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:
- Synthesis Gas Production
- Fischer-Tropsch Reactor
- Upgrading Unit

Ideal Case: Thermodynamically possible but very far from being practical

\[ nCH_4 + \frac{n}{2}O_2 \rightarrow (-CH_2-)_n + nH_2O \]
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.
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Main reactions in GTL process

SynGas unit

Auto Thermal Reforming (ATR)

\[ CH_4 + \frac{3}{2}O_2 \rightleftharpoons CO + 2H_2O \quad \Delta H = -519.32 \frac{kJ}{mol} \quad \Delta G = -562.65 \frac{kJ}{mol} \]

\[ CH_4 + H_2O \rightleftharpoons CO + 3H_2 \quad \Delta H = +206.13 \frac{kJ}{mol} \quad \Delta G = +151.65 \frac{kJ}{mol} \]

\[ CO + H_2O \rightleftharpoons CO_2 + H_2 \quad \Delta H = -41.39 \frac{kJ}{mol} \quad \Delta G = -19.09 \frac{kJ}{mol} \]

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

\[ nCO + 2nH_2 \rightarrow (-CH_2-)_n + nH_2O \quad \Delta H = -165 \frac{kJ}{mol} \]

FT temperature is 220-230 °C

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
Resulting flowsheet of a GTL process
Process design

Effect of %CO$_2$ removal on (1) H$_2$/CO in syngas and (2) production of liquid fuels
Process design
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Skogestad’s procedure for plantwide control

Self-optimizing control

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

![Diagram of cost versus disturbance with marked optimal costs](image-url)

Self-optimizing control procedure

Step 1: Define an objective function and constraints
Step 2: Degrees of freedom (DOFs)
Step 3: Disturbances
Step 4: Optimization (nominally and with disturbances)
Step 5: Identification of controlled variables (CVs) for unconstrained DOFs
Step 6: Evaluation of loss
Step 1: Define an objective function and constraints

Objective function: max. Liquids fuel production

Operational constraints that should be satisfied:
(a) The H₂O/NG ratio should be larger than 0.3 to avoid soot formation in ATR.
(b) The fired heater outlet temperature should not exceed 675°C 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:

- $u_1$: Water flowrate?
- $u_2$: Oxygen flowrate?
- $u_3$: Inlet temp. to ATR?
- $u_4$: CO$_2$ removal %?
- $u_5$: CO$_2$ recycle %
- $u_6$: recycle % to FT reactor
- $u_7$: recycle % to ATR
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
First disturbance: Change in flowrate of natural gas (±10%)
Second disturbance: Change in composition of natural gas (-10%)
Third disturbance: Change in FT kinetics
(±10% in kinetic parameter a)
Fourth disturbance: Change in inlet temperature to ATR (±25°C)
Summary of loss for various disturbances

<table>
<thead>
<tr>
<th>no.</th>
<th>Disturbance</th>
<th>Worst case of each disturbance</th>
<th>Loss (%)</th>
<th>Loss (%), if all DOFs are constant except of O₂ flowrate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Flowrate of natural gas</td>
<td>+10%</td>
<td>20.6</td>
<td>1.3</td>
</tr>
<tr>
<td>2</td>
<td>Inlet temperature to ATR</td>
<td>-25 ºC</td>
<td>3.8</td>
<td>0.1</td>
</tr>
<tr>
<td>3</td>
<td>Hydrocarbons in the feed</td>
<td>-10%</td>
<td>3.3</td>
<td>0.8</td>
</tr>
<tr>
<td>4</td>
<td>Kinetic FT parameter a</td>
<td>+5%</td>
<td>0.8</td>
<td>-</td>
</tr>
</tbody>
</table>

It seems that we can always keep constant all the DOFs except of the O₂ flowrate.

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

Implementation error: inaccuracy in control device

Effect of CV implementation error on objective function (loss)

<table>
<thead>
<tr>
<th>CVs</th>
<th>Implementation error</th>
<th>Loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>Recycled flue gas % to ATR</td>
<td>-15%</td>
<td>13.55%</td>
</tr>
<tr>
<td>H$_2$O flowrate</td>
<td>-10%</td>
<td>1.9%</td>
</tr>
<tr>
<td>Recycled flue gas % to FT</td>
<td>-15%</td>
<td>0.51%</td>
</tr>
<tr>
<td>CO$_2$ removal%</td>
<td>-5%</td>
<td>0.21%</td>
</tr>
<tr>
<td>Recycled CO$_2$% to ATR</td>
<td>-15%</td>
<td>0.02%</td>
</tr>
</tbody>
</table>

2 more unconstrained DOFs (flowrate of water and recycled flue gas % to ATR)
Conclusion of self-optimizing so far

Keep 4 DOFs constant in their optimal nominal points
- u3: Inlet temperature to ATR
- u4: CO₂ removal %
- u5: CO₂ recycle %
- u6: Recycle % to FT reactor

3 unconstrained DOFs
- u1: H₂O flowrate
- u2: O₂ flowrate
- u3: Recycle % to ATR

Candidate CVs: ATR temperature, H₂/CO in syngas etc.
Current work: Finding the best self-optimizing variables

Exact local method

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

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

\( M_n = J_{uu}^{1/2} G^{-1} H W_n \)

\( G = H G^y \quad G_d = H G^y_d \)

Worst case loss

\[ L_{\text{worst}} = \frac{1}{2} \bar{\sigma} \left( \begin{bmatrix} M_d & M_n \end{bmatrix} \right)^2 \]

Minimizing \( L_{\text{worst}} \) = Minimizing maximum singular value

\[ y = G^y u + G^y_d W_d d + W_n n \]

\[ c = H y \]

\[ c = (H G^y u + H G^y_d W_d d + H W_n n) \]

\[ c = G u + G_d W_d d + H W_n n \]

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

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✓ Conceptual design and simulation of a GTL process

✓ Optimal operation and self-optimizing control

✓ 7 DOFs (4 keep constants+3 unconstrained)
Thank you for your attention