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.\(^3\)

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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

1. estimating reaction rates from concentration and temperature via the concept of variants,
2. using feedback linearization and these estimated rates to effectively control the temperature by manipulating the exchanged heat.

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Description of the reaction system

Mole and heat balance equations

- 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:\textsuperscript{5}

\[
\dot{\mathbf{n}}(t) = \begin{bmatrix} N^T \end{bmatrix} \mathbf{r}_v(t) + \begin{bmatrix} \mathbf{A} \end{bmatrix} \dot{\mathbf{b}} + \begin{bmatrix} \mathbf{W}_{in} \end{bmatrix} \mathbf{u}_{in}(t) - \mathbf{C} \mathbf{z}(t),
\]

\[
\mathbf{z}(0) = \mathbf{z}_0.
\]

- 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, $\Delta H$ $R$ heats of reaction,
  $\mathbf{W}_{in}$ ($S \times p$) inlet composition, $\tilde{T}_{in}$ $p$ inlet specific heats.

\textsuperscript{5}Rodrigues, D. et al. \textit{Comp. Chem. Eng.} \textbf{2015}, 73, 23–33
Description of the reaction system
Transformation to reaction-variant states

- If \( \text{rank}(\mathcal{A}) = R \), there exists an \( R \times (S + 1) \) transformation matrix \( T \) such that
  \[
  TA = I_R,
  \]
  where \( \mathcal{A} = \begin{bmatrix} N^T \\ (-\Delta H)^T \end{bmatrix} \).

- Apply \( T \) to the balance equations and define \( y_r(t) := Tz(t) \):
  \[
  \dot{y}_r(t) = r_v(t) + (Tb) q_{ex}(t) + (TC) u_{in}(t) - \omega(t) y_r(t), \quad y_r(0) = Tz_0.
  \]

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

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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 $r_v$ via differentiation of $y_r$ that is obtained by transformation of $z$, and the knowledge of $q_{ex}$, $u_{in}$ and $\omega$.

- Reformulate the dynamic equations of $y_r$:

$$r_v(t) = \dot{y}_r(t) - (\mathcal{T} b) q_{ex}(t) - (\mathcal{T} C) u_{in}(t) + \omega(t) y_r(t).$$

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

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

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

\[
\dot{Q}(t) = (\Delta H)^T r_v(t) + q_{ex}(t) + \hat{T}_{in}^T u_{in}(t) - \omega(t)Q(t) \overset{!}{=} v(t).
\]

The relationship between the new input \( v \) and \( q_{ex} \) is known:

\[
q_{ex}(t) = v(t) - (\Delta H)^T \hat{r}_v(t) - \hat{T}_{in}^T u_{in}(t) + \omega(t)Q(t).
\]
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
  \[ v(t) = \dot{Q}_s(t) + \gamma (Q_s(t) - Q(t)) \]
  forces the error $e(t) := Q_s(t) - Q(t)$ to converge exponentially to zero at a rate $\gamma$:
  \[ \dot{e}(t) = -\gamma e(t), \quad e(0) = Q_s(0) - Q(0). \]

- The output of the feedback controller is $v$, which determines $q_{ex}$ according to
  \[ q_{ex}(t) = v(t) - (\Delta H)^T \hat{r}_v(t) - \hat{T}_{in}^T u_{in}(t) + \omega(t)Q(t). \]
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 \(\bar{u}_{in} = \begin{bmatrix} \bar{u}_{in,A} \\ \bar{u}_{in,B} \end{bmatrix}\).

- **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 \(q_{ex}\).

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Simulated CSTR

Data treatment

Following values are assumed to be known:
- Stoichiometry $N$.
- Heats of reaction $\Delta H$.
- Inlet composition $W_{in}$.
- Inlet specific enthalpies $\tilde{T}_{in}$.

Measurements of $z$, $q_{ex}$, $u_{in}$ and $\omega$ are available at the sampling time $h_s = 0.4$ s.

Standard deviation of added measurement noise
- $n$: 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 $\gamma = 5 \text{ min}^{-1}$.
- **PI control** with gain $K_p = 5 \text{ min}^{-1}$ and integral time constant $\tau_I = 0.2$ min.

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Simulated CSTR
Results (without measurement noise)

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\textsuperscript{9}, the estimated reaction rates are either too imprecise (due to differentiation of $z$) or delayed (due to a larger window size $q$), and the advantage of feedback linearization over PI control becomes less clear.

\textsuperscript{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 \( \text{rank}(A) = R \).

- 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 \( \gamma \).
  - 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


Thank you for your attention!
Let us approximate the derivative $\dot{y}_r(t)$ using the first-order differentiation Savitzky-Golay filter, denoted as $D_q(y_r, t)$, 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 $y_r$ is Lipschitz continuous, $D_q(y_r, t)$ can be reformulated as
\[
D_q(y_r, t) = \sum_{k=0}^{q-2} b_{k+1} \int_k^{k+1} \dot{y}_r(t_\xi) d\xi
\]
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 $\dot{y}_r(t) = r_v(t) + (Tb)q_{ex}(t) + (TC)u_{in}(t) - \omega(t)y_r(t)$. 

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

$$D_q(y_r, t) = \sum_{k=0}^{q-2} b_{k+1} \int_k^{k+1} (r_v(t_\xi) + (Tb) q_{ex}(t_\xi) + (TC) u_{in}(t_\xi) - \omega(t_\xi)y_r(t_\xi)) \, d\xi$$

$$\approx r_v(t) + \sum_{k=0}^{q-2} b_{k+1} ((Tb) q_{ex}(t_k) + (TC) u_{in}(t_k) - \omega(t_k)y_r(t_k)),$$

where $t_k := t - \Delta t + k h_s$.

A1: $r_v(t)$ approximately constant on $[t - \Delta t, t]$.
A2: $q_{ex}(t), u_{in}(t)$ and $\omega(t)y_r(t)$ approximately constant on each $[t_k, t_{k+1}]$.

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

$$\hat{r}_v(t) = D_q(\tilde{y}_r, t) - (Tb) W_q(\tilde{q}_{ex}, t) - (TC) W_q(\tilde{u}_{in}, t) + W_q(\tilde{\omega} \tilde{y}_r, t)$$

This approximates $r_v(t)$ for measured quantities and is used to compute $q_{ex}(t)$. 