

Extent-based Incremental Identification of Reaction Kinetics from Spectroscopic Data

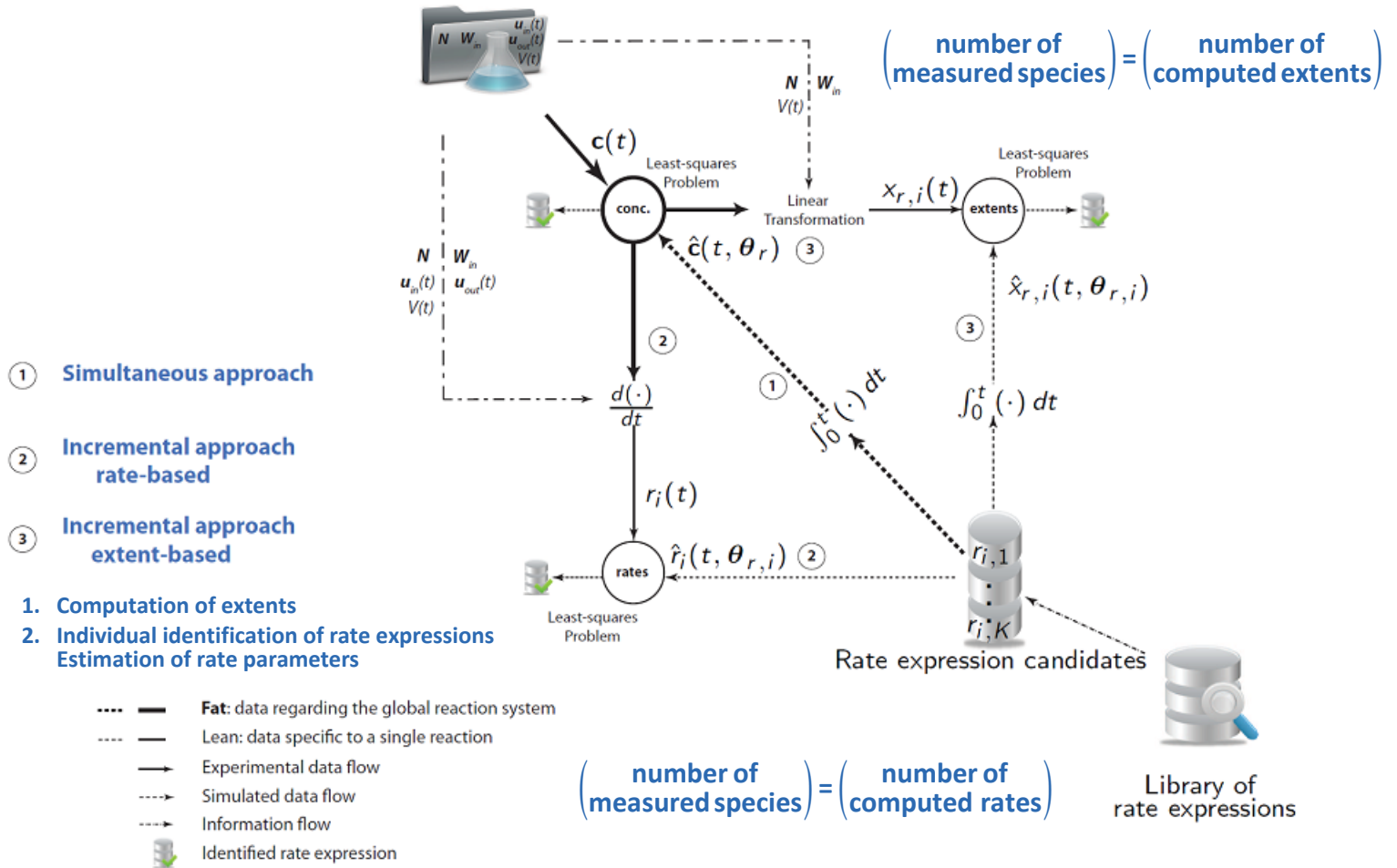
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Kinetic investigation From data to rate expressions

Experiments, measurements
and required information



Homogeneous reaction systems

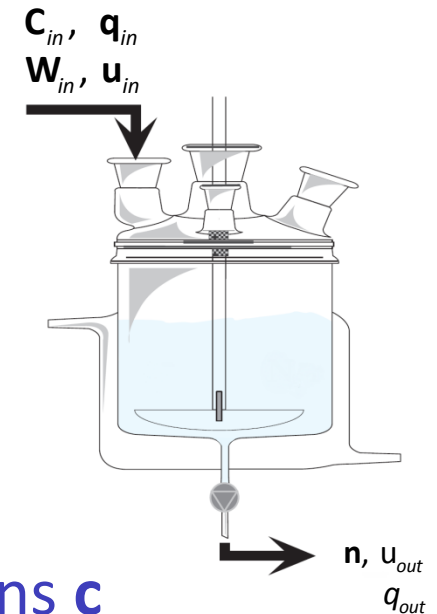
Balance equations

Homogeneous reaction system containing S species, R independent reactions, p inlets and 1 outlet

Mole balance for S species

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

$$(S \times 1) \quad (S \times R)(R \times 1) \quad (S \times p)(p \times 1)$$



Mass m , density ρ , volume V and concentrations \mathbf{c}

$$m(t) = \mathbf{1}_S^T \mathbf{M}_w \mathbf{n}(t), \quad \rho(t) = \phi(\mathbf{n}(t), \mathbf{M}_w, \rho_i), \quad V(t) = \frac{m(t)}{\rho(t)}, \quad \mathbf{c}(t) = \frac{\mathbf{n}(t)}{V(t)}$$

Homogeneous reaction systems

4-way decomposition into extents

Assumption: $\text{rank} \left(\begin{bmatrix} \mathbf{N}^T & \mathbf{W}_{in} & \mathbf{n}_0 \end{bmatrix} \right) = R + p + 1$

$$\mathbf{n} \xrightarrow{\psi} \begin{bmatrix} \mathbf{x}_r \\ \mathbf{x}_{in} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{S}_0^T \\ \mathbf{M}_0^T \\ \mathbf{q}_0^T \end{bmatrix} \mathbf{n}$$

