scale all variables such that the scaled variable has a value close to one
3. Scale all equations such that the absolute value of the elements of the first order derivatives, corresponding to the equation and variable pairing, is close to one.
4. Scale the objective function such that the largest element of the first order derivative $\widetilde{J}(\tilde{z})$ has an absolute value close to one.

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Scaling

$P(i,j) = 1$ if variable number j is paired with equation number i

$$\tilde{z} = S_v^{-1} z \approx 1$$

$$S_{f_i} = \left| \left[I \times \left(\frac{\partial f_i(z)}{\partial z} S_v P_{ni}^{\mathrm{T}} \right) \right]^{-1} \right|$$

$$S_o = 1/\max \left| \frac{\partial J(z)}{\partial z} S_v \right| \qquad (1)$$

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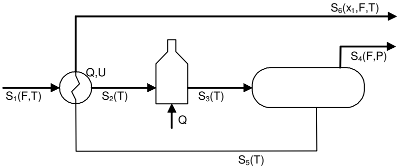
Example



	Cond.no. $\widetilde{H}$	Number of iterations Rec.	Opt.	d_{est}	J_{opt}	Active Constraints
Unscaled	5.0E+09	23	11	2.99	-9.34	$x_6(1)$
Method 1	4.8E+05	14	7	0.30	-9.85	$P_4, x_6(1), Q_{HT}$
Method 2	7.0E+09	9	3	3.49	-5.84	Q_{HT}
Method 3	4.0E+03	28	10	0.30	-9.85	$P_4, x_6(1), Q_{HT}$
New method	5.1E+01	12	5	0.30	-9.85	$P_4, x_6(1), Q_{HT}$

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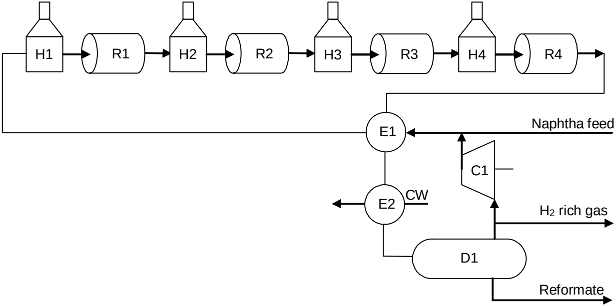
Optimal operation of a naphtha reformer



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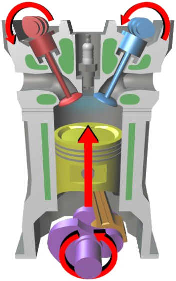
Optimal operation of a naphtha reformer

Octane number

The octane number is a measure of the autoignition resistance of gasoline.



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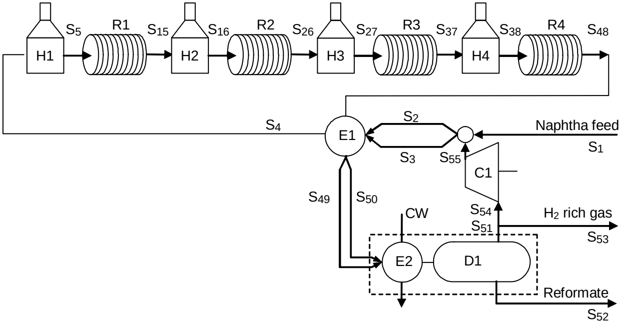
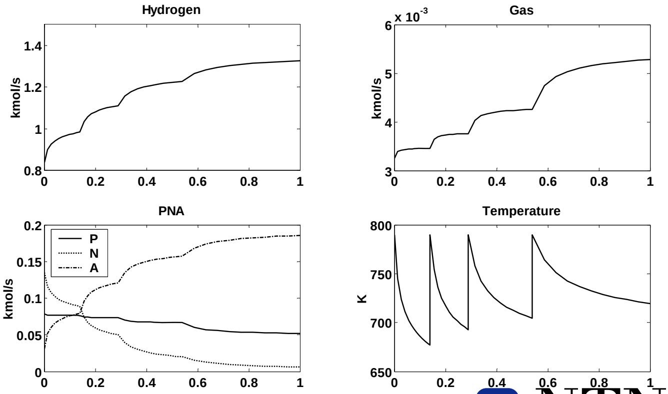
Optimal operation of a naphtha reformer

