ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Laboratoire d'Automatique

On the Use of Extents for Process Monitoring and Fault Diagnosis

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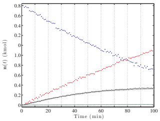
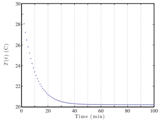
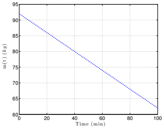
Outline

Problem Statement

- Measurements of numbers of moles $\mathbf{n}(t)$, mass $m(t)$ and reactor temperature $T(t)$ are available







- Assumption: Stoichiometry, inlet composition and initial conditions are known but no information is available on the reaction kinetics
- Can we detect faults using only data from the current batch?
- The answer is Yes, using the extent-based approach...

Material Balance Equations

- For a reaction system with S species, R reactions, p inlets and one outlet,

Mole balances for S species

$$\dot{\mathbf{n}}(t) = \mathbf{N}^{\mathrm{T}} \, V(t) \, \mathbf{r}(t) + \mathbf{W}_{in} \, \mathbf{u}_{in}(t) - \frac{u_{out}(t)}{m(t)}\mathbf{n}(t), \quad \mathbf{n}(0) = \mathbf{n}_0$$

(S) $(S \times R)$ (R) $(S \times p)$ (p)

where,

$$\dot{m}(t) = \mathbf{1}_p^{\mathrm{T}} \mathbf{u}_{in}(t) - u_{out}(t), \qquad m(0) = m_0,$$

$$\omega(t) = -\frac{u_{out}(t)}{m(t)}$$

Energy Balance Equations

- The energy balance equation can be written as:

Heat balance

$$\dot{Q}(t) = (-\Delta\,\mathbf{H})^{\mathrm{T}}\,\mathbf{r}_v(t) + q_{ex}(t) + \check{\mathbf{T}}_{in}^{\mathrm{T}}\,\mathbf{u}_{in}(t) - \omega(t)\;Q(t) \qquad Q(0) = Q_0$$

where $Q(t) = m(t)c_p T(t)$ is the heat power

$\check{\mathbf{T}}_{in}^{\mathrm{T}}$ contains the specific heats of the inlet streams

Balance Equations

- Combining both equations

Combined material and energy balance

$$\dot{\mathbf{z}}(t) = \mathcal{A}\,\mathbf{r}_v(t) + \mathbf{b}\; q_{ex}(t) + \mathcal{C}\,\mathbf{u}_{in}(t) - \omega(t)\,\mathbf{z}(t)$$

$$\mathbf{z} = \begin{bmatrix} \mathbf{n} \\ Q \end{bmatrix} \text{and} \;\; \mathbf{z}_0 = \begin{bmatrix} \mathbf{n}_0 \\ Q_0 \end{bmatrix}.$$

$$\mathcal{A} = \begin{bmatrix} \mathbf{N}^{\mathrm{T}} \\ (-\Delta\,\mathbf{H})^{\mathrm{T}} \end{bmatrix},\; \mathbf{b} = \begin{bmatrix} \mathbf{0}_S \\ 1 \end{bmatrix},\; \mathcal{C} = \begin{bmatrix} \mathbf{W}_{in} \\ \check{\mathbf{T}}_{in}^{\mathrm{T}} \end{bmatrix}$$

Linear Transformation

- The linear transformation $\mathcal{T} = \left[\mathcal{A} \;\; \mathbf{b} \;\; \mathcal{C} \;\; \mathbf{z}_0 \;\; \mathbf{P}\right]^{-1}$ gives,

$$\begin{bmatrix} \mathbf{x}_r(t) \\ x_{ex}(t) \\ \mathbf{x}_{in}(t) \\ x_{ic}(t) \\ \mathbf{x}_{iv}(t) \end{bmatrix} = \mathcal{T}\,\mathbf{z}(t)$$

- The matrix $\mathbf{P}$ describes the q-dimensional null space of the matrix $\left[\mathcal{A} \;\; \mathbf{b} \;\; \mathcal{C} \;\; \mathbf{z}_0\right]$, with $q = S - R - p - 1\,.$