Vessel extents of reaction \mathbf{x}_r and of flow (\mathbf{x}_{in} and x_{out})

$$\begin{aligned} \dot{\mathbf{x}}_r &= \underbrace{\mathbf{S}_0^T \mathbf{N}^T}_{\mathbf{I}_R} \mathbf{V}r + \underbrace{\mathbf{S}_0^T \mathbf{W}_{in}}_{\mathbf{0}_{R \times p}} \mathbf{u}_{in} - \frac{u_{out}}{m} \mathbf{x}_r & \mathbf{x}_r(0) &= \mathbf{0}_R \\ \dot{\mathbf{x}}_{in} &= \underbrace{\mathbf{M}_0^T \mathbf{N}^T}_{\mathbf{0}_R} \mathbf{V}r + \underbrace{\mathbf{M}_0^T \mathbf{W}_{in}}_{\mathbf{I}_p} \mathbf{u}_{in} - \frac{u_{out}}{m} \mathbf{x}_{in} & \mathbf{x}_{in}(0) &= \mathbf{0}_p \\ \dot{\lambda} &= \underbrace{\mathbf{q}_0^T \mathbf{N}^T}_{\mathbf{0}_{1 \times R}} \mathbf{V}r + \underbrace{\mathbf{q}_0^T \mathbf{W}_{in}}_{\mathbf{0}_{1 \times p}} \mathbf{u}_{in} - \frac{u_{out}}{m} \lambda & \lambda(0) &= 1 \\ x_{out} &= 1 - \lambda & x_{out}(0) &= 0 \\ \mathbf{x}_{iv} &= \mathbf{0}_{S-R-p} \end{aligned}$$

Homogeneous reaction systems

4-way decomposition into extents

Assumption: $\text{rank} \left(\begin{bmatrix} \mathbf{N}^T & \mathbf{W}_{in} & \mathbf{n}_0 \end{bmatrix} \right) = R + p + 1$

$$\mathbf{n} \xrightarrow{\Psi} \begin{bmatrix} \mathbf{x}_r \\ \mathbf{x}_{in} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{S}_0^T \\ \mathbf{M}_0^T \\ \mathbf{q}_0^T \end{bmatrix} \mathbf{n}$$

Vessel extents of reaction \mathbf{x}_r and of flow (\mathbf{x}_{in} and x_{out})

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

Reconstruction:

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

Homogeneous reaction systems

Reaction Variant (RV) form

When $\text{rank}\left(\begin{bmatrix} \mathbf{N}^T & \mathbf{W}_{in} & \mathbf{n}_0 \end{bmatrix}\right) < R + p + 1$

- Compute \mathbf{x}_{in} and x_{out} using \mathbf{u}_{in} , u_{out} and m

$$\begin{aligned} \dot{\mathbf{x}}_{in} &= \mathbf{u}_{in} - \frac{u_{out}}{m} \mathbf{x}_{in} & \mathbf{x}_{in}(0) &= \mathbf{0}_p \\ \dot{x}_{out} &= \frac{u_{out}}{m} (1 - x_{out}) & x_{out}(0) &= 0 \end{aligned}$$

- Compute \mathbf{n}^{RV} (RV-form of \mathbf{n})

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

- Compute \mathbf{x}_r from \mathbf{n}^{RV}

$$\mathbf{x}_r(t) = \mathbf{N}^{T+} \mathbf{n}^{RV}(t) = \mathbf{N}^{T+} \left(\mathbf{n}(t) - \mathbf{n}_0 - \mathbf{W}_{in} \mathbf{x}_{in}(t) + \mathbf{n}_0 x_{out}(t) \right)$$

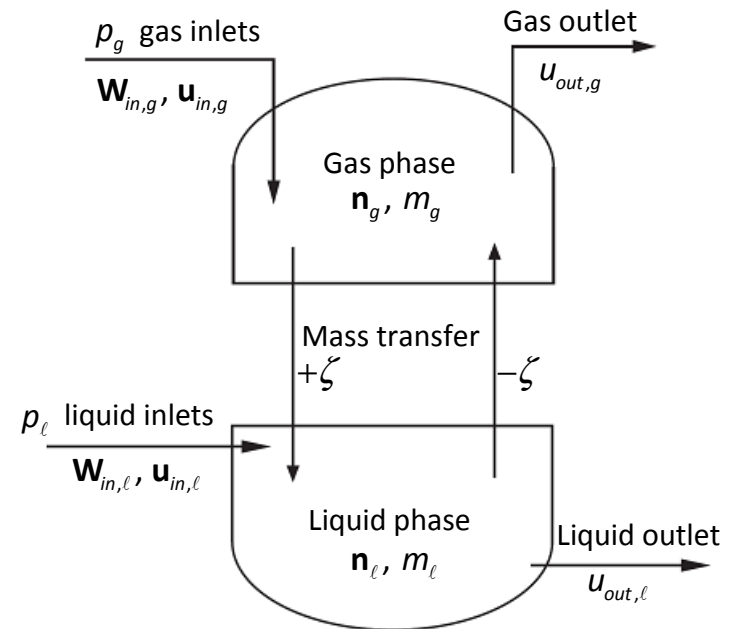
Gas-liquid reaction systems

Assumptions

Gas-liquid reaction system containing p_g inlets and 1 outlet in the gas phase, and p_ℓ inlets and 1 outlet in the liquid phase. The two phases are connected with p_m mass transfer rates ζ . By convention, a positive sign (+) is assigned to a mass transfer from the gas to the liquid.

