

DATA RECONCILIATION USING THE CONCEPT OF EXTENTS

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INTRODUCTION

- Measurements of concentrations made during the course of the reaction are vital for efficient reactor operation
- Process monitoring, control and optimization can be carried out using measurements by building first-principles kinetic models, data-driven models, or combining these two approaches

DATA RECONCILIATION VIA NUMBERS OF MOLES

- The representation of a reaction system in terms of numbers of moles is given by a set of S differential equations:

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

- The redundancy in these S differential equations is expressed by algebraic constraints
- The number and nature of these constraints depend on the operating mode of the reactor

Table 1: Algebraic constraints under different operating modes

Operation	# constraints	Constraint derivation	Constraints
Batch	$q = S - R$	$\mathbf{P}^T [\mathbf{N}^T] = \mathbf{0}_{q \times R}$	$\mathbf{P}^T \mathbf{n}(t) = \mathbf{P}^T \mathbf{n}_0$
Fed-batch	$q = S - R - p$	$\mathbf{P}^T [\mathbf{N}^T \mathbf{W}_{in}] = \mathbf{0}_{q \times (R+p)}$	$\mathbf{P}^T \mathbf{n}(t) = \mathbf{P}^T \mathbf{n}_0$
Open	$q = S - R - p - 1$	$\mathbf{P}^T [\mathbf{N}^T \mathbf{W}_{in} \mathbf{n}_0] = \mathbf{0}_{q \times (R+p+1)}$	$\mathbf{P}^T \mathbf{n}(t) = \mathbf{0}_q$

S : # species, R : # independent reactions, p : # independent flows

- Usually, due to noise, the measured numbers of moles ($\hat{\mathbf{n}}$) violate the algebraic constraints
- The data reconciliation problem in terms of concentrations can be formulated as:

$$\begin{aligned} \min_{\hat{\mathbf{n}}(t_i)} \quad & (\hat{\mathbf{n}}(t_i) - \hat{\mathbf{n}}(t_i))^T \mathbf{W}(t_i) (\hat{\mathbf{n}}(t_i) - \hat{\mathbf{n}}(t_i)) \\ \text{s.t.} \quad & \mathbf{P}^T \hat{\mathbf{n}}(t_i) = \mathbf{0}_q, \\ & \hat{\mathbf{n}}(t_i) \geq \mathbf{0}_S \end{aligned}$$

- **Advantages:** The DR problems for different time instants are decoupled, that is, the reconciled number of moles ($\hat{\mathbf{n}}$) can be estimated independently at each time instant

MOTIVATION

- Concentrations/numbers of moles measured are corrupted with noise, which reduces the quality of their information
- The aim is to reduce the **noise** in the concentration measurements using data reconciliation (DR) [1]
- An alternative procedure for data reconciliation via extents instead of concentrations is presented

DATA RECONCILIATION VIA EXTENTS

- The numbers of moles can be converted into variant/invariant state variables called extents via a linear transformation [2,3]

$$\begin{bmatrix} \mathbf{x}_r(t) \\ \mathbf{x}_{in}(t) \\ x_{ic}(t) \\ \mathbf{x}_{iv}(t) \end{bmatrix} = \mathcal{T} \mathbf{n}(t) := \begin{bmatrix} \mathbf{R} \\ \mathbf{F} \\ \mathbf{i}^T \\ \mathbf{Q} \end{bmatrix} \mathbf{n}(t),$$

$$\mathcal{T} = [\mathbf{N}^T \mathbf{W}_{in} \mathbf{n}_0 \mathbf{P}]^{-1} \quad \mathbf{P}^T [\mathbf{N}^T \mathbf{W}_{in} \mathbf{n}_0] = \mathbf{0}_{q \times (R+p+1)}$$

- The system representation in terms of extents is given by a set of $R + p + 1$ differential equations and q algebraic constraints

$$\begin{aligned} \dot{\mathbf{x}}_r(t) &= V(t) \mathbf{r}(t) - \frac{u_{out}(t)}{m(t)} \mathbf{x}_r(t) & \mathbf{x}_r(0) &= \mathbf{0}_R \\ \dot{\mathbf{x}}_{in}(t) &= \mathbf{u}_{in}(t) - \frac{u_{out}(t)}{m(t)} \mathbf{x}_{in}(t) & \mathbf{x}_{in}(0) &= \mathbf{0}_p \\ \dot{x}_{ic}(t) &= -\frac{u_{out}(t)}{m(t)} x_{ic}(t) & x_{ic}(0) &= 1 \\ \mathbf{x}_{iv}(t) &= \mathbf{0}_q \end{aligned}$$