Process model



Optimal operation of a naphtha reformer

Nominal operation



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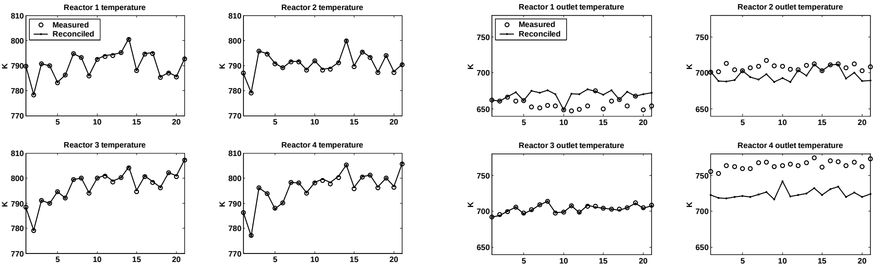
Optimal operation of a naphtha reformer

Data reconciliation results



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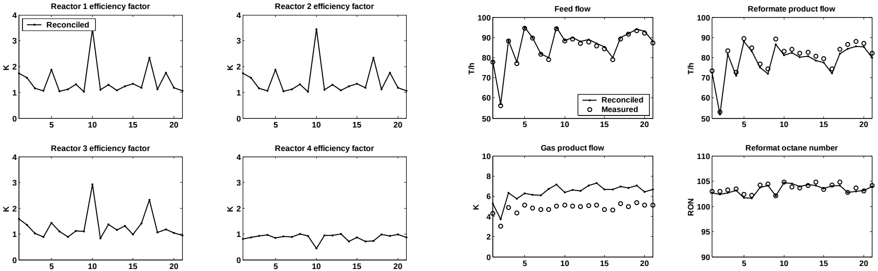
Optimal operation of a naphtha reformer

Data reconciliation results



Optimal operation of a naphtha reformer

Optimal operation

Description	Variable	Unit	Min.	Max.	Rec.	Case 1	Case 2	Price
Feed flow	$\widetilde{F}_1$	t/h			89.2	95.6	84.1	-60.0
Reformate flow	$\widetilde{F}_{52}$	t/h			84.2	90.6	79.7	**100.0
Gas flow (LPG)	$\widetilde{F}_{53}(G)$	t/h			1.2	1.0	0.9	50.0
H_2 mass flow	$\widetilde{F}_{53}(H)$	t/h	3.5		3.8	4.0	*3.5	
Reformat octane	RON		103.0		103.9	*103.0	*103.0	
Reactor 1 temp.	T_5	K		810.0	794.0	790.7	794.1	
Reactor 2 temp.	T_{16}	K		810.0	788.6	782.7	788.8	
Reactor 3 temp.	T_{27}	K		810.0	801.2	799.9	798.8	
Reactor 4 temp.	T_{38}	K		810.0	799.6	791.6	780.4	
Heater 1 duty	Q_1	MW		9.5	9.3	*9.5	8.6	-0.015
Heater 2 duty	Q_2	MW		13.0	12.7	*13.0	12.2	-0.015
Heater 3 duty	Q_3	MW		13.0	12.1	*13.0	11.3	-0.015
Heater 4 duty	Q_4	MW		10.0	10.0	*10.0	7.6	-0.015
Compressor duty	W	MW			0.88	0.48	0.39	-0.015
Feed H_2/HC ratio	H2/HC		3.0		5.0	*3.0	*3.0	
Separator pres.	P_{53}	bar	8.0	10.0	8.0	*10.0	*10.0	
Profit		$/h			2638	2883	-249	

(* = active constraint, ** = in case 2 the price of reformate is 65$/t)

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Optimal operation of a naphtha reformer