Assumptions:

- the gas and liquid phases are homogeneous
- the reactions take place in the liquid bulk
- the mass transfer is described by the two-film theory with no accumulation in the boundary layer



Gas-liquid reaction systems

Balance equations

Mole balance in the **Liquid** phase

$$\dot{\mathbf{n}}_l(t) = \mathbf{N}^T V_l(t) \mathbf{r}(t) + \mathbf{W}_{m,l} \zeta(t) + \mathbf{W}_{in,l} \mathbf{u}_{in,l}(t) - \frac{u_{out,l}(t)}{m_l(t)} \mathbf{n}_l(t), \quad \mathbf{n}_l(0) = \mathbf{n}_{l0}$$

Mole balance in the **Gas** phase

$$\dot{\mathbf{n}}_g(t) = -\mathbf{W}_{m,g} \zeta(t) + \mathbf{W}_{in,g} \mathbf{u}_{in,g}(t) - \frac{u_{out,g}(t)}{m_g(t)} \mathbf{n}_g(t), \quad \mathbf{n}_g(0) = \mathbf{n}_{g0}$$

Mass m_l , density ρ_l , volumes V_l and V_g , and concentrations \mathbf{c}_l

$$m_l(t) = \mathbf{1}_S^T \mathbf{M}_{w,l} \mathbf{n}_l(t), \quad V_l(t) = \frac{m_l(t)}{\rho_l(t)}, \quad \mathbf{c}_l(t) = \frac{\mathbf{n}_l(t)}{V_l(t)}$$

$$\rho_l(t) = \phi(\mathbf{c}_l(t), \mathbf{M}_{w,l}, \mathbf{p}_{li}) \quad V_g(t) = V_{tot} - V_l(t)$$

Gas-liquid reaction systems

5-way decomposition into extents

Assumption: $\text{rank} \left(\begin{bmatrix} \mathbf{N}^\top & \mathbf{W}_{m,l} & \mathbf{W}_{in,l} & \mathbf{n}_{\ell 0} \end{bmatrix} \right) = R + p_m + p_\ell + 1$

$$\mathbf{n}_\ell \xrightarrow{\Psi} \begin{bmatrix} \mathbf{x}_r \\ \mathbf{x}_{m,l} \\ \mathbf{x}_{in,l} \\ \lambda_\ell \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{\ell 0}^\top \\ \mathbf{M}_{m,l}^\top \\ \mathbf{M}_{in,l}^\top \\ \mathbf{q}_{\ell 0}^\top \end{bmatrix} \mathbf{n}_\ell$$

Vessel extents of reaction \mathbf{x}_r and of flow (\mathbf{x}_{in} and \mathbf{x}_{out})

$$\begin{aligned} \dot{\mathbf{x}}_r &= V_\ell \mathbf{r} - \frac{u_{out,l}}{m_\ell} \mathbf{x}_r & \mathbf{x}_r(0) &= \mathbf{0}_R \\ \dot{\mathbf{x}}_{m,l} &= \zeta - \frac{u_{out,l}}{m_\ell} \mathbf{x}_{m,l} & \mathbf{x}_{m,l}(0) &= \mathbf{0}_{p_m} \\ \dot{\mathbf{x}}_{in,l} &= \mathbf{u}_{in,l} - \frac{u_{out,l}}{m_\ell} \mathbf{x}_{in,l} & \mathbf{x}_{in,l}(0) &= \mathbf{0}_{p_\ell} \\ \dot{\lambda}_\ell &= -\frac{u_{out,l}}{m_\ell} \lambda_\ell & \lambda_\ell(0) &= 1 \\ \mathbf{x}_{out,l} &= 1 - \lambda_\ell & \mathbf{x}_{out,l}(0) &= 0 \end{aligned}$$

Reconstruction:

$$\mathbf{n}_\ell(t) = \mathbf{n}_{\ell 0} + \mathbf{N}^\top \mathbf{x}_r(t) + \mathbf{W}_{m,l} \mathbf{x}_{m,l}(t) + \mathbf{W}_{in,l} \mathbf{x}_{in,l}(t) - \mathbf{n}_{\ell 0} \mathbf{x}_{out,l}(t)$$

Gas-liquid reaction systems

Reaction & Mass-transfer Variant (RMV) form

When $\text{rank}\left(\begin{bmatrix} \mathbf{N}^\top & \mathbf{W}_{m,l} & \mathbf{W}_{in,l} & \mathbf{n}_{l,0} \end{bmatrix}\right) < R + p_m + p_l + 1$

- Compute $\mathbf{x}_{in,l}$ and $x_{out,l}$ using $\mathbf{u}_{in,l}$, $u_{out,l}$ and m_l

$$\dot{\mathbf{x}}_{in,l} = \mathbf{u}_{in,l} - \frac{u_{out,l}}{m_l} \mathbf{x}_{in,l} \quad \mathbf{x}_{in,l}(0) = \mathbf{0}_{p_l}$$

$$\dot{x}_{out,l} = \frac{u_{out,l}}{m_l} (1 - x_{out,l}) \quad x_{out,l}(0) = 0$$

- Compute \mathbf{n}_l^{RMV} (RMV-form of \mathbf{n}_l)

$$\mathbf{n}_l^{RMV}(t) = \mathbf{n}_l(t) - \mathbf{n}_{l0} - \mathbf{W}_{in,l} \mathbf{x}_{in,l}(t) + \mathbf{n}_{l0} x_{out,l}(t) = \mathbf{N}^\top \mathbf{x}_r(t) + \mathbf{W}_{m,l} \mathbf{x}_{m,l}(t)$$

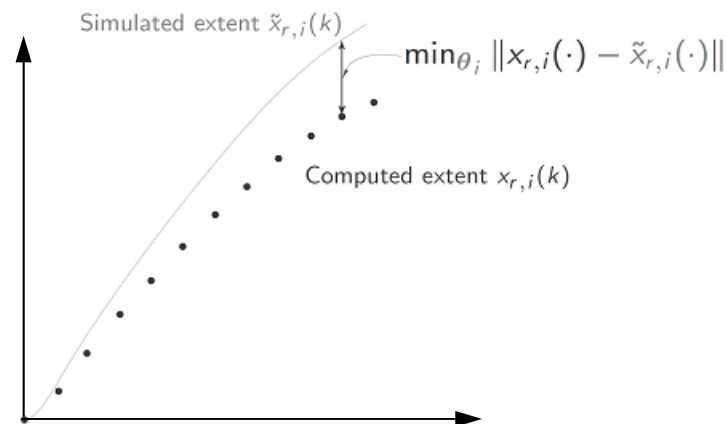
- Compute \mathbf{x}_r and $\mathbf{x}_{m,l}$ from \mathbf{n}_l^{RMV}

$$\begin{bmatrix} \mathbf{x}_r(t) \\ \mathbf{x}_{m,l}(t) \end{bmatrix} = \begin{bmatrix} \mathbf{N}^\top & \mathbf{W}_{m,l} \end{bmatrix}^+ \mathbf{n}_l^{RMV}(t) = \begin{bmatrix} \mathbf{N}^\top & \mathbf{W}_{m,l} \end{bmatrix}^+ (\mathbf{n}_l(t) - \mathbf{n}_{l0} - \mathbf{W}_{in,l} \mathbf{x}_{in,l}(t) + \mathbf{n}_{l0} x_{out,l}(t))$$