- The numbers of moles can be reconstructed from extents as:

$$\mathbf{n}(t) = \mathbf{N}^T \mathbf{x}_r(t) + \mathbf{W}_{in} \mathbf{x}_{in}(t) + \mathbf{n}_0 x_{ic}(t)$$

- The data reconciliation problem in terms of extents can then be formulated as:

$$\begin{aligned} \min_{\substack{\hat{\mathbf{x}}_r(t_1), \dots, \hat{\mathbf{x}}_r(t_H) \\ \hat{\mathbf{x}}_{in}(t_1), \dots, \hat{\mathbf{x}}_{in}(t_H) \\ \hat{x}_{ic}(t_1), \dots, \hat{x}_{ic}(t_H)}} \quad & \sum_{i=1}^H (\hat{\mathbf{n}}(t_i) - \hat{\mathbf{n}}(t_i))^T \mathbf{W}(t_i) (\hat{\mathbf{n}}(t_i) - \hat{\mathbf{n}}(t_i)) \\ \text{s.t.} \quad & \hat{x}_{ic}(t_i) - \hat{x}_{ic}(t_{i-1}) \leq 0 \quad \forall i > 1, \\ & \hat{\mathbf{n}}(t_i) \geq \mathbf{0}_S, \quad \hat{\mathbf{x}}_r(t_i) \geq \mathbf{0}_R, \quad \hat{\mathbf{x}}_{in}(t_i) \geq \mathbf{0}_p, \quad \hat{x}_{ic}(t_i) \geq 0 \end{aligned}$$

- **Advantages:** Monotonicity constraints can be imposed on the DR problem. In the absence of an outlet stream, all extents are monotonically increasing.

SIMULATED EXAMPLE

- Let us consider the acetoacetylation of pyrrole, a reaction system with four reactions, operated in a batch reactor in the presence of a catalyst (K)



- Each concentration is corrupted with additive independent zero-mean Gaussian noise of standard deviation corresponding to 10% of its maximum concentration

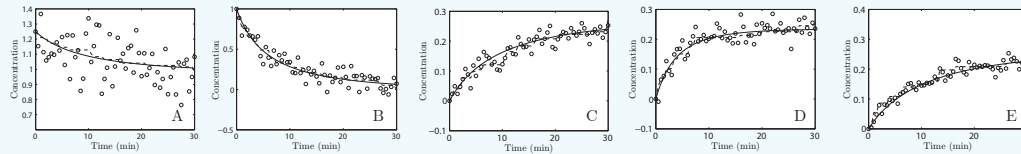


Figure 1: Simulated (—), measured (○) and extent-based reconciled (···) concentrations of the species A to E.

Table 2: Residual sums of squares between the true and the reconciled concentrations

Species	Measurements	Data reconciliation	
		via concentrations	via extents
A	0.9164	0.0332	0.0108
B	0.4615	0.1317	0.0355
C	0.0316	0.0332	0.0109
D	0.0392	0.0268	0.0062
E	0.0162	0.0155	0.0115

CONCLUSIONS

- Formulating the reconciliation problem in terms of extents allows exploiting additional monotonicity constraints
- **Future work:** Extend the DR formulation to the extents of reaction and of mass transfer in the context of open heterogeneous reaction systems

REFERENCES

- [1] S. Narasimhan and C. Jordache., Data Reconciliation and Gross Error Detection, Elsevier, 1999.
- [2] D. Rodrigues, S. Srinivasan, J. Billeter and D. Bonvin., Variant and invariant states for reaction systems, Comp & Chem. Eng., 73: 23-33, 2015
- [3] S. Srinivasan, J. Billeter and D. Bonvin., Extent-based incremental identification of reaction systems using concentration and calorimetric measurements, Chem. Eng. J. 208, 785 - 793, 2012