Linear Transformation

- The transformed system reads

$$\begin{aligned} \dot{\mathbf{x}}_r(t) &= \mathbf{r}_v(t) - \omega(t)\,\mathbf{x}_r(t) & \mathbf{x}_r(0) &= \mathbf{0}_R \\ \dot{x}_{ex}(t) &= q_{ex}(t) - \omega(t)\,x_{ex}(t) & x_{ex}(0) &= 0 \\ \dot{\mathbf{x}}_{in}(t) &= \mathbf{u}_{in}(t) - \omega(t)\,\mathbf{x}_{in}(t) & \mathbf{x}_{in}(0) &= \mathbf{0}_p \\ \dot{x}_{ic}(t) &= -\omega(t)\,x_{ic}(t) & x_{ic}(0) &= 1 \\ \mathbf{x}_{iv}(t) &= \mathbf{0}_q\ , \end{aligned}$$

- The numbers of moles $\mathbf{n}(t)$ and the heat $Q(t)$ can be reconstructed from the transformed variables:

$$\begin{bmatrix} \mathbf{n}(t) \\ Q(t) \end{bmatrix} = \begin{bmatrix} \mathbf{N}^{\mathrm{T}} \\ (-\Delta\,\mathbf{H})^{\mathrm{T}} \end{bmatrix} \mathbf{x}_r(t) + \begin{bmatrix} \mathbf{0}_S \\ 1 \end{bmatrix} x_{ex}(t) + \begin{bmatrix} \mathbf{W}_{in} \\ \check{\mathbf{T}}_{in}^{\mathrm{T}} \end{bmatrix} \mathbf{x}_{in}(t) + \begin{bmatrix} \mathbf{n}_0 \\ Q_0 \end{bmatrix} x_{ic}(t).$$

Fault Detection

- Objective Use extents to identify faults in:

  1. Outlet flowrates $u_{out}(t)$
  2. Inlet flowrates $\mathbf{u}_{in}(t)$
  3. Heat exchange $q_{ex}(t)$

- *Note:* In order to identify faults in reactions, we need either historical data or a kinetic model

Fault Detection - Fault in Flowrates

- Compute the reference mass $m_{ref}(t)$

$$\dot{m}_{ref}(t) = \mathbf{1}_p^T \mathbf{u}_{in,ref}(t) - u_{out,ref}(t) \qquad m_{ref}(0) = m_{ref,0}$$

- Compare $m_{ref}(t)$ with the measured mass $m(t)$ using either z-test or t-test
- If an error is detected, fault either in $\mathbf{u}_{in}(t)$ and/or $u_{out}(t)$

Fault Detection - Fault in Flowrates

- Compute the extents by applying the linear transformation
- Compute $x_{ic,ref}(t)$

$$x_{ic,ref}(t) = -\frac{u_{out,ref}(t)}{m_{ref}(t)} x_{ic,ref}(t)$$

- Compare $x_{ic,ref}(t)$ with $x_{ic}(t)$ - Error in outlet flowrate?
- Compute $\mathbf{x}_{in,ref}(t)$

$$\mathbf{x}_{in,ref}(t) = \mathbf{u}_{in,ref}(t) - \frac{u_{out,ref}(t)}{m_{ref}(t)} \mathbf{x}_{in,ref}(t)$$

- Compare $\mathbf{x}_{in,ref}(t)$ with $\mathbf{x}_{in}(t)$ - Error in inlet flowrates?

Fault Detection - Fault in Heat transfer

- Compute $x_{ex,ref}(t)$

$$x_{ex,ref}(t) = q_{ex,ref}(t) - \frac{u_{out,ref}(t)}{m_{ref}(t)} x_{ex,ref}(t)$$

- Compare $x_{ex,ref}(t)$ with $x_{ex}(t)$ - Error in heat transfer?