Individual identification of reaction rates from the extents of reaction

Identification of the rate expression r_i and estimation of the associated kinetic parameters θ_i for each i -th reaction by comparing the computed extents $x_{r,i}(t)$ and the simulated extents $\tilde{x}_{r,i}(t)$ of reaction

$$\dot{\tilde{x}}_{r,i} = V_\ell(t) r_i(\theta_i, \mathbf{c}_\ell(t)) - \frac{u_{out,\ell}(t)}{m_\ell(t)} \tilde{x}_{r,i}(t) \quad \tilde{x}_{r,i}(0) = 0$$



Incremental identification using spectroscopic data

Homogeneous
reaction systems

Gas-liquid
reaction systems

Calibration step

$$\mathbf{F}_{prog} = \varphi(\mathbf{C}_c, \mathbf{Y}_c)$$

$$\mathbf{F}_{prog} = \varphi(\mathbf{C}_{\ell,c}, \mathbf{Y}_{\ell,c})$$

Numbers of moles

$$\hat{\mathbf{n}}(t) = \mathbf{F}_{prog} \mathbf{a}_v(t)$$

$$\hat{\mathbf{n}}_{\ell}(t) = \mathbf{F}_{prog} \mathbf{a}_v(t)$$

Extents using $\hat{\mathbf{n}}$

$$\mathbf{x}_r(t) = \mathbf{S}_0^T \hat{\mathbf{n}}(t)$$

$$\begin{bmatrix} \mathbf{x}_r(t) \\ \mathbf{x}_{m,\ell}(t) \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{\ell 0}^T \\ \mathbf{M}_{m,\ell 0}^T \end{bmatrix} \hat{\mathbf{n}}_{\ell}(t)$$

using $\hat{\mathbf{n}}^{RV}$ or $\hat{\mathbf{n}}_{\ell}^{RMV}$

$$\mathbf{x}_r(t) = \mathbf{N}^{T+} \hat{\mathbf{n}}^{RV}(t)$$

$$\begin{bmatrix} \mathbf{x}_r(t) \\ \mathbf{x}_{m,\ell}(t) \end{bmatrix} = \begin{bmatrix} \mathbf{N}^T & \mathbf{W}_{m,\ell} \end{bmatrix}^+ \hat{\mathbf{n}}_{\ell}^{RMV}(t)$$

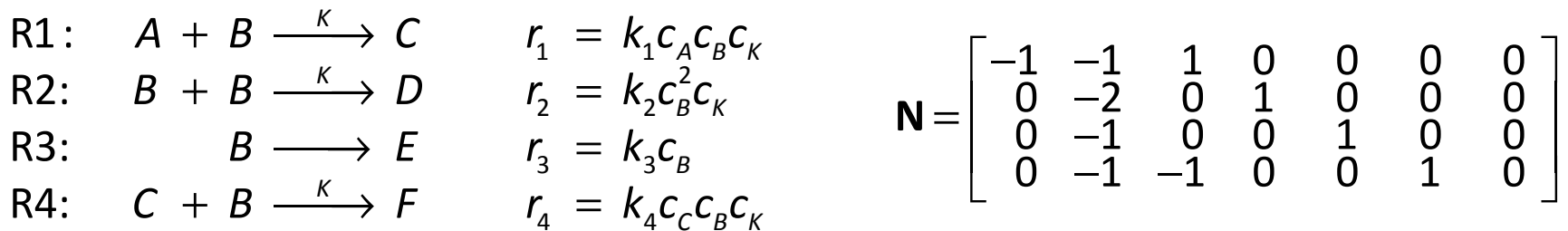
Extents can subsequently be used for model identification

\mathbf{F}_{prog} is the prognostic matrix ($S \times L$) from calibration, $\mathbf{a}_v(t) = \mathbf{a}(t)V_{\ell}(t)$ with dimension ($L \times 1$)

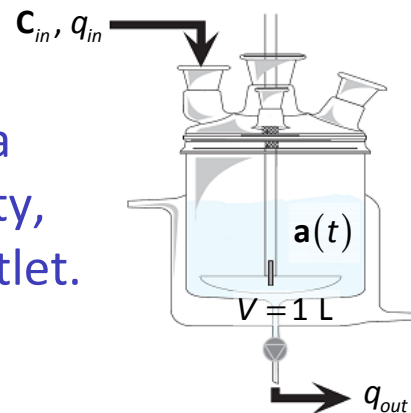
Homogeneous reaction systems

Acetoacetylation of pyrrole

The acetoacetylation of Pyrrole (*A*) with Diketene (*B*) catalyzed by Pyridine (*K*) involves seven species ($S = 7$). Four reactions ($R = 4$) produce 2-acetoacetyl pyrrole (*C*), Dehydroacetic acid (*D*), Oligomers (*E*) and a By-product (*F*).



The experiment is performed in a CSTR, assuming a constant density, with one inlet ($p = 1$) and one outlet.



