HDA case study

• S. Skogestad, May 2006
• Thanks to Antonio Araújo
Process Description

• Benzene production from thermal-dealkalination of toluene (high-temperature, non-catalytic process).

• Main reaction:

\[
\text{CH}_3\begin{array}{c}
\text{Toluene} \\
+ \text{H}_2 \rightarrow \text{Benzene} \\
+ \text{CH}_4 + \text{Heat}
\end{array}
\]

• Side reaction

\[
2\begin{array}{c}
\text{Diphenyl} \\
\leftrightarrow \end{array} \rightarrow \begin{array}{c}
\text{Diphenyl} \\
+ \text{H}_2
\end{array}
\]

• Excess of hydrogen is needed to repress the side reaction and coke formation.

• References for HDA process:
  • McKetta (1977) – first reference on the process;
  • Douglas (1988) – design of the process;
  • Wolff (1994) – discuss the operability of the process.

• No references on the optimization of the process for control structure design purposes.
Process Description

- **Mixer**
- **FEHE**
- **Furnace**
- **PFR**
- **Quench**
- **Separator**
- **Compressor**

Reactants and Products:
- $\text{H}_2 + \text{CH}_4$
- Toluene
- Benzene
- CH$_4$

Flow Diagram:
- $\text{H}_2 + \text{CH}_4$ enters the system and reacts with Toluene.
- The reaction products flow through the FEHE, Furnace, and PFR.
- The cooled products enter the Separator.
- Purge ($\text{H}_2 + \text{CH}_4$) is added to the system.

Products:
- Toluene
- Benzene
- CH$_4$
- Diphenyl
Steady-state operational degrees of freedom

<table>
<thead>
<tr>
<th>Process units</th>
<th>DOF</th>
</tr>
</thead>
<tbody>
<tr>
<td>External feed streams (feed rate)</td>
<td>2</td>
</tr>
<tr>
<td>Heat exchangers duties (including 1 furnace)</td>
<td>3</td>
</tr>
<tr>
<td>Splitters</td>
<td>2</td>
</tr>
<tr>
<td>Compressor duty</td>
<td>1</td>
</tr>
<tr>
<td>Adiabatic flash(*)</td>
<td>0</td>
</tr>
<tr>
<td>Gas phase reactor(*)</td>
<td>0</td>
</tr>
<tr>
<td>Distillation columns</td>
<td>6</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>14</td>
</tr>
</tbody>
</table>

**Equality constraint**

- Quencher outlet temperature: -1

**Remaining degrees of freedom at steady state**: 13

(*) No adjustable valves (assumed fully open valve before flash)
Steady-state operational degrees of freedom
Cost Function and Constraints

• The following profit is maximized (Douglas’s EP):

\[-J = \text{p}_{\text{ben}} D_{\text{ben}} - \text{p}_{\text{tol}} F_{\text{tol}} - \text{p}_{\text{gas}} F_{\text{gas}} - \text{p}_{\text{fuel}} Q_{\text{fuel}} - \text{p}_{\text{cw}} Q_{\text{cw}} - \text{p}_{\text{power}} W_{\text{power}} - \text{p}_{\text{steam}} Q_{\text{steam}} + \sum (p_{v,i} F_{v,i})\]

• Constraints during operation:
  – Production rate: \(D_{\text{ben}} \geq 265 \text{ lbmol/h.}\)
  – Hydrogen excess in reactor inlet: \(F_{\text{Hyd}} / (F_{\text{ben}} + F_{\text{tol}} + F_{\text{diph}}) \geq 5.\)
  – Bound on toluene feed rate: \(F_{\text{tol}} \leq 300 \text{ lbmol/h.}\)
  – Reactor pressure: \(P_{\text{reactor}} \leq 500 \text{ psia.}\)
  – Reactor outlet temperature: \(T_{\text{reactor}} \leq 1300 \degree \text{F.}\)
  – Quencher outlet temperature: \(T_{\text{quencher}} = 1150 \degree \text{F.}\)
  – Product purity: \(x_{\text{Dben}} \geq 0.9997.\)
  – Separator inlet temperature: \(95 \degree \text{F} \leq T_{\text{flash}} \leq 105 \degree \text{F.}\)

  – + Distillation constraints

• Manipulated variables are bounded.
## Disturbances

<table>
<thead>
<tr>
<th>Disturbance</th>
<th>Unit</th>
<th>Nominal</th>
<th>Lower</th>
<th>Upper</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene feed flow rate</td>
<td>lbmol/h</td>
<td>300</td>
<td>285</td>
<td>315</td>
</tr>
<tr>
<td>Gas feed composition</td>
<td>mol% of H₂</td>
<td>95</td>
<td>90</td>
<td>100</td>
</tr>
<tr>
<td>Benzene price</td>
<td>$/lbmol</td>
<td>9.04</td>
<td>8.34</td>
<td>9.74</td>
</tr>
<tr>
<td>Energetic value of fuel to the furnace</td>
<td>MBTU/lbmol</td>
<td>0.1247</td>
<td>0.12</td>
<td>0.13</td>
</tr>
</tbody>
</table>
Optimization

Profit (M$/year)

Disturbance

Nominal

Gas feed composition (lower)

Gas feed composition (upper)

Benzene price (lower)

Benzene price (upper)

Toluene feed rate (lower)

Toluene feed rate (upper)

Energetic value of fuel (lower)

Energetic value of fuel (upper)

