Self-optimizing Control of a GTL process

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Outline

- ❑ Introduction
- ❑ Conceptual design of a GTL process
- ❑ Optimal operation and self-optimizing control
- ❑ Summary

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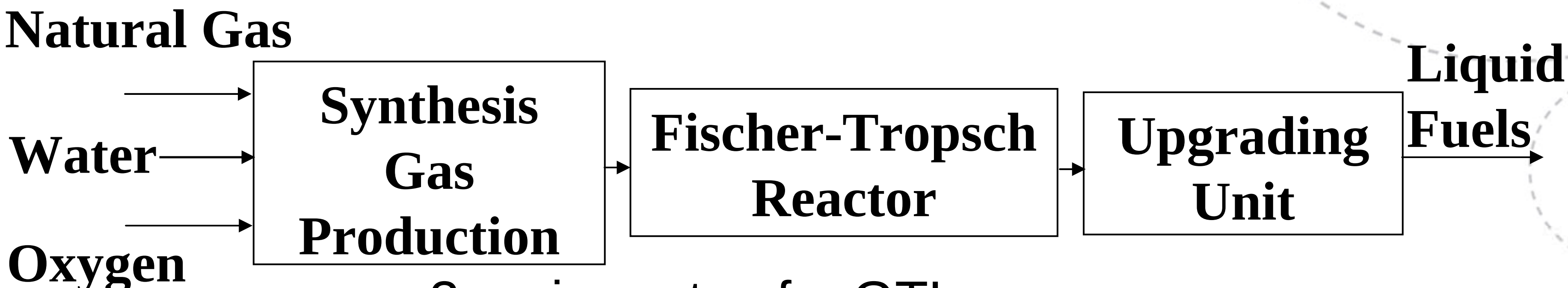
GTL is converting of natural gas to synthetic liquid fuels via Fischer-Tropsch (FT) reactions



3 main parts of a GTL process

Ideal Case: Thermodynamically possible but very far from being practical

$$nCH_4 + \frac{n}{2}O_2 \rightarrow (-CH_2-)_n + nH_2O$$

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Skogestad's procedure for plantwide control

Self-optimizing control

Mode I: maximize efficiency

Mode II: maximize throughput

Self-optimizing control is when we can achieve acceptable loss with constant setpoint values for the controlled variables without the need to reoptimize the plant when disturbances occur

Skogestad, S., 2004, Control Structure Design for Complete Chemical Plants, Computers and Chemical Engineering, 28, 219-234

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Main reactions in GTL process

SynGas unit

Auto Thermal Reforming (ATR)

$$CH_4 + \frac{3}{2}O_2 \Leftrightarrow CO + 2H_2O \qquad \Delta H = -519.32\frac{kJ}{mol} \qquad \Delta G = -562.65\frac{kJ}{mol}$$

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2 \qquad \Delta H = +206.13\frac{kJ}{mol} \qquad \Delta G = +151.65\frac{kJ}{mol}$$

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \qquad \Delta H = -41.39\frac{kJ}{mol} \qquad \Delta G = -19.09\frac{kJ}{mol}$$

Desired $\frac{H_2}{CO}$ is 2-2.3 for FT reactor using Cobalt catalyst in a SBCR. ATR temperature is around 1000°C

FT reactions

$$nCO + 2nH_2 \rightarrow (\text{-}CH_2\text{-})_n + nH_2O \qquad \Delta H = -165\frac{kJ}{mol}$$

FT temperature is 220-230 °C

Yates, I. C. and C. N. Satterfield,1991, Intrinsic Kinetics of the Fischer-Tropsch Synthesis on a Cobalt Catalyst, Energy & Fuels, 5, 168-173

Process design basis

- One train of the biggest current GTL plant
- Equilibrium reactions in syngas unit
- Satterfield & Yates kinetic in FT reactor
- Industrial scale ratios of water and oxygen to natural gas in feedstock and volume of the FT reactor