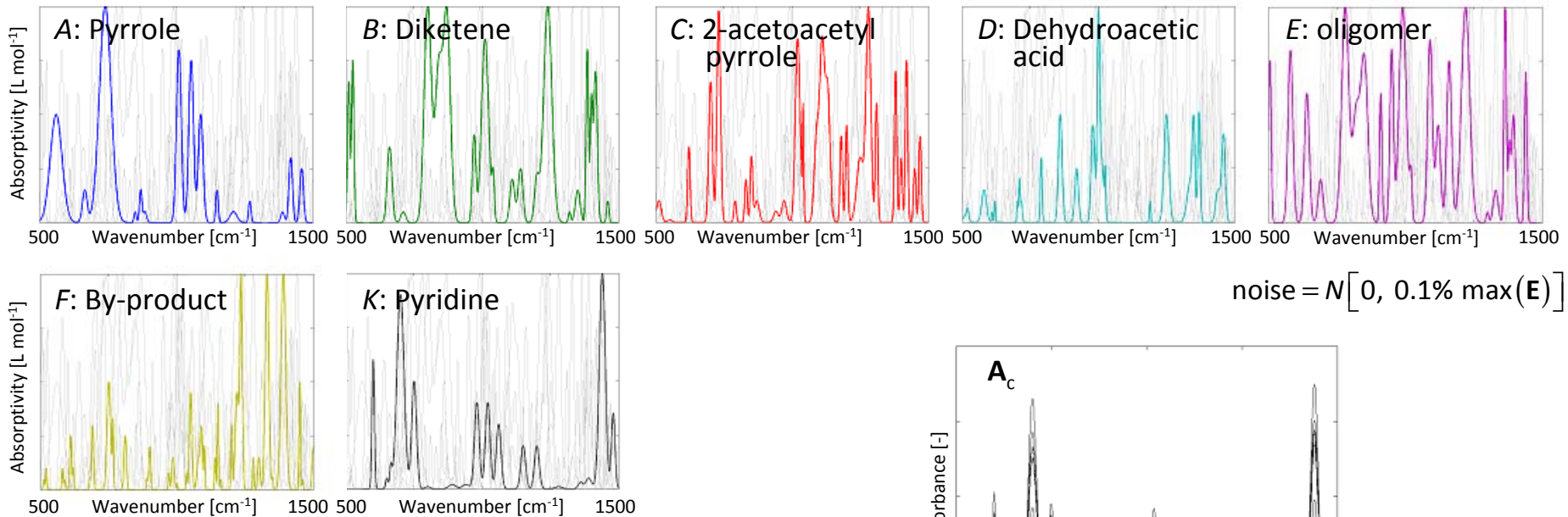
$$\mathbf{n}_0 = \begin{bmatrix} 0.72 \\ 0.09 \\ 0.01 \\ 0.02 \\ 0 \\ 0 \\ 5 \end{bmatrix}$$

$$\mathbf{c}_{in} = \begin{bmatrix} 0 \\ 0.58 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

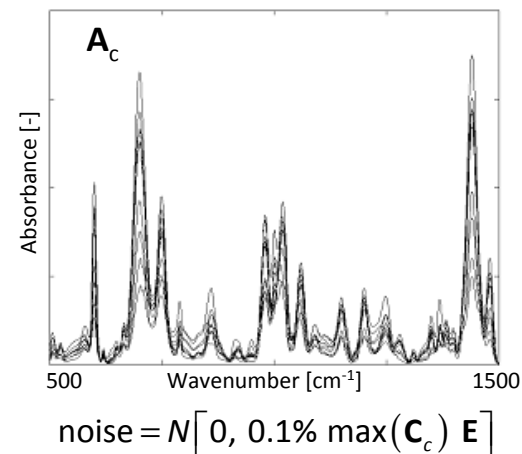
Homogeneous reaction systems

Acetoacetylation of pyrrole

Pure Component Spectra : $\mathbf{F}_{prog} = \mathbf{E}^+$ ($S = 7 \times L = 1000$)



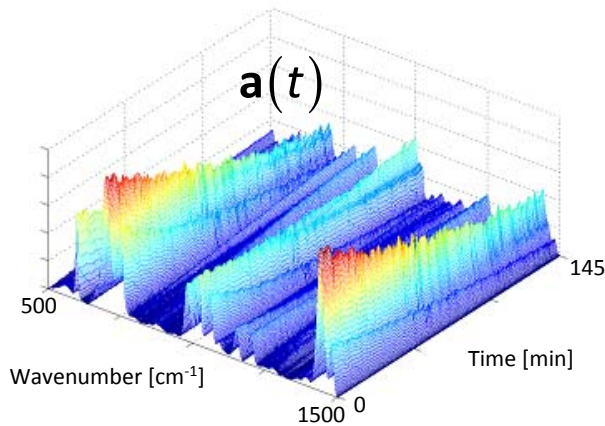
Calibration set (10 spectra):



Homogeneous reaction systems

Acetoacetylation of pyrrole

$$\text{rank}\left(\begin{bmatrix} \mathbf{N}^T & \mathbf{C}_{in} & \mathbf{n}_0 \end{bmatrix}\right) = 6 = R + p + 1 \quad \checkmark$$

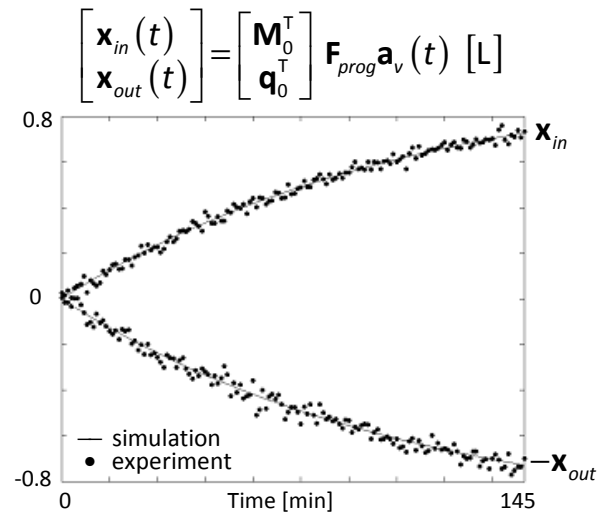
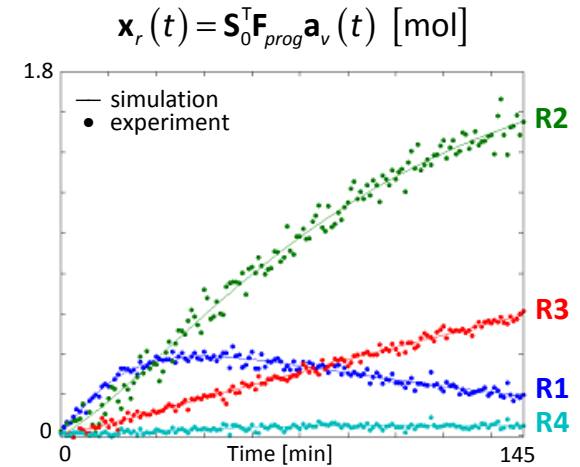


$$\mathbf{a}_v(t) = \mathbf{a}(t)\mathbf{V}(t)$$

$$\text{noise} = N\left[0, 3\% \max(\mathbf{c}(t)) \mathbf{E}\right]$$

$$\psi(\mathbf{N}, \mathbf{C}_{in}, \mathbf{n}_0) = \begin{bmatrix} \mathbf{S}_0^T \\ \mathbf{M}_0^T \\ \mathbf{q}_0^T \end{bmatrix} \mathbf{F}_{prog}$$