Benzene price
Optimization

- **14 steady-state degrees of freedom**

- **10 active constraints:**
  1. Pure toluene feed rate (UB)
  2. By-pass valve around FEHE (LB)
  3. Reactor inlet hydrogen-aromatics ratio (LB)
  4. Flash inlet temperature (LB)
  5. Methane mole fraction in stabilizer bottom (UB)
  6. Benzene mole fraction in stabilizer distillate (UB)
  7. Toluene mole fraction in benzene column bottom (LB)
  8. Benzene mole fraction in benzene column distillate (LB)
  9. Diphenyl mole fraction in toluene column bottom (LB)
  10. Toluene mole fraction in toluene column distillate (LB)

- **1 equality constraint:**
  11. Quencher outlet temperature

- **3 remaining unconstrained degrees of freedom.**
Optimization – Active Constraints

- **Mixer**
- **Compressor**
- **Furnace**
- **FEHE**
- **Cooler**
- **Reactor**
- **Separator**

**Purge (H₂ + CH₄)**

**Equality**

1. Toluene
2. H₂ + CH₄
3. Benzene
4. CH₄
5. Diphenyl
6. Toluene
7. Benzene
8. Benzene
9. Toluene Column
10. Toluene Column
11. Quencher
Candidate Controlled Variables

- Candidate controlled variables:
  - Pressure differences;
  - Temperatures;
  - Compositions;
  - Heat duties;
  - Flow rates;
  - Combinations thereof.

- 138 candidate controlled variables might be selected.
- 14 degrees of freedom.
- Number of different sets of controlled variables:
  \[
  \frac{138!}{14!14!} \approx 5.3 \times 10^{18}
  \]

- 10 active constraints + 1 equality constraint leaving 3 DOF:
  \[
  \frac{127!}{3!124!3!} = 333,375
  \]

- What should we do with the remaining 3 DOF?
  - **Self-optimizing control!!!**
## Analysis of the linear model

a. All measurements ($\sigma(G_{\text{full}}) = 1.58$):

| Branch-and-bound: $\sigma(G_{3x3}) = 0.864$ |
|-----------------------------------|------------------|
| I  | Quencher outlet benzene mole fraction |
| II | Compressor power                     |
| III| Liquid (cooling) flow to quencher    |

| Branch-and-bound: $\sigma(G_{3x3}) = 0.853$ |
|-----------------------------------|------------------|
| I  | Separator liquid outlet benzene mole fraction |
| II | Compressor power                     |
| III| Liquid (cooling) flow to quencher    |

| Branch-and-bound: $\sigma(G_{3x3}) = 0.852$ |
|-----------------------------------|------------------|
| I  | Benzene mole fraction in stabilizer bottom |
| II | Compressor power                     |
| III| Liquid (cooling) flow to quencher    |
Optimal self-optimizing variables

1. Toluene
2. FEHE
3. Furnace
4. Compressor
5. Stabilizer
6. Diphenyl
7. Benzene Column
8. Toluene Column
9. Toluene
10. Toluene
11. Purge ($H_2 + CH_4$)

Flow

$X_{benzene}$
Analysis of the linear model

b. Separator pressure constant ($\sigma(G_{full}) = 1.50$):

| Branch-and-bound: $\sigma(G_{3x3}) = 0.835$
<table>
<thead>
<tr>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
</tr>
<tr>
<td>II</td>
</tr>
<tr>
<td>III</td>
</tr>
</tbody>
</table>
Alternative self-optimizing variables

Self-Optimizing Control

Mixer
FEHE
Furnace
Compressor
Reactor
Cooler
Separator
Quencher
Purge (H₂ + CH₄)

\[ \text{Toluene} \]
\[ \text{Benzene} \]
\[ \text{CH₄} \]

\[ \text{Diphenyl} \]

\[ \text{P} \]
Conclusion steady-state analysis

• Many similar alternatives in terms of loss

• Need to consider dynamics (Input-output controllability analysis):
  – RHP-zeros
  – RHP-poles
  – Input saturation
  – Easy of implementation (decentralized control of final 3x3 supervisory control problem)!

• Now: Consider “bottom-up” design of control system
Bottom-up design of control system

• Start with stabilizing control
  – Levels
  – Pressure
  – Temperatures

• Normally start with fastest loops (often pressure)
  – but let is start with levels
“Bottom-up”: Proposed Control Structure
Stabilizing Control: Control 7 liquid levels

LV-configuration assumed for columns
Avoiding “Drift” I – 4 Pressure loops

Pressure with purge

Purge (H₂ + CH₄)

Column pressures are given
Avoiding “Drift” II – 4 Temperature loops
Now suggest pairings for supervisory control
Control of 11 active constraints.
Control of 3 self-optimizing variables: Optimal set

Difficult supervisory control problem:
Control of 3 self-optimizing variables: Near-Optimal set: SIMPLE

H₂ + CH₄

Toluene

Mixer

FEHE

Furnace

Reactor

Cooler

Separator

Compressor

Purge (H₂ + CH₄)

X_{benzene}

T_{p}

Ts

I

xbenzene

III'

II

FC

SP

SP

TC

TC

CC

CC

CC

SP

ps

PC

SP

SP

SP

SP

ps

ps

ps

ps

ps
Conclusion HDA

• Follow systematic procedure
• May want to keep several candidate sets of “almost” self-optimizing variables
• Final evaluation: Non-linear steady-state simulations + Dynamic simulations