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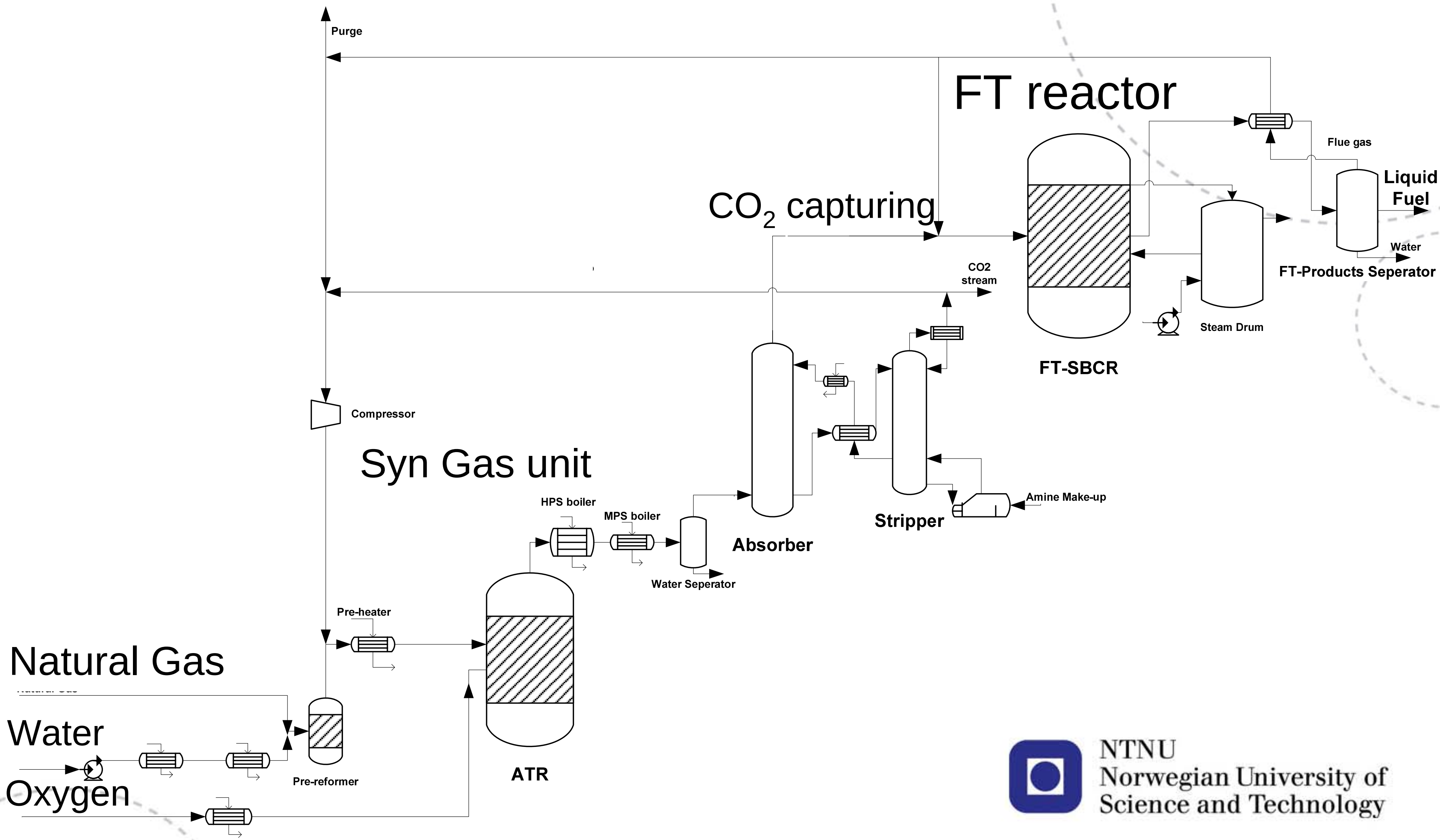
Resulting flowsheet of a GTL process



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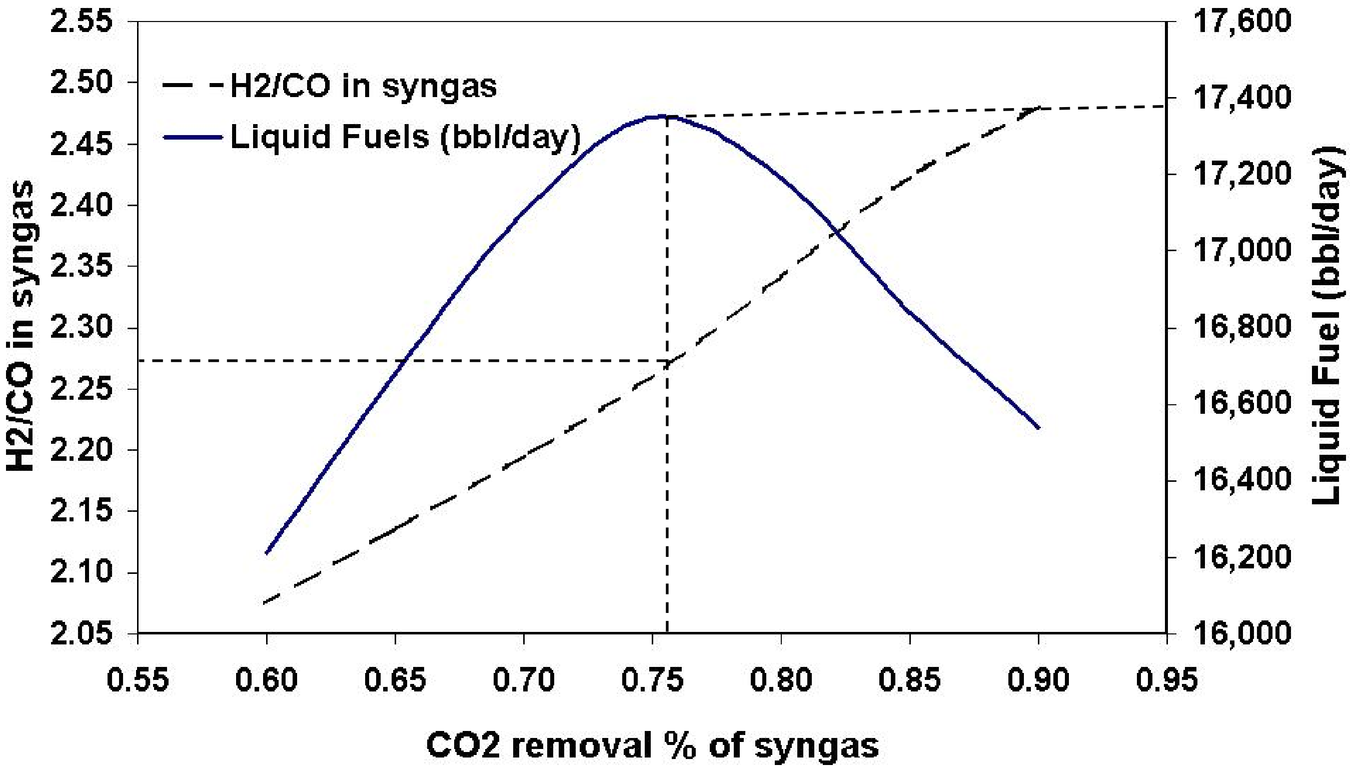
Process design



