Control of Reaction Systems via Rate Estimation and Feedback Linearization

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- Efficient control of reaction systems typically requires kinetic models, whose identification can be difficult and time consuming.

- One can infer reaction rates from measurements, without a kinetic model, if the rates are decoupled.[1]

- Reaction variants/invariants decouple reaction rates, thereby facilitating analysis and control.[2]

- More generally, variant/invariant states can decouple dynamic effects via a linear transformation to vessel extents.[3]

[1] Mhamdi, A.; Marquardt, W. In *ADCHEM 2003, Hong Kong, China*, 2004, pp 171–176.

[2] Asbjørnsen, O. A.; Fjeld, M. *Chem. Eng. Sci.* **1970**, *25*, 1627–1636.

[3] Rodrigues, D. et al. *Comp. Chem. Eng.* **2015**, *73*, 23–33.

- Various control strategies for open reactors are based on reaction variants and extensive variables.[4]
- There is no systematic control method that takes advantage of multiple measurements, in particular without a kinetic model.
- The control of chemical reactors **without kinetic models** is possible, by
  - (i) estimating reaction rates from concentration and temperature via the concept of variants,
  - (ii) using feedback linearization and these estimated rates to effectively control the temperature by manipulating the exchanged heat.

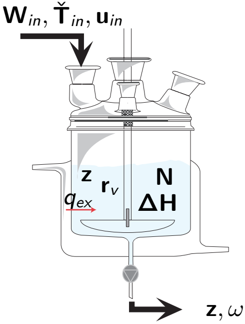
[4] Georgakis, C. *Chem. Eng. Sci.* **1986**, *41*, 1471–1484; Farschman, C. A. et al. *AIChE J.* **1998**, *44*, 1841–1857.

- Open homogeneous reactor with S species, R independent reactions, p inlet streams and 1 outlet stream.
- The S-dimensional vector of numbers of moles $\mathbf{n}$, and the heat energy $Q = mc_p(T - T_{ref})$ are state variables.
- Mole and heat balance equations:[5]

$$\underbrace{\begin{bmatrix}\dot{\mathbf{n}}(t)\\ \dot{Q}(t)\end{bmatrix}}_{\dot{\mathbf{z}}(t)} = \underbrace{\begin{bmatrix}\mathbf{N}^{\mathrm{T}}\\ (-\boldsymbol{\Delta}\mathbf{H})^{\mathrm{T}}\end{bmatrix}}_{\mathcal{A}}\mathbf{r}_v(t) + \underbrace{\begin{bmatrix}\mathbf{0}_S\\ 1\end{bmatrix}}_{\mathbf{b}}q_{ex}(t) + \underbrace{\begin{bmatrix}\mathbf{W}_{in}\\ \check{\mathbf{T}}_{in}^{\mathrm{T}}\end{bmatrix}}_{\mathcal{C}}\mathbf{u}_{in}(t) - \omega(t)\underbrace{\begin{bmatrix}\mathbf{n}(t)\\ Q(t)\end{bmatrix}}_{\mathbf{z}(t)},$$

$$\mathbf{z}(0) = \mathbf{z}_0.$$

  - Time-variant signals
    $\mathbf{r}_v(t)$ R reaction rates, $q_{ex}(t)$ exchanged heat power,
    $\mathbf{u}_{in}(t)$ p inlet flowrates, $\omega(t)$ inverse of residence time.
  - Structural information
    $\mathbf{N}$ $(R \times S)$ stoichiometry, $\boldsymbol{\Delta}\mathbf{H}$ R heats of reaction,
    $\mathbf{W}_{in}$ $(S \times p)$ inlet composition, $\check{\mathbf{T}}_{in}$ p inlet specific heats.



[5] Rodrigues, D. et al. *Comp. Chem. Eng.* **2015**, *73*, 23–33

- If $\text{rank}(\mathcal{A}) = R$, there exists an $R \times (S+1)$ transformation matrix $\mathcal{T}$ such that

$$\mathcal{T}\mathcal{A} = \mathbf{I}_R,$$

where $\mathcal{A} = \begin{bmatrix} \mathbf{N}^{\mathsf{T}} \\ (-\mathbf{\Delta H})^{\mathsf{T}} \end{bmatrix}$.