Simulated Example

- Consider the hydrodealkylation reaction system

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$$
$$2\,C_6H_6 \rightarrow C_{12}H_{10} + H_2$$

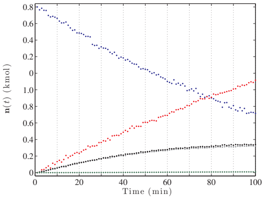
- Both reactions are exothermic
- Simplification: Hydrogen is considered as a dissolved species fed directly into the liquid phase

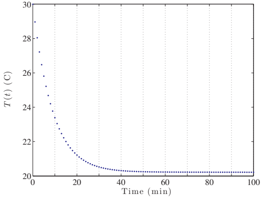
Fault Detection - Simulated Example

Extents for Process Monitoring

Motivation
Problem Statement
System Description
Material Balance Equations
Energy Balance Equations
Transformation to Vessel Extents
Fault Detection
Conclusion

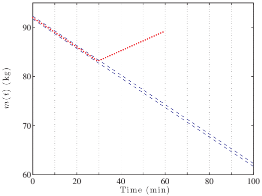
- For the hydrodealkylation example, under normal operating conditions (NOC), $\mathbf{n}$ and T vary with time
- The measurements are corrupted with 1% zero-mean gaussian white noise

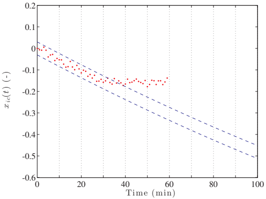




Fault Detection - Fault in u_{out}

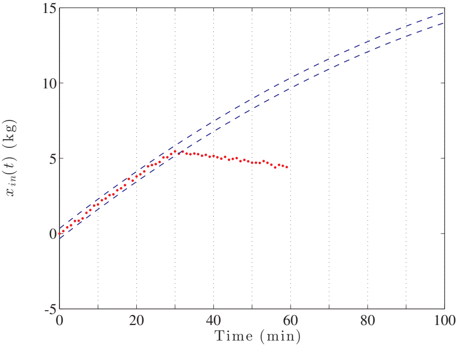
- NOC: $u_{out}(t) = 0.5\,kg\,min^{-1}$ AOC: $u_{out}(t) = 0\,kg\,min^{-1}$
- Fault introduced at time $t = 30$ min.





Fault Detection - Fault in $\mathbf{u}_{in}$

- NOC: $\mathbf{u}_{in}(t) = 0.2\, kg\ min^{-1}$ AOC: $\mathbf{u}_{in}(t) = 0\, kg\ min^{-1}$
- Fault introduced at time $t = 30$ min.



Fault Detection - Fault in $q_{ex}(t)$

Extents for Process Monitoring

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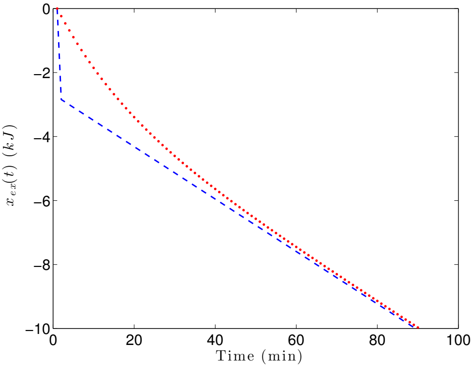
- The wrong heat transfer coefficient (UA) was used
- NOC: $UA = 500\ W\ K^{-1}$ AOC: $UA = 5\ W\ K^{-1}$



Conclusion

- The transformation to extents gives variables that depend on a single rate process → easier to detect a fault associated with that rate
- This allows isolation of faults *without knowledge of kinetics*
- The method requires a proper statistical framework - Generalized Likelihood Ratio (GLR) tests
- GLR also helps detect sensor faults
- Thank you for your attention!

References

- M. Amrhein, N. Bhatt , B.Srinivasan and D. Bonvin, Extents of Reaction and Flow for Homogeneous Reaction Systems with Inlet and Outlet Streams, AIChE Journal, 56(11), 2873 - 2866 (2010)
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- S. Narasmihan and R. S. H. Mah, Generalized likelihood ratios for gross error identification in dynamic processes, AIChE Journal, 34(8), 1321 - 1331 (1988)