Effect of %CO_2 removal on (1) H_2/CO in syngas and (2) production of liquid fuels

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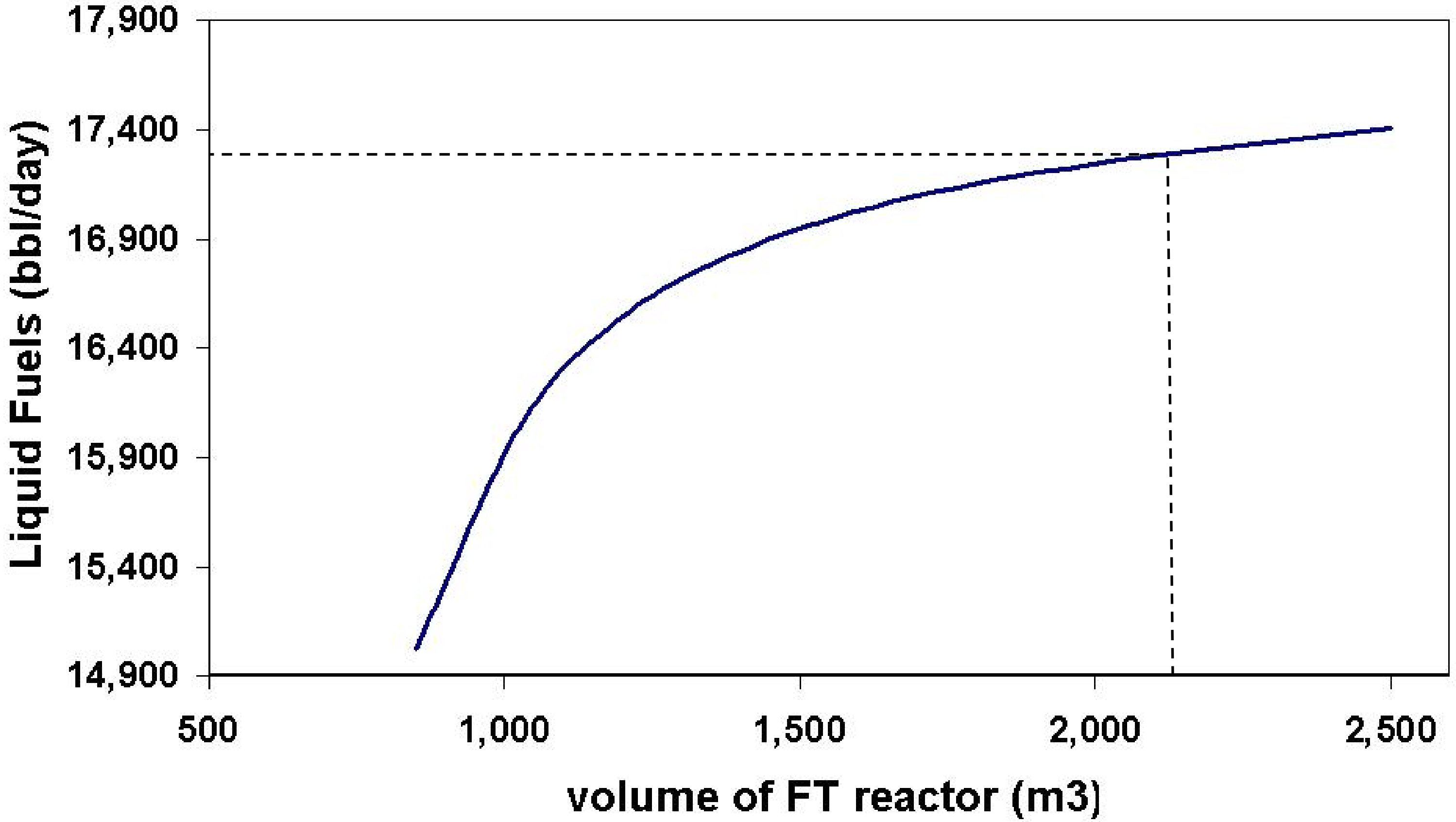
Process design