$\xrightarrow{\mathbf{F}_{prog} = \mathbf{E}^+}$



Homogeneous reaction systems

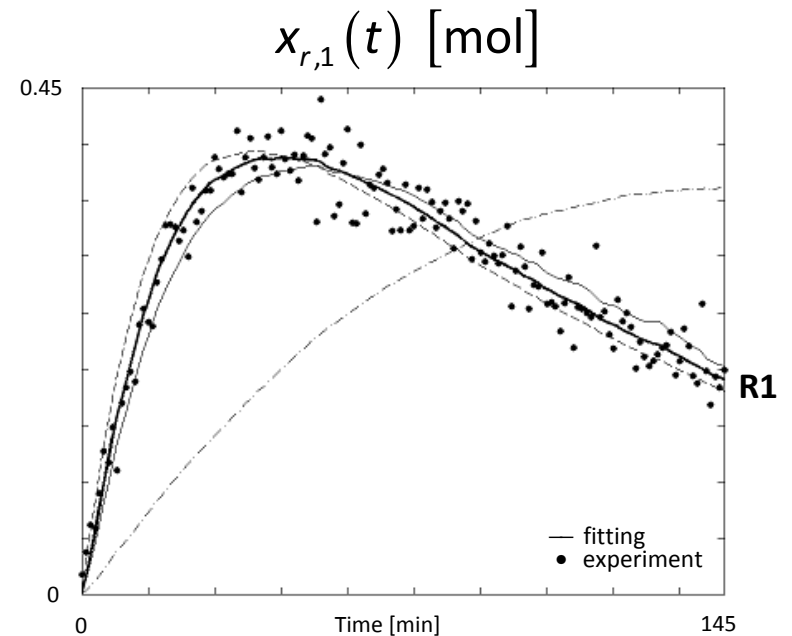
Acetoacetylation of pyrrole

Fitting of each extent individually

	Simulation		Fitting		
	Model	k	Model	k	CI (99%)
R1	M1	0.0530	E : M1	0.0525	0.0516 – 0.0534
			PCR : M1	0.0536	0.0528 – 0.0543
			PLS : M1	0.0536	0.0528 – 0.0543
R2	M2	0.1280	E : M2	0.1287	0.1269 – 0.1304
			PCR : M2	0.1294	0.1278 – 0.1309
			PLS : M2	0.1294	0.1278 – 0.1309
R3	M3	0.0280	E : M3	0.0280	0.0276 – 0.0283
			PCR : M3	0.0280	0.0276 – 0.0285
			PLS : M3	0.0280	0.0276 – 0.0285
R4	M4	0.0030	E : M4	0.0029	0.0027 – 0.0031
			PCR : M4	0.0030	0.0028 – 0.0032
			PLS : M4	0.0030	0.0028 – 0.0032

M1: $r = k c_A c_B c_K$, M2: $r = k c_B^2 c_K$, M3: $r = k c_B$, M4: $r = k c_C c_B c_K$

PCR and PLS calibrations performed with 7 factors

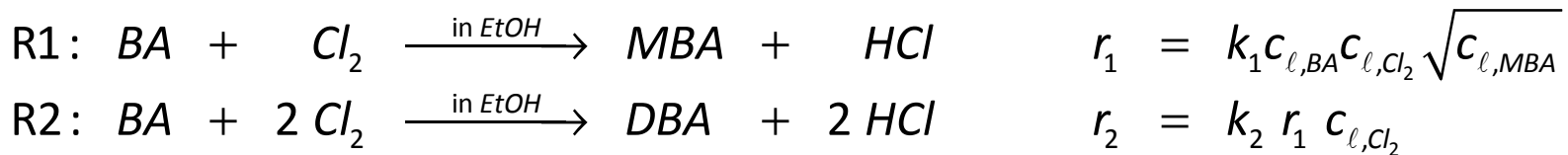


r_1	$k c_B c_K$	$k c_A c_K$	$k c_A c_B$	$k c_A c_B c_K$
ssq	2.802	0.114	0.100	0.064
line	-----	-----	—————	—————

Gas-liquid reaction systems

Chlorination of butanoic acid

The reaction of Butanoic acid (BA) with chlorine (Cl_2) involves seven species ($S = 7$). Two reactions ($R = 2$) produce α -mono-chloro-butanoic acid (MBA), α -di-chloro-butanoic acid (DBA) and Hydrochloric acid (HCl). Ethanol (EtOH) is used as liquid solvent and Air is initially present in the reactor.



$$\mathbf{N} = \begin{bmatrix} -1 & -1 & 1 & 1 & 0 & 0 & 0 \\ -1 & -2 & 0 & 2 & 1 & 0 & 0 \end{bmatrix}$$

