

# ON THE USE OF EXTENTS FOR PROCESS MONITORING AND FAULT DIAGNOSIS

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## CONTEXT

Process monitoring and fault diagnosis are used to control quality and enforce safety compliance in industrial processes. Processes are monitored by comparing abstract or physical variables to set points representing Normal Operating Conditions (NOC) and faults (AOC) are detected based on deviations from statistical thresholds.

Mole and energy balance equations of open reactors exhibit an inherent structure in which the dynamics of the  $R$  reactions ( $\mathbf{r}_v$ ),  $p$  inlet flows ( $\mathbf{u}_m$ ), of the heat exchange ( $q_{ex}$ ) and outlet flow ( $\omega = u_{out}/m$ ) are weighted by static information, i.e. the reaction stoichiometry and enthalpy ( $\mathbf{N}$ ,  $\Delta\mathbf{H}_r$ ), and the composition and heat of inlet flows ( $\mathbf{W}_{in}$ ,  $\mathbf{T}_{in}$ ). Moreover, the initial conditions ( $\mathbf{n}_0$ ,  $Q_0$ ) are usually known.

$$\begin{bmatrix} \dot{\mathbf{n}}(t) \\ \dot{Q}(t) \end{bmatrix} = \begin{bmatrix} \mathbf{N}^T \\ -\Delta\mathbf{H}_r^T \end{bmatrix} \mathbf{r}_v \left( \frac{\mathbf{n}(t)}{V(t)}, \mathbf{k} \right) + \begin{bmatrix} \mathbf{W}_{in} \\ \mathbf{T}_{in}^T \end{bmatrix} \mathbf{u}_m(t) + \begin{bmatrix} \mathbf{0}_S \\ 1 \end{bmatrix} q_{ex}(T(t), UA) - \begin{bmatrix} \mathbf{n}(t) \\ Q(t) \end{bmatrix} \omega(t),$$

$$\dot{m}(t) = \mathbf{1}_p^T \mathbf{u}_m(t) - u_{out}(t), \quad m(0) = m_0 \quad \text{with } Q(t) = m(t)c_p T(t) \text{ and } \begin{bmatrix} \mathbf{n}(0) \\ Q(0) \end{bmatrix} = \begin{bmatrix} \mathbf{n}_0 \\ m_0 c_p T_0 \end{bmatrix}$$

Static process information of the mole balance equation ( $\mathbf{N}$ ,  $\mathbf{W}_{in}$  and  $\mathbf{n}_0$ ) can be tested by Target Factor Analysis (TFA) [1].

$$\mathbf{n}(t) \approx \bar{\mathbf{U}}\bar{\mathbf{S}}\bar{\mathbf{V}}^T, \quad \min_{\mathbf{t}^T = \mathbf{N}_{ic}, \mathbf{W}_{ic,j}, \mathbf{n}_0^T} \mathbf{t}^T (\mathbf{I}_S - \bar{\mathbf{V}}\bar{\mathbf{V}}^T), \quad i = 1, \dots, R, \quad j = 1, \dots, p \quad \text{and for } \mathbf{n}_0$$

Exploiting the structure of differential balance equations, a transformation is used to separate data - numbers of moles [2], heat power [2-3] or absorbance spectra [4] - to extents, using typically known process information ( $\mathbf{N}$ ,  $\Delta\mathbf{H}_r$ ,  $\mathbf{W}_{in}$ ,  $\mathbf{T}_{in}$ ,  $\mathbf{n}_0$  and  $Q_0$ ).

$$\begin{bmatrix} \mathbf{n}(t) \\ Q(t) \end{bmatrix} \rightarrow \mathbf{x}(t) = \begin{bmatrix} \mathbf{x}_r(t) \\ \mathbf{x}_m(t) \\ x_{ex}(t) \\ x_{ic}(t) \end{bmatrix} := \underbrace{\begin{bmatrix} \mathbf{N}^T & \mathbf{W}_{in} & \mathbf{0}_S & \mathbf{n}_0 \\ -\Delta\mathbf{H}_r^T & \mathbf{T}_{in}^T & 1 & Q_0 \end{bmatrix}^+}_{\text{rank}([\cdot])=R+p+2} \begin{bmatrix} \mathbf{n}(t) - \mathbf{n}_0 \\ Q(t) - Q_0 \end{bmatrix}$$

The resulting extents capture the effects of each individual reaction (in  $\mathbf{x}_r$ ), inlet flow (in  $\mathbf{x}_m$ ), exchange heat (in  $x_{ex}$ ) and outlet flow (in  $x_{ic}$ ).