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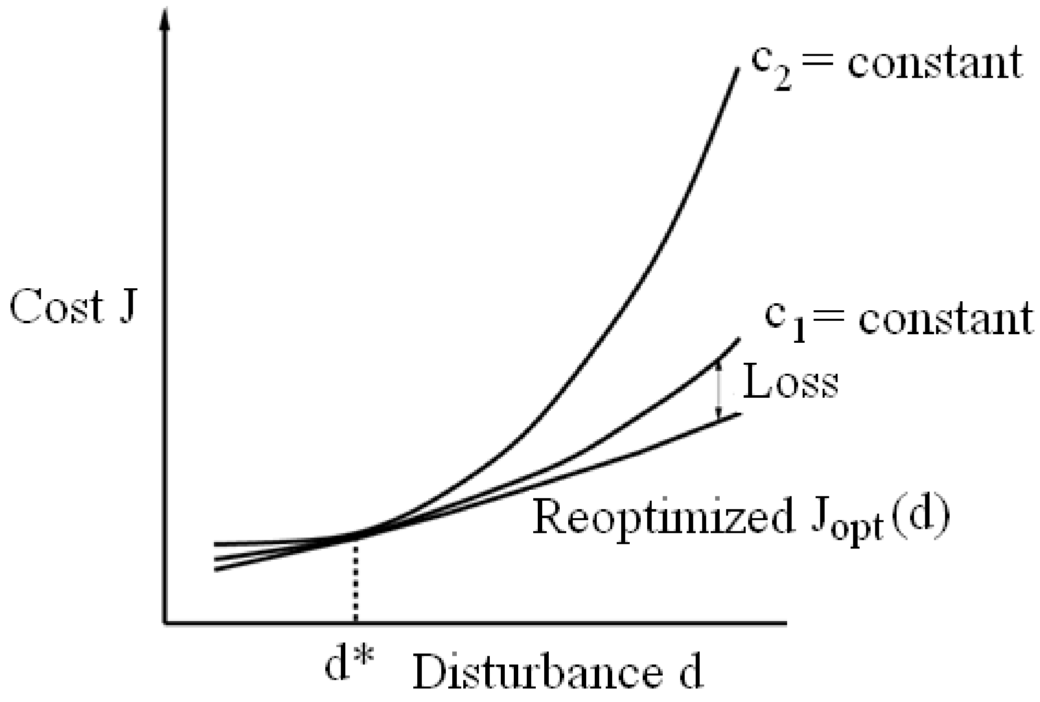
Skogestad's procedure for plantwide control

Self-optimizing control

Mode I: maximize efficiency (here natural gas is given)



Skogestad, S., I. Postlethwaite, 2005, Multivariable Feedback Control Analysis and Design, 2nd edition

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Self-optimizing control procedure

Step 1: Define an objective function and constraints

Step 2: Degrees of freedom (DOFs)

Step3: Disturbances

Step 4: Optimization (nominally and with disturbances)

Step 5: Identification of controlled variables (CVs) for unconstrained DOFs

Step 6: Evaluation of loss

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Step 1: Define an objective function and constraints

Objective function: max. Liquids fuel production

Operational constraints that should be satisfied:

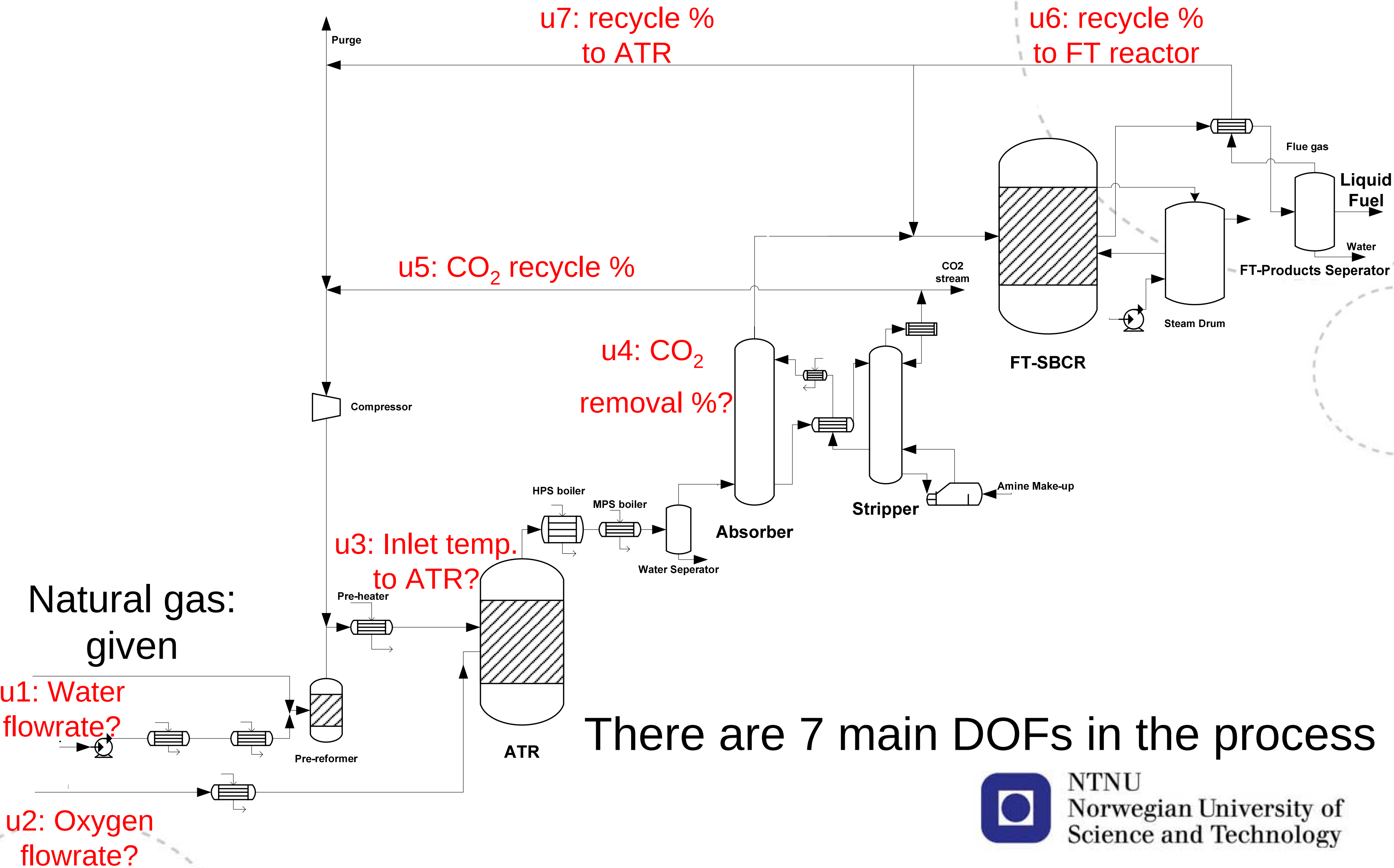
(a) The H_2O/NG ratio should be larger than 0.3 to avoid soot formation in ATR.