Species in the Liquid phase ($S_l = 6$): BA, Cl_2, MBA, HCl, DBA and EtOH

Species in the Gas phase ($S_g = 3$): $Cl_2, HCl, (\text{Air})$

Transferring species ($p_m = 2$): Cl_2, HCl

Gas-liquid reaction systems

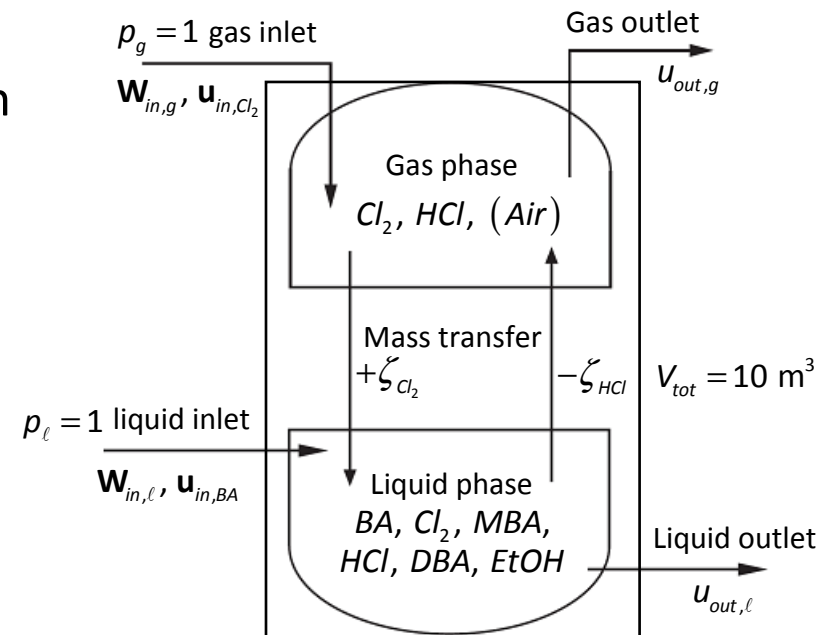
Chlorination of butanoic acid

Liquid phase

One inlet of BA ($p_\ell = 1$) and one outlet
 The density changes with the composition
 The outlet is *regulated* to maintain the mass of the liquid constant

Gas phase

One inlet of Cl_2 ($p_g = 1$) and one outlet
 The outlet is *regulated* to maintain the total pressure at 10 bar



$$\mathbf{n}_{l0} = \begin{bmatrix} 0 \\ 0 \\ 10^{-5} \\ 0 \\ 0 \\ 100 \end{bmatrix} \text{ kmol}$$

$$\mathbf{W}_{m,l} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\mathbf{n}_{g0} = \begin{bmatrix} 0 \\ 0 \\ 0.095 \end{bmatrix} \text{ kmol}$$

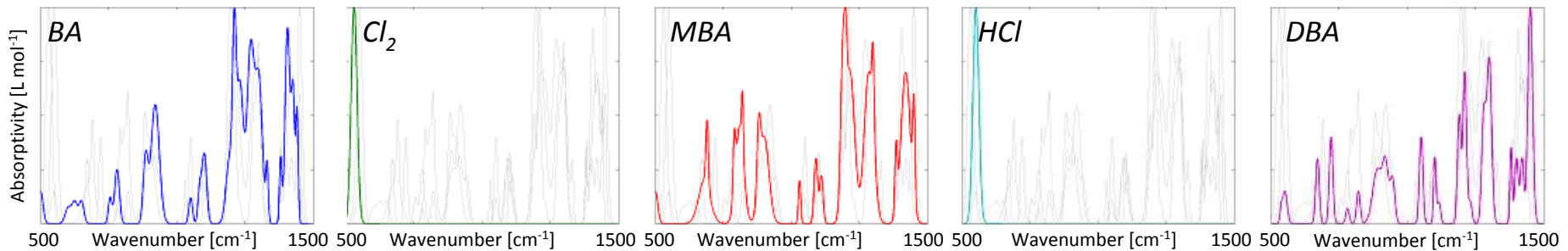
$$\mathbf{W}_{in,g} = \begin{bmatrix} 0.0141 \\ 0 \\ 0 \end{bmatrix}$$

$$\mathbf{W}_{m,g} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Gas-liquid reaction systems

Chlorination of butanoic acid

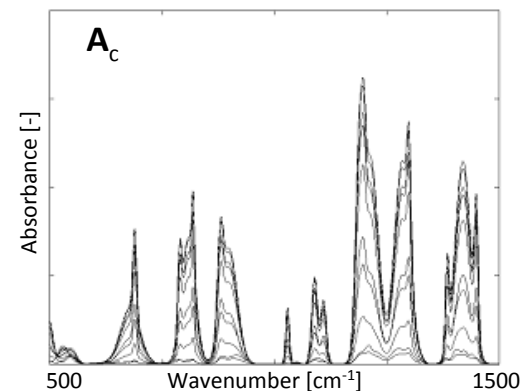
Pure Component Spectra : $F_{prog} = E^+$ ($S_a = 5 \times L = 1000$)



*The pure spectrum of EtOH is treated as background spectrum
Air does not absorb*

$$\text{noise} = N[0, 0.1\% \max(\mathbf{E})]$$

Calibration set (10 spectra):

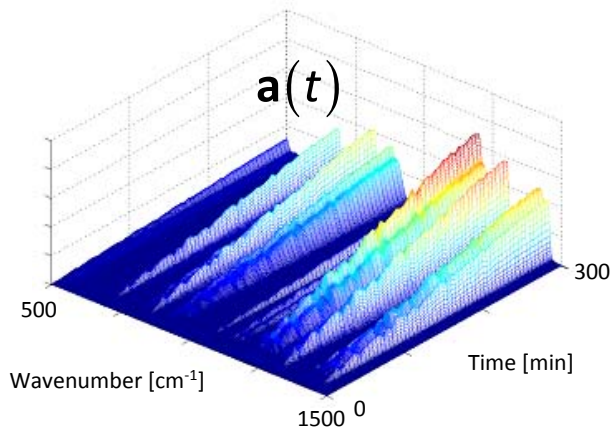


$$\text{noise} = N[0, 0.1\% \max(\mathbf{C}_c) \mathbf{E}]$$

Gas-liquid reaction systems

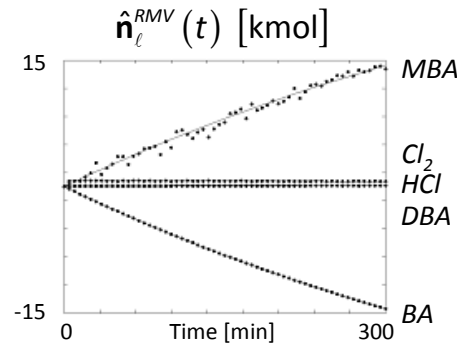
Chlorination of butanoic acid

$$\text{rank}\left(\begin{bmatrix} \mathbf{N}^T & \mathbf{W}_{m,\ell} & \mathbf{W}_{in,\ell} & \mathbf{n}_{\ell 0} \end{bmatrix}\right) = 5 < R + p_m + p_\ell + 1 = 6 \quad \times$$