Control

Manipulated variables	Controlled variables Case 1	Controlled variables Case 2
Feed flow	Reformate RON	H_2 product flow
Heater 1 duty	Maximum*	Reformate RON
Heater 2 duty	Maximum*	T_{R1_i}-T_{R2_i}(=0)
Heater 3 duty	Maximum*	T_{R2_i}-T_{R3_i}(=0)
Heater 4 duty	Maximum*	T_{R3_i}-T_{R4_i}(=0)
Pressure	Maximum*	Maximum*
Compressor work	H_2/HC ratio	H_2/HC ratio

(* Manipulated variable fixed at maximum value)

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Summary

— Modeling framework simplifies the development of on-line models.

— Proposed scaling shows promising results, also for larger models.

— Data reconciliation and problem analysis gives useful knowledge of the measurements and process behavior.

— Proper selection of controlled variables simplifies the implementation of the optimal result.

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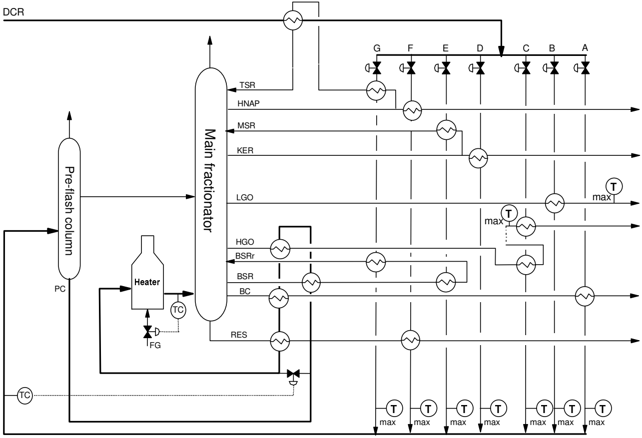
Crude unit heat exchanger network



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Models for effective on-line applications

Scaling

Method 1. Scaling based on variable bounds and initial equation residual

$$S_{v_{jj}} = 2^{a_j} \quad \text{where } a_j = \text{int}[\log_2(z_{\max_i} - z_{\min_i})] \qquad (2)$$

$$S_{n_{ii}} = 2^{-a_i} \quad \text{where } a_i = \text{int}[\log_2(|f(z_0)|_i)] \qquad (3)$$

$$S_{l_{ii}} = 2^{-a_i} \quad \text{where } a =_i \text{int}[\log_2(|A_s z_0 - b_s|_i)] \qquad (4)$$

where z_0 is the initial value. The equation scaling factor is limited to some maximum value in case the equation residual is close to zero.

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Scaling

Method 2. Scaling based on first order derivatives

$$\mathbb{C} = \begin{bmatrix} \frac{\partial f(z_0)}{\partial z} \\ A_s \end{bmatrix} \quad (5)$$

$$S_{v_{jj}} = ||\mathbb{C}_j||_2^{-1} \quad \text{where } j = 1...n_z \quad (6)$$

$$S_{n_{ii}} = ||\mathbb{C}_i||_2^{-1} \quad \text{where } i = 1...n_f \quad (7)$$

$$S_{l_{ii}} = ||\mathbb{C}_i||_2^{-1} \quad \text{where } j = n_f + 1...n_f + n_s \quad (8)$$

where $\mathbb{C}_j$ and $\mathbb{C}_i$ denotes the columns and rows of $\mathbb{C}$ respectively.

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Scaling

Method 3. Scaling based on order of magnitude

$$S_{v_{jj}} = 10^{-a_j} \quad \text{where } a_j = \mathrm{int}[\log_{10}(z_0)_j] \tag{9}$$

The equation scaling factor is the reciprocal of an integer power of 10 of the value of a given term or group of terms, normally related to the scale factor of a relevant variable.

As an example, let a typical value of a mass balance term $x_i F$ be $0.5 \cdot 0.3 = 0.15$. The scaling factor for the mass balance equation is then $10^{(-\mathrm{int}(\log_{10}(0.15)))} = 10$. The objective scaling factor is divided by an integer power of 10 close to its typical value.

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