(b) The fired heater outlet temperature should not exceed 675ºC due to limitations on construction material.

Aasberg-Petersen, K., T. S. Christensen, C. Stud Nielsen and I. Dybkjær, 2003, Recent developments in authothermal reforming and pre-reforming for synthesis gas production in GTL applications, Fuel Processing Technology, 83, 253-261

Bakkerud, P. K., 2005, Update on synthesis gas production for GTL, Catalysis Today, 106, 30-33

Step2: Degrees of freedom (DOFs)



There are 7 main DOFs in the process

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Step3: Disturbances

1. Flowrate of natural gas (±10%)
2. Composition of hydrocarbons in feed (-10%)
3. Change in FT kinetics (±10% in kinetic parameter a)
4. Change in inlet temperature to ATR (±25°C)

Step3: Reoptimization for Disturbances

- Reoptimization of the process in presence of different disturbances
- Only one active constraint (inlet temperature to ATR)
- 6 CVs associated with the 6 unconstrained DOFs
- Keep some of CVs in their optimal nominal points
- Ideal case: no need to reoptimize any of DOFs in presence of disturbances

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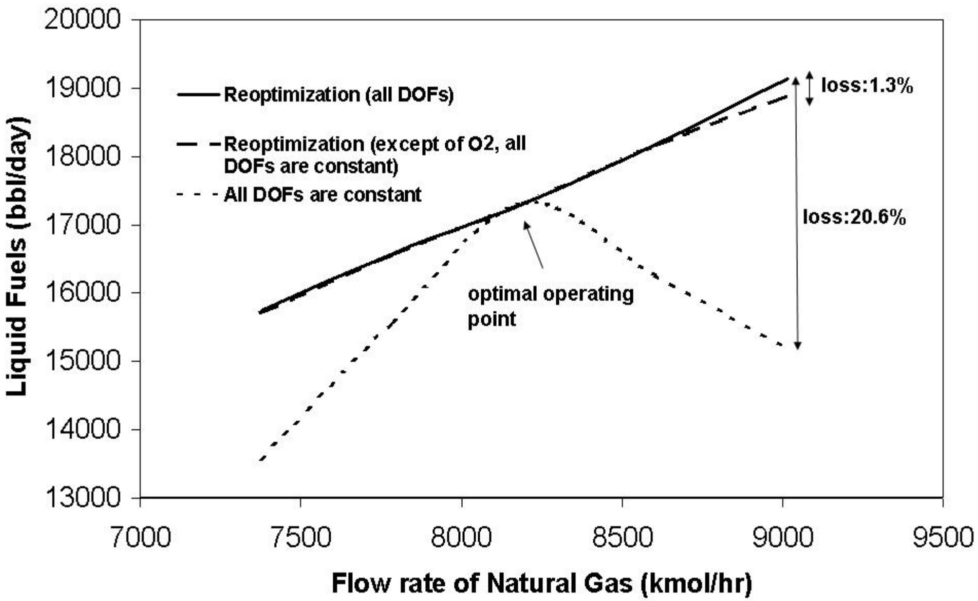
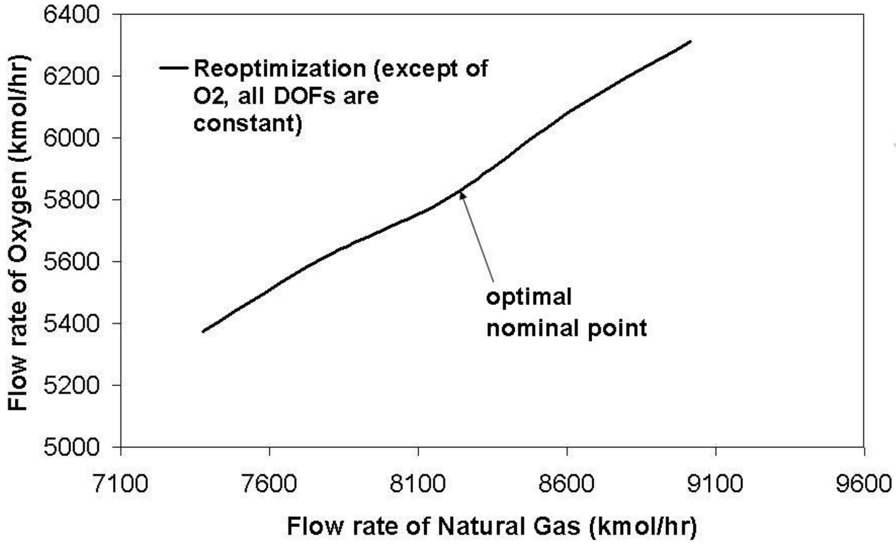
First disturbance: Change in flowrate of natural gas (±10%)