- Apply $\mathcal{T}$ to the balance equations and define $\mathbf{y}_r(t) := \mathcal{T}\,\mathbf{z}(t)$:

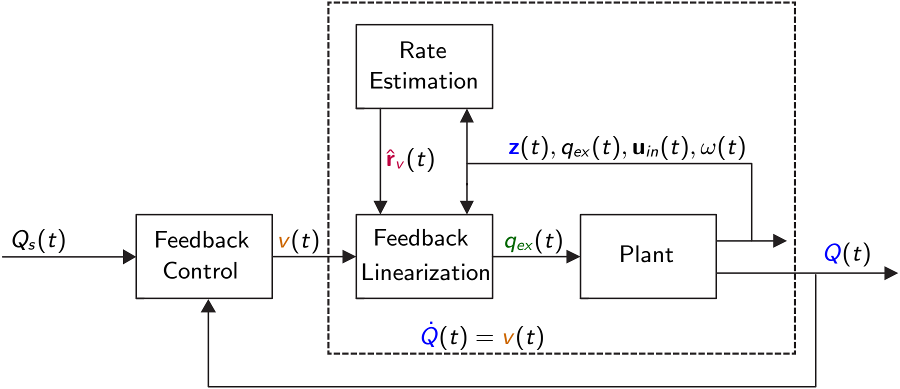
$$\dot{\mathbf{y}}_r(t) = \mathbf{r}_v(t) + (\mathcal{T}\mathbf{b})\,q_{ex}(t) + (\mathcal{T}\mathcal{C})\,\mathbf{u}_{in}(t) - \omega(t)\,\mathbf{y}_r(t), \qquad \mathbf{y}_r(0) = \mathcal{T}\mathbf{z}_0.$$

- The transformed states $\mathbf{y}_r$ are reaction variants, with each state $y_{r,i}$ $(i = 1, \ldots, R)$ depending on the corresponding rate $r_{v,i}$.[6]

[6] Asbjørnsen, O. A.; Fjeld, M. *Chem. Eng. Sci.* **1970**, *25*, 1627–1636.

- **Objective:** control the heat Q (indirectly temperature) to the setpoint Q_s by manipulating q_{ex}.

- **Method:**



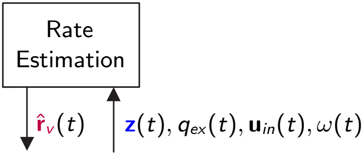
Control problem

Estimation of reaction rates

- Estimation of $\mathbf{r}_v$ via differentiation of $\mathbf{y}_r$ that is obtained by transformation of $\mathbf{z}$, and the knowledge of q_{ex}, $\mathbf{u}_{in}$ and ω.

- Reformulate the dynamic equations of $\mathbf{y}_r$:

$$\mathbf{r}_v(t) = \dot{\mathbf{y}}_r(t) - (\mathcal{T}\mathbf{b})\, q_{ex}(t) - (\mathcal{T}\mathcal{C})\, \mathbf{u}_{in}(t) + \omega(t)\mathbf{y}_r(t).$$



- The transformation $\mathcal{T}$ requires that at least R elements of $\mathbf{z}$ be measured.

- Different transformations $\mathcal{T}$ satisfy $\mathcal{T}\mathcal{A} = \mathbf{I}_R$, e.g. $\mathcal{T} = \mathcal{A}^{\dagger}$ (Moore-Penrose).

- With noisy measurements of $\mathbf{z}$, a maximum-likelihood estimator is obtained with $\mathcal{T} = (\mathcal{A}^{\mathsf{T}}\mathbf{\Sigma}^{-1}\mathcal{A})^{-1}\mathcal{A}^{\mathsf{T}}\,\mathbf{\Sigma}^{-1}$, where $\mathbf{\Sigma}$ is the variance-covariance matrix.

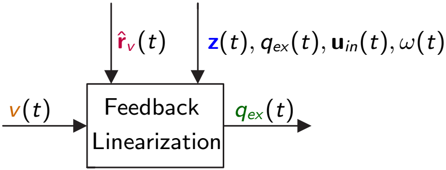
Control problem

Feedback linearization

- Feedback linearization (linear, first-order relationship between v and Q).

- Define the new input v as the right-hand side of the heat balance equation:

$$\dot{Q}(t) = (-\boldsymbol{\Delta}\mathbf{H})^{\mathrm{T}}\mathbf{r}_v(t) + q_{ex}(t) + \check{\mathbf{T}}_{in}^{\mathrm{T}}\mathbf{u}_{in}(t) - \omega(t)Q(t) \stackrel{!}{=} v(t).$$



- The relationship between the new input v and q_{ex} is known:

$$q_{ex}(t) = v(t) - (-\boldsymbol{\Delta}\mathbf{H})^{\mathrm{T}}\hat{\mathbf{r}}_v(t) - \check{\mathbf{T}}_{in}^{\mathrm{T}}\mathbf{u}_{in}(t) + \omega(t)Q(t).$$

Control problem

Feedback control of the temperature

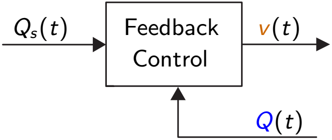
- Design of a feedback controller for the system $\dot{Q}(t) = v(t)$, using pole placement or loop shaping (closed-loop transfer function $\frac{Q(s)}{Q_s(s)} = 1$).