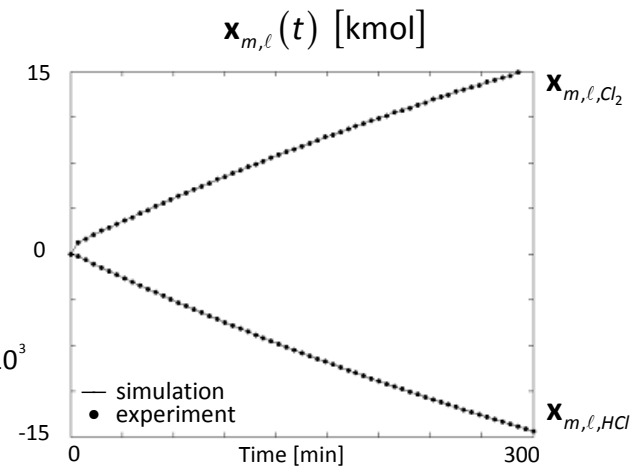
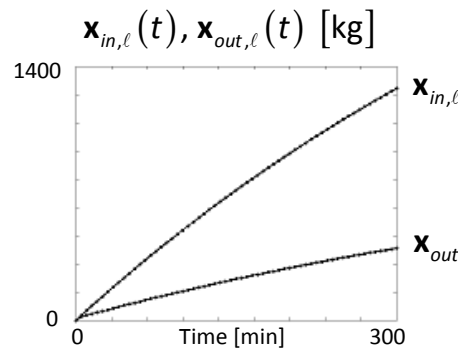
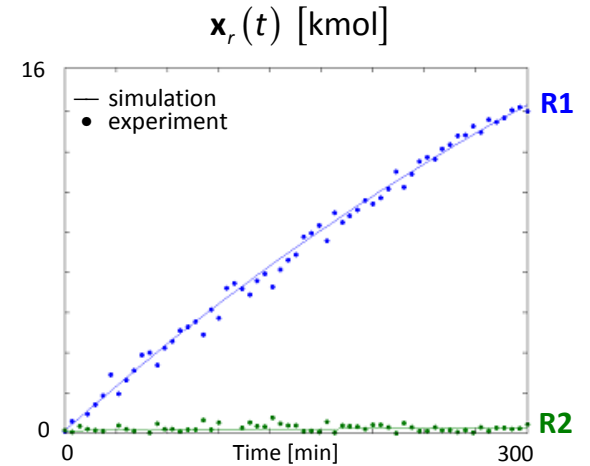


$$\mathbf{a}_v(t) = \mathbf{a}(t)V(t)$$

$$\text{noise} = N\left[0, 3\% \max(\mathbf{c}(t)) \mathbf{E}\right]$$



$$\begin{bmatrix} \mathbf{N}^T & \mathbf{W}_{m,\ell} \end{bmatrix}^+ \hat{\mathbf{n}}_\ell^{RMV}(t) \rightarrow \mathbf{F}_{prog} = \mathbf{E}^+$$



Gas-liquid reaction systems

Chlorination of butanoic acid

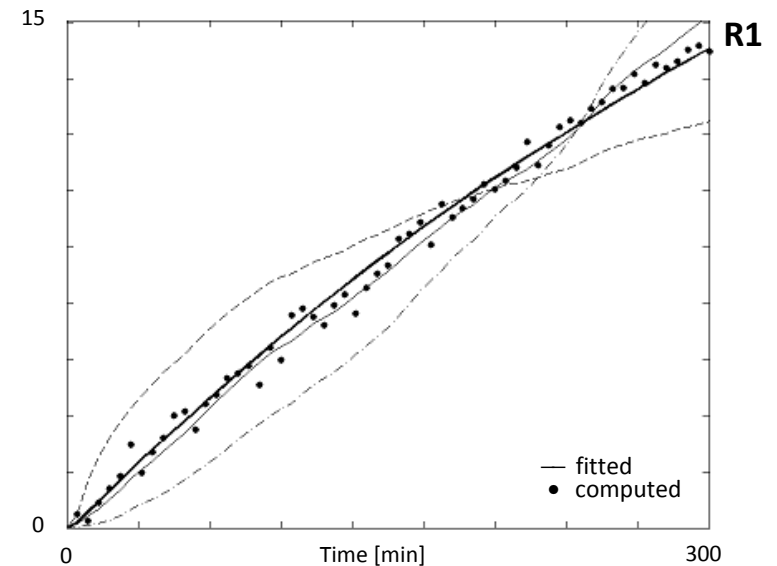
Fitting of each extent individually

	Simulation		Fitting		
	Model	k	Model	k	CI (99%)
R1	M1	1.358	E : M1	1.335	1.310 – 1.361
			PCR : M1	1.353	1.331 – 1.374
			PLS : M1	1.353	1.331 – 1.374
R2	M2	0.100	E : M2	0.119	0.037 – 0.201
			PCR : M2	0.128	0.049 – 0.206
			PLS : M2	0.128	0.049 – 0.206

M1: $r = k c_{\ell,BA} c_{\ell,Cl_2} \sqrt{c_{\ell,MBA}}$, M2: $r = k c_{\ell,BA} c_{\ell,Cl_2}^2 \sqrt{c_{\ell,MBA}}$

PCR and PLS calibrations performed with 5 factors

$x_{r,1}(t)$ [kmol]



r_1	$kc_{BA}c_{Cl_2}c_{MBA}$	$kc_{BA}c_{Cl_2}$	kc_{Cl_2}	$kc_{BA}c_{Cl_2}\sqrt{c_{MBA}}$
ssq	159.4	147.4	11.6	8.1
line	-----	-----	—————	—————

Conclusions

Extent-based incremental identification

- decouples each reaction from other reactions and mass transfers
- allows investigating each reaction individually
- leads to model reduction:

Homogeneous reaction systems: $S \rightarrow R + p + 1$

Gas-liquid reaction systems: $S_\ell \rightarrow R + p_m + p_\ell + 1$

Extension to spectroscopic data with calibration

- requires computing a minimum number of concentrations (liquid phase)

Homogeneous reaction systems: R

Gas-liquid reaction systems: $R + p_m$

or requires an additional source of measurements in the liquid/gas phase

Outlook: is a calibration-free approach possible?

Thank you for you attention

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