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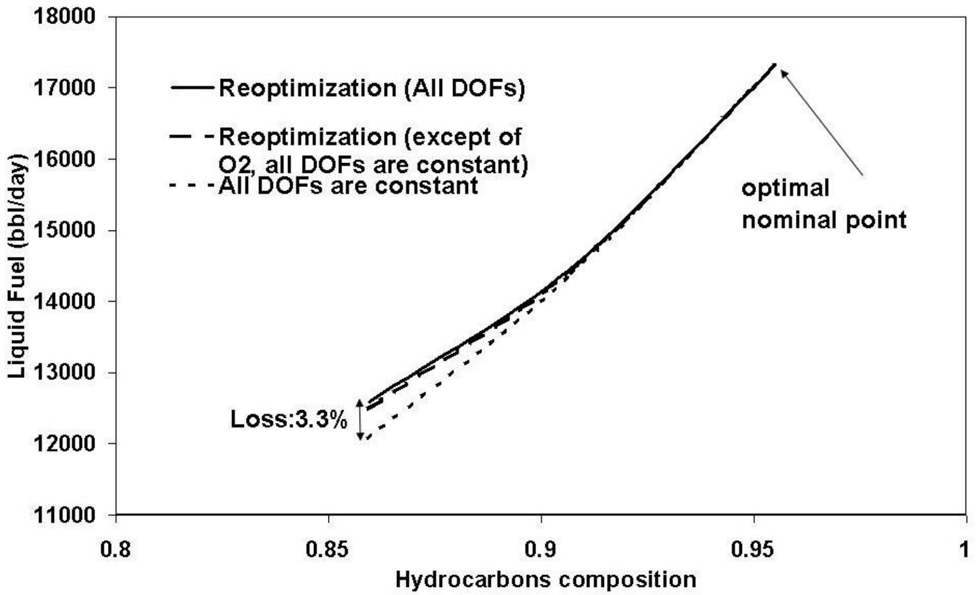
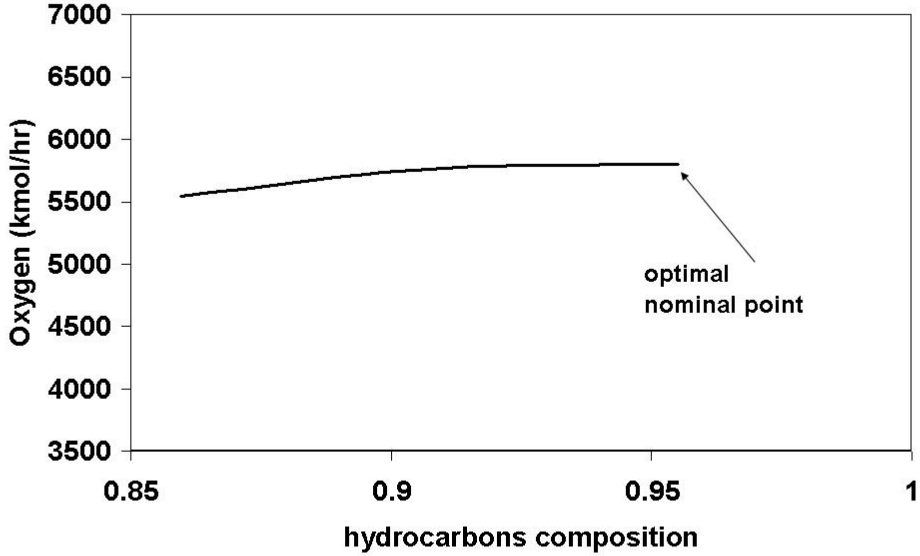
Second disturbance: Change in composition of natural gas (-10%)