- The feedback controller using the control law

$$v(t) = \dot{Q}_s(t) + \gamma\left(Q_s(t) - Q(t)\right)$$

forces the error $e(t) := Q_s(t) - Q(t)$ to converge exponentially to zero at a rate γ:

$$\dot{e}(t) = -\gamma\, e(t), \qquad e(0) = Q_s(0) - Q(0).$$



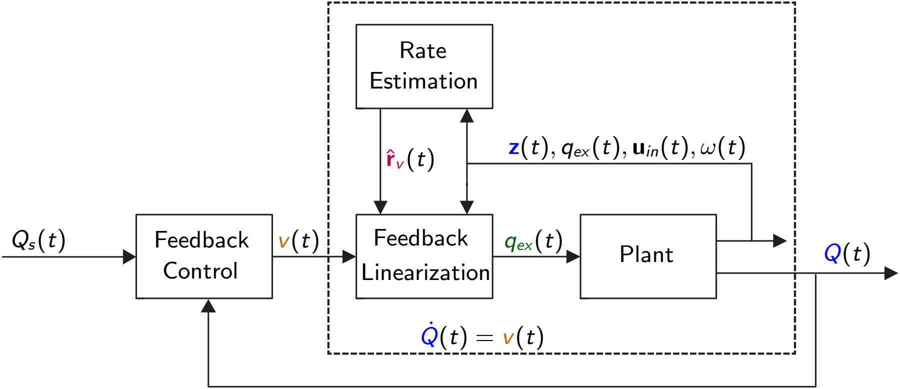
- The output of the feedback controller is v, which determines q_{ex} according to

$$q_{ex}(t) = v(t) - (-\boldsymbol{\Delta}\mathbf{H})^{\mathrm{T}}\hat{\mathbf{r}}_v(t) - \check{\mathbf{T}}_{in}^{\mathrm{T}}\mathbf{u}_{in}(t) + \omega(t)Q(t).$$

Control problem

Objective and method

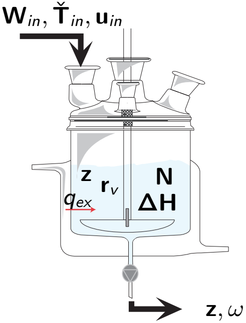
- **Objective:** control the heat Q (indirectly temperature) to the setpoint Q_s by manipulating q_{ex}.
- **Method:**



Simulated CSTR

Physical description

- Acetoacetylation of pyrrole in a homogeneous CSTR:[7]
  - $S = 4$ species (A: pyrrole; B: diketene).
  - $R = 2$ reactions (A + B $\rightarrow$ 2-acetoacetylpyrrole, 2B $\rightarrow$ dehydroacetic acid).
  - $p = 2$ inlets (of A and B).
  - 1 outlet (flowrate adjusted to keep constant volume).
  - Constant heat capacity mc_p.
  - Heat exchange only with the jacket.



- Reaction rates are complex and unknown.

- The system is initially at a steady state corresponding to $\bar{q}_{ex}$ and $\bar{\mathbf{u}}_{in} = \begin{bmatrix} \bar{u}_{in,A} \\ \bar{u}_{in,B} \end{bmatrix}$.

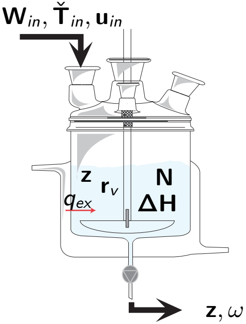
- **Control objective:**
  Reject effect on the temperature T of 15 kg min^{-1} step disturbance in $u_{in,B}$ (with $\bar{u}_{in,B} = 15$ kg min^{-1}) by manipulating q_{ex}.

[7] Ruppen, D. et al. *Comp. Chem. Eng.* **1998**, *22*, 185–189.