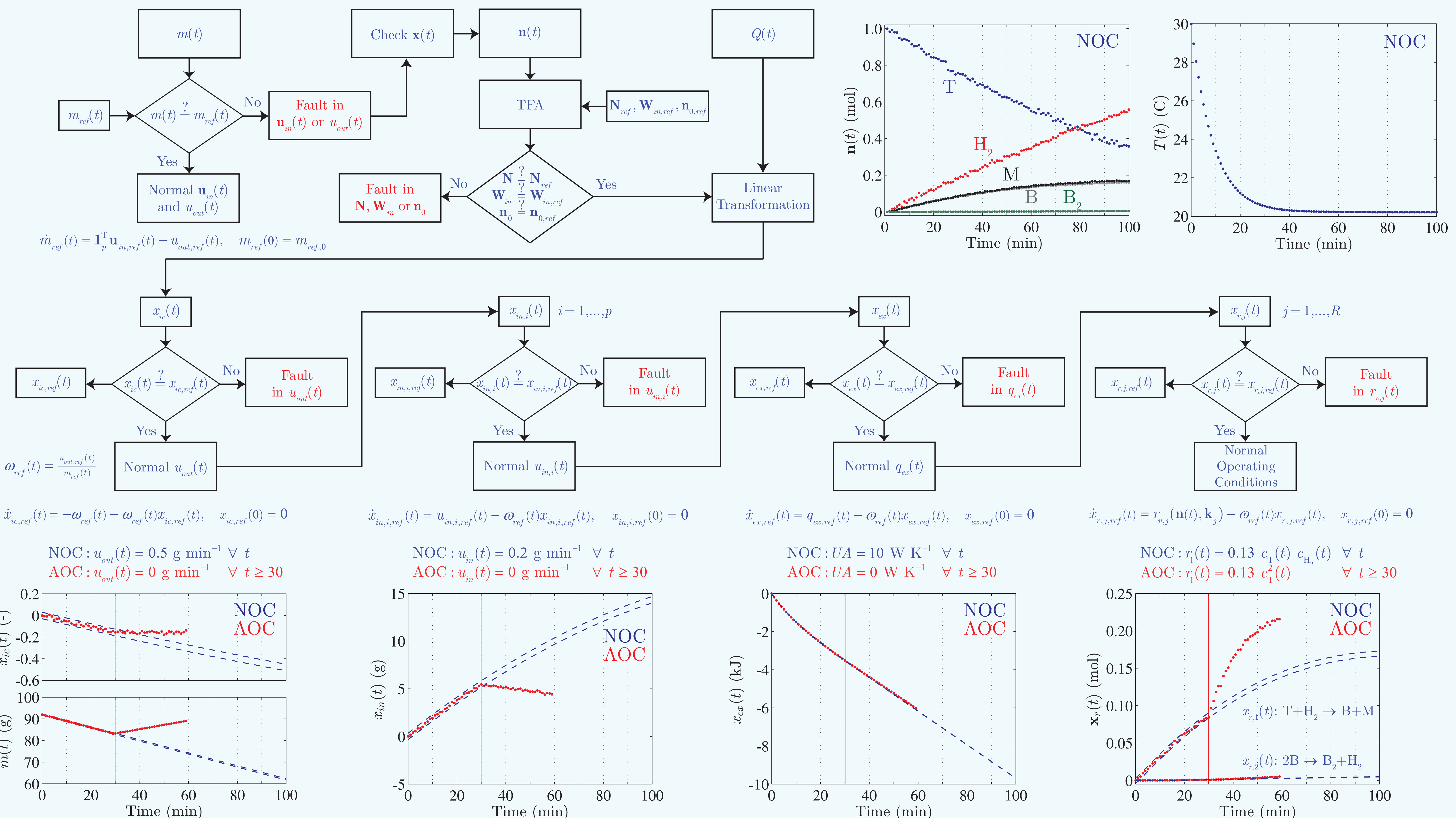
$$\mathbf{x}(t) = \begin{bmatrix} \dot{\mathbf{x}}_r(t) \\ \dot{\mathbf{x}}_m(t) \\ \dot{x}_{ex}(t) \\ \dot{x}_{ic}(t) \end{bmatrix} := \begin{bmatrix} \mathbf{r}_v \left( \frac{\mathbf{n}(t)}{V(t)}, \mathbf{k} \right) \\ \mathbf{u}_m(t) \\ q_{ex}(T(t), UA) \\ -\omega(t) \end{bmatrix} - \omega(t) \begin{bmatrix} \mathbf{x}_{r,f}(t) \\ \mathbf{x}_m(t) \\ x_{ex}(t) \\ x_{ic}(t) \end{bmatrix}, \quad \begin{bmatrix} \mathbf{x}_r(0) \\ \mathbf{x}_m(0) \\ x_{ex}(0) \\ x_{ic}(0) \end{bmatrix} = \begin{bmatrix} \mathbf{0}_R \\ \mathbf{0}_p \\ 0 \\ 0 \end{bmatrix}$$

Hence, these decoupled quantities -  $\mathbf{x}(t)$  - represent ideal state variables for the **monitoring and fault isolation of each dynamic effect**.

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

## METHODOLOGY AND EXAMPLE

The methodology is presented with the simulated example of the hydrogenation of toluene (T) to benzene (B) and methane (M) followed by the dimerization of benzene to phenylbenzene ( $B_2$ ) in an open reactor (initially at 30°C) operated under non-isothermal conditions. Both reactions are exothermic. Hydrogen is treated as a dissolved species fed directly in the liquid phase. This system has  $R = 2$  reactions,  $p = 1$  inlet (hydrogen at 30°C), 1 heat transfer with the environment (at 20°C) and 1 outlet. The numbers of moles of all  $S = 5$  species (obtained by PLS calibration of absorbance spectra), the heat power (temperature) and the mass of the reactor are assumed to be measured.



## REFERENCES

- [1] Bonvin and Rippin, Chem. Eng. Sci. 45 (1990), 3417
- [2] Srinivasan et al., IFAC Proceedings, TFMST 1 (2013), 102
- [3] Srinivasan et al., Chem. Eng. J. 207-208 (2012), 785
- [4] Billeter et al., Anal. Chim. Acta 767 (2013), 21

## PERSPECTIVES

- Improvement of statistical tests and thresholds
- Introduction of a suitable method to detect sensor faults
- Extension of the methodology to Gas-Liquid reaction systems