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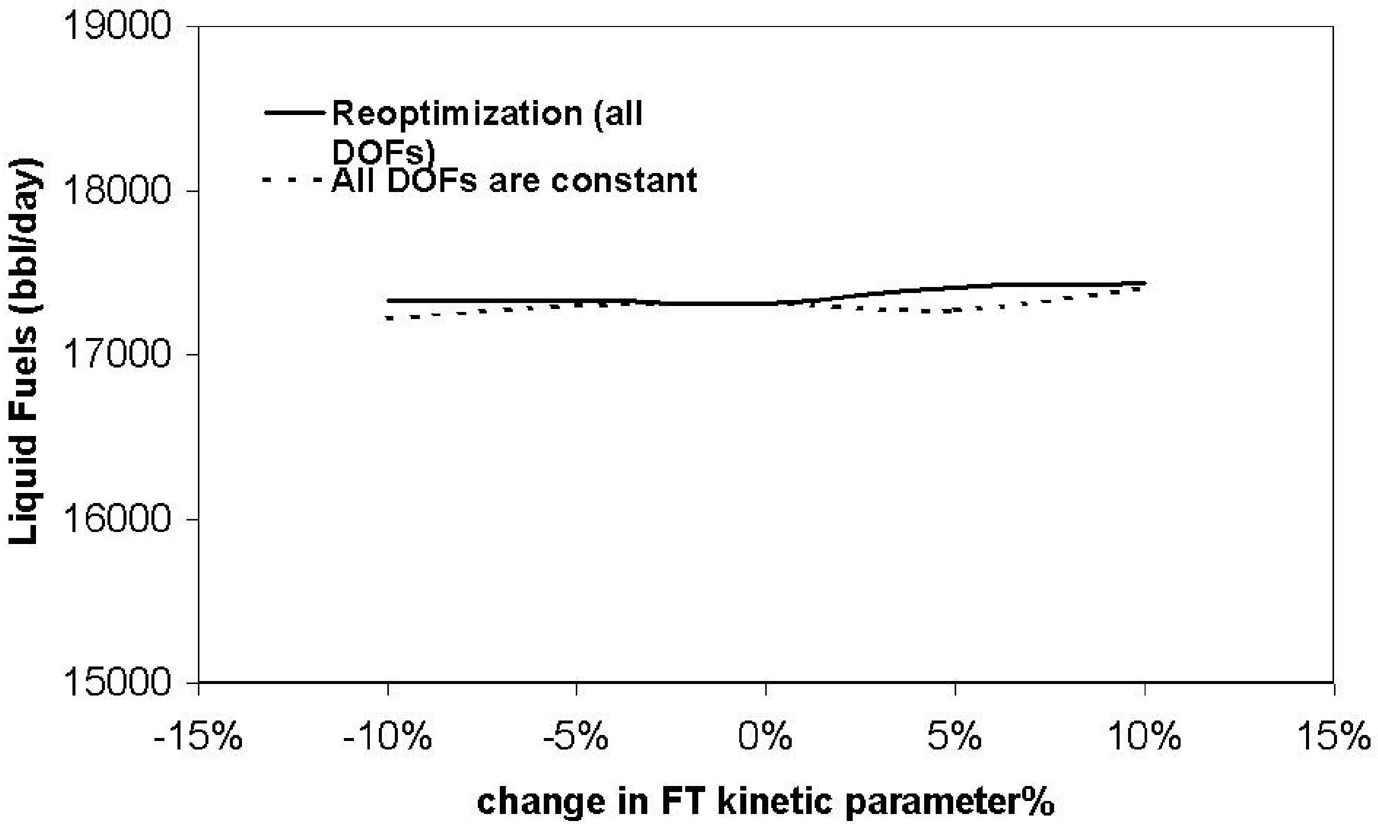
Third disturbance: Change in FT kinetics

(±10% in kinetic parameter a)