Simulated CSTR

Data treatment

- Following values are assumed to be known:
  - Stoichiometry $\mathbf{N}$.
  - Heats of reaction $\mathbf{\Delta H}$.
  - Inlet composition $\mathbf{W}_{in}$.
  - Inlet specific enthalpies $\check{\mathbf{T}}_{in}$.
- Measurements of $\mathbf{z}$, q_{ex}, $\mathbf{u}_{in}$ and ω are available at the sampling time $h_s = 0.4$ s.
- Standard deviation of added measurement noise
  - $\mathbf{n}$: 0.5% (relative to maximum value for each species).
  - Q: 0.5 K.
- Savitzky-Golay differentiation filter (of order 1 and window size $q = 25$) is used.[8]



- **Benchmark comparison:**
  FL control with convergence rate $\gamma = 5$ min^{-1}.
  PI control with gain $K_p = 5$ min^{-1} and integral time constant $\tau_I = 0.2$ min.

[8] Savitzky, A.; Golay, M. *Anal. Chem.* **1964**, *36*, 1627–1639.

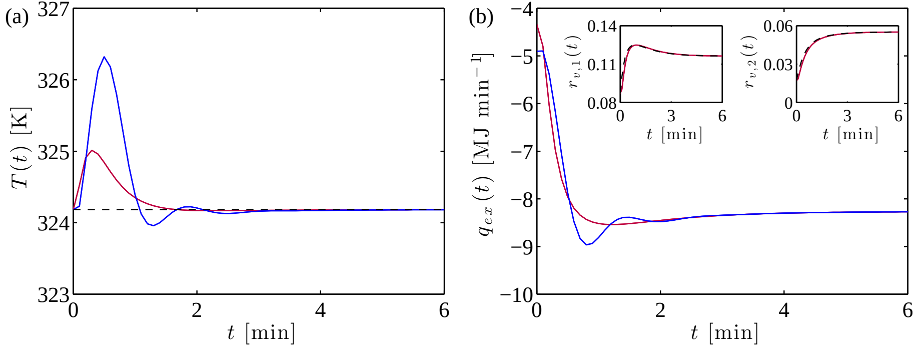


Figure 1: (a): Temperature for FL control and PI control, with the setpoint shown by the dashed line; (b): Exchanged heat power and, insets, estimated (solid lines) and true (dashed lines) reaction rates.

Simulated CSTR

Results (with measurement noise)

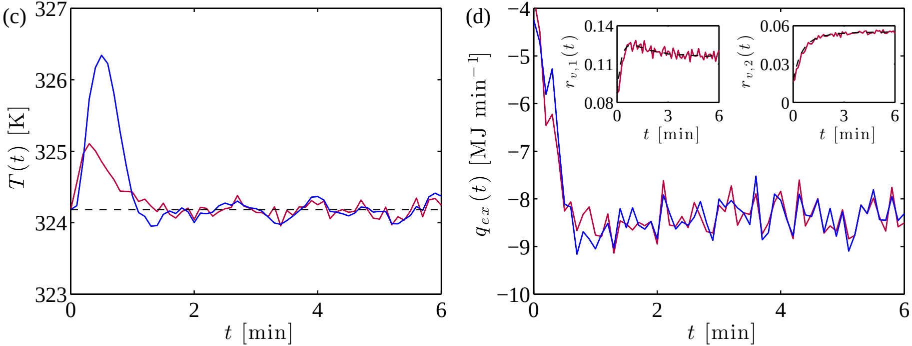


Figure 1: (c): Temperature for FL control and PI control, with the setpoint shown by the dashed line; (d): Exchanged heat power and, insets, estimated (solid lines) and true (dashed lines) reaction rates.

- **Pros:**
  The feedback-linearization scheme rejects the disturbance more quickly than the PI controller, because feedback linearization generates first-order dynamics between v and Q, whereas PI control needs to deal with $(R + p + 1)$-order dynamics between q_{ex} and Q.

- **Cons:**
  If the standard deviation of the concentration measurement noise is too large[9], the estimated reaction rates are either too imprecise (due to differentiation of $\mathbf{z}$) or delayed (due to a larger window size q), and the advantage of feedback linearization over PI control becomes less clear.

[9] In this example, about 1% of the maximum for each species.

Conclusions

- Control of the heat Q (and indirectly of the temperature T) by manipulating the exchanged heat power q_{ex} in an open homogeneous reactor is implemented **without a kinetic model**.
- Straightforward extension to control of reactant concentrations by manipulating the inlet flowrates.
- The proposed control scheme includes
  - estimation of reaction rates via differentiation of reaction variants that are computed from measured states,
  - feedback linearization using the estimated reaction rates, thereby simplifying control design significantly.
- This approach implementing feedback linearization allows tracking a trajectory by forcing an exponential decay of the control error.
- In the case of low measurement noise, feedback-linearization control can outperform PI control for the purpose of disturbance rejection.

Conclusions

- Good performance for the case of frequent and precise concentration measurements.
- The control approach requires at least as many measured states as there are reaction rates ($\text{rank}(\mathcal{A}) = R$).
- Parameters of the feedback-linearization controller are mostly determined by readily available information – stoichiometry, heats of reaction, inlet composition/specific heat, and inlet/outlet flow rates.
- Two controller parameters need to be tuned to guarantee closed-loop stability:
  - The exponential convergence rate γ.
  - The parameter(s) of the differentiation filter used for rate estimation.

Take-home message:
Control of reaction systems without kinetic models is made possible by decoupling the dynamic effects and estimating the reaction rates.

References

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Ruppen, D.; Bonvin, D.; Rippin, D. W. T. *Comp. Chem. Eng.* **1998**, *22*, 185–189.

Savitzky, A.; Golay, M. *Anal. Chem.* **1964**, *36*, 1627–1639.

Thank you for your attention!

Appendix: estimation of reaction rates (1/2)

- Let us approximate the derivative $\dot{\mathbf{y}}_r(t)$ using the first-order differentiation Savitzky-Golay filter, denoted as $\mathcal{D}_q(\mathbf{y}_r, t)$, where
  - q is the window size expressed in number of samples on $[t - \Delta t, t]$,
  - h_s is the sampling time,
  - $\Delta t := (q-1)h_s$.

- Since $\mathbf{y}_r$ is Lipschitz continuous, $\mathcal{D}_q(\mathbf{y}_r, t)$ can be reformulated as

$$\mathcal{D}_q(\mathbf{y}_r, t) = \sum_{k=0}^{q-2} b_{k+1} \int_k^{k+1} \dot{\mathbf{y}}_r(t_\xi) d\xi$$

with $b_{k+1} = \frac{6(q-1-k)(k+1)}{q(q^2-1)} > 0$, such that $\sum_{k=0}^{q-2} b_{k+1} = 1$, and $t_\xi := t - \Delta t + \xi\, h_s$.

- One also knows that $\dot{\mathbf{y}}_r(t) = \mathbf{r}_v(t) + (\mathcal{T}\mathbf{b})\, q_{ex}(t) + (\mathcal{T}\mathcal{C})\, \mathbf{u}_{in}(t) - \omega(t)\, \mathbf{y}_r(t)$.

Appendix: estimation of reaction rates (2/2)

- Replacing $\dot{\mathbf{y}}_r$ by its expression:

$$\mathcal{D}_q(\mathbf{y}_r, t) = \sum_{k=0}^{q-2} b_{k+1} \int_k^{k+1} \left(\mathbf{r}_v(t_\xi) + (\mathcal{T}\mathbf{b})\, q_{ex}(t_\xi) + (\mathcal{T}\mathcal{C})\, \mathbf{u}_{in}(t_\xi) - \omega(t_\xi)\mathbf{y}_r(t_\xi)\right) d\xi$$

$$\overset{A1,A2}{\approx} \mathbf{r}_v(t) + \sum_{k=0}^{q-2} b_{k+1} \left((\mathcal{T}\mathbf{b})\, q_{ex}(t_k) + (\mathcal{T}\mathcal{C})\, \mathbf{u}_{in}(t_k) - \omega(t_k)\, \mathbf{y}_r(t_k)\right),$$

where $t_k := t - \Delta t + k\, h_s$.
A1: $\mathbf{r}_v(t)$ approximately constant on $[t - \Delta t, t]$.
A2: $q_{ex}(t)$, $\mathbf{u}_{in}(t)$ and $\omega(t)\, \mathbf{y}_r(t)$ approximately constant on each $[t_k, t_{k+1}[$.

- Defining the operator $\mathcal{W}_q(f, t) := \sum_{k=0}^{q-2} b_{k+1} f(t_k)$ for any function $f(t)$, rearranging for $\mathbf{r}_v(t)$ and using measured quantities $(\tilde{\cdot})$:

$$\hat{\mathbf{r}}_v(t) = \mathcal{D}_q(\tilde{\mathbf{y}}_r, t) - (\mathcal{T}\mathbf{b})\, \mathcal{W}_q(\tilde{q}_{ex}, t) - (\mathcal{T}\mathcal{C})\, \mathcal{W}_q(\tilde{\mathbf{u}}_{in}, t) + \mathcal{W}_q(\tilde{\omega}\, \tilde{\mathbf{y}}_r, t)$$

- This approximates $\mathbf{r}_v(t)$ for measured quantities and is used to compute $q_{ex}(t)$.