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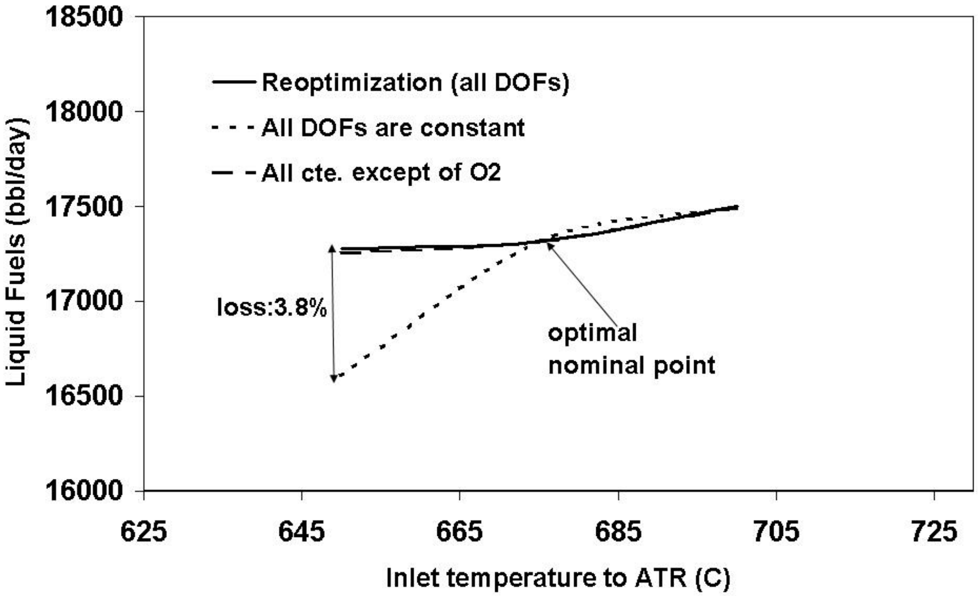
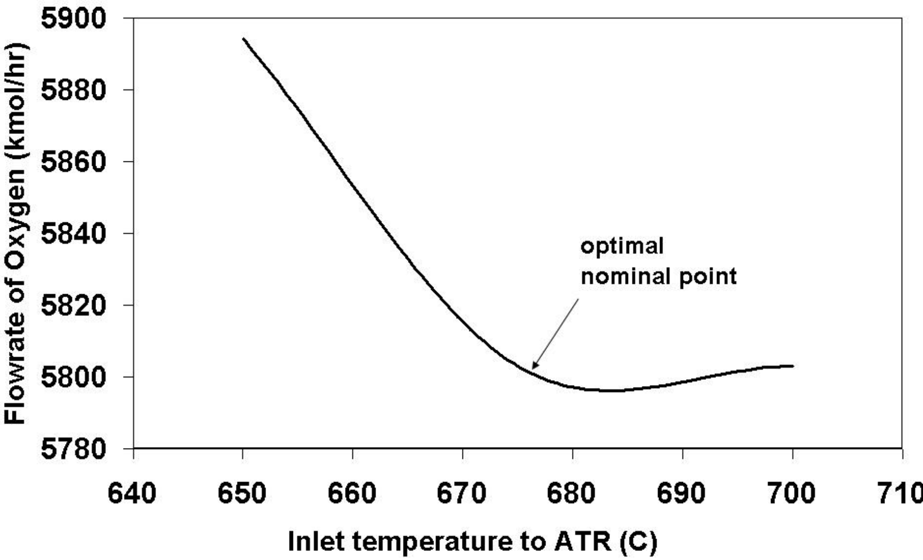
Fourth disturbance: Change in inlet temperature to ATR (±25°C)





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Summary of loss for various disturbances

no.	Disturbance	Worst case of each disturbance		Loss (%), if all DOFs are constant except of O_2 flowrate
		Change from nominal point	Loss (%)	
1	Flowrate of natural gas	+10%	20.6	1.3
2	Inlet temperature to ATR	-25 ºC	3.8	0.1
3	Hydrocarbons in the feed	-10%	3.3	0.8
4	Kinetic FT parameter a	+5%	0.8	-

It seems that we can always keep constant all the DOFs except of the O_2 flowrate.

We should also examine effect of implementation error in each controlled variables on objective function.

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Implementation error of CVs

Implementation error: inaccuracy in control device

Effect of CV implementation error on objective function (loss)

CVs	Implementation error %	Loss %
Recycled flue gas % to ATR	-15	**13.55**
H_2O flowrate	-10	**1.9**
Recycled flue gas % to FT	-15	0.51
CO_2 removal%	-5	0.21
Recycled CO_2% to ATR	-15	0.02

2 more unconstrained DOFs (flowrate of water and recycled flue gas % to ATR)

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Conclusion of self-optimizing so far

Keep 4 DOFs constant in their optimal nominal points

- u3: Inlet temperature to ATR
- u4: CO_2 removal %
- u5: CO_2 recycle %
- u6: Recycle % to FT reactor

3 unconstrained DOFs

- u1: H_2O flowrate
- u2: O_2 flowrate
- u3: Recycle % to ATR

Candidate CVs: ATR temperature, H_2/CO in syngas etc.

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Current work: Finding the best self-optimizing variables

Exact local method

$$L = \frac{1}{2}\left\| [M_d \ M_n] \begin{bmatrix} d \\ n \end{bmatrix} \right\|_2^2$$

$$\text{where } M_d = J_{uu}^{1/2}(J_{uu}^{-1}J_{ud} - G^{-1}G_d)W_d$$

$$M_n = J_{uu}^{1/2}G^{-1}HW_n$$

$$G = HG^y \quad G_d = HG_d^y$$

$$y = G^y u + G_d^y W_d d + W_n n$$

$$c = Hy$$

$$c = (HG^y u + HG_d^y W_d d + HW_n n)$$

$$c = Gu + G_d W_d d + HW_n n$$

Worst case loss $L_{worst} = \frac{1}{2}\bar{\sigma}([M_d \ M_n])^2$

Minimizing L_{worst} = Minimizing maximum singular value

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I.J. Halvorsen, S. Skogestad, J.C. Morud and V. Alstad,

``Optimal selection of controlled variables'', *Ind. Eng. Chem. Res.*, **42** (14), 3273-3284 (2003)

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Summary

✓ Conceptual design and simulation of a GTL process

✓ Optimal operation and self-optimizing control

✓ 7 DOFs (4 keep constants+3 unconstrained)

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Thank you for your attention

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