TRACKING-ERROR-BASED CONTROL OF A CHEMICAL REACTOR USING DECOUPLED DYNAMIC VARIABLE

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Outline

1 Introduction
   - Stabilization problem of continuous stirred tank reactor (CSTR)
   - Control Strategy

2 Preliminaries
   - An overview of port-Hamiltonian representation
   - Tracking-error-based control via quadratic affine PH representation
   - CSTR modeling

3 Main Results
   - Hamiltonian view on the decoupled model of CSTR
   - Controller design
   - Simulations and Discussion

4 Conclusion and Future Work
   - Conclusion
   - Future Work
Motivation, challenges and objective

Consider a first-order reaction system:

\[ v_A A \rightarrow v_B B \]

taking place in a continuous stirred tank reactor (CSTR)

Motivation

The continuous operation via CSTR is common in the industry

Challenges

- High nonlinearity due to reaction kinetics and thermal effects
- Exhibition of multiplicity behavior under certain conditions
- Instability if operated without controller
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Stabilization of the first-order reaction system at desired set point (including unstable-middle steady state)
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Concepts of Reaction Variant/Invariants

- Dynamics of reaction system can be partitioned into 2 parts by a linear transformation: (i) reaction variant (ii) invariant

- Reaction variant:
  - Having the same dimension as the number of linearly independent reactions
  - Containing the information of nonlinear reaction kinetics

- Invariant:
  - Being independent of reaction kinetics
  - Asymptotically converging to origin without control

- These features will ease the control design of tracking-error method in PH representation
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The variants/invariants-based model is derived by a suitable linear transformation.

The transformed model is then formulated into the quadratic affine PH representation.

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Port Hamiltonian (PH) Formulation With Dissipation

Let consider a lumped multivariable nonlinear system

\[
\frac{dx}{dt} = f(x) + g(x)u, \quad x(t = 0) = x_0 \quad \text{and} \quad y = h(x)
\]

where

- \( x = x(t) \) is the state vector in the operating region \( \mathbb{D} \in \mathbb{R}^n \)
- \( f(x) \in \mathbb{R}^n \) expresses the smooth (nonlinear) function with respect to \( x \)
- The input-state map and the control input are represented by \( g(x) \in \mathbb{R}^{n \times m} \) and \( u \in \mathbb{R}^m \) respectively
- \( y \) (or \( h(x) \)) \( \in \mathbb{R}^m \) is the output of the system
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\]

If \( f(x) \) satisfies the \textit{separability condition}, this system can be formulated into \textbf{PH representation}:

\[
\frac{dx}{dt} = \left[ J(x) - R(x) \right] \frac{\partial \mathcal{H}(x)}{\partial x} + g(x)u \quad \text{and} \quad y = g(x)^\top \frac{\partial \mathcal{H}(x)}{\partial x}
\]

where

- \( J(x) = -J^\top(x) \) is the \textit{interconnection matrix}
- \( R(x) = R^\top(x) \geq 0 \) is the \textit{damping matrix}
- The Hamiltonian \( \mathcal{H}(x) : \mathbb{R}^n \rightarrow \mathbb{R} \) is the \textit{storage function}
Let consider a lumped multivariable nonlinear system

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If \(f(x)\) satisfies the **separability condition**, this system can be formulated into **PH representation**:

\[
\frac{dx}{dt} = \left[ J(x) - R(x) \right] \frac{\partial H(x)}{\partial x} + g(x)u \quad \text{and} \quad y = g(x)^\top \frac{\partial H(x)}{\partial x}
\]

**Power-Balance Equation or Dissipation Inequality**

Because \(R(x)\) is positive semi-define, the inequality is fulfilled

\[
\frac{dH(x)}{dt} = -\left[ \frac{\partial H(x)}{\partial x} \right]^\top R(x) \frac{\partial H(x)}{\partial x} + u^\top y \leq u^\top y
\]
The quadratic affine PH Representation

Assume that

- The nonlinear dynamics is rendered into PH with a priori quadratic storage function

\[ \mathcal{H}(x) := \frac{1}{2} x^\top R_d i x \]

- \( x_d \) is a reference trajectory passing through a set-point or containing the desired profile
The quadratic affine PH Representation

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Proposition 1

If the dynamics of $x_d$ is governed by

$$\frac{dx_d}{dt} = \left[ J(x) - R(x) \right] \frac{\partial \mathcal{H}(x_d)}{\partial x_d} + R_I(x) \frac{\partial \mathcal{H}(e)}{\partial e} + g(x)u$$

where

- $e = x - x_d$ is the error state vector
- $\mathcal{H}(e) = \frac{1}{2} e^\top R_{di} e$
- $R_I(x)$ is assigned suitably such that

$$\left( R(x) + R_I(x) \right) = \left( R(x) + R_I(x) \right)^\top > 0$$

then $x$ converge exponentially to $x_d$
Mathematical model

Let reconsider the first-order reaction system $\nu_A A \rightarrow \nu_B B$, taking place in a CSTR.

Under some modeling assumptions, the mathematical model is given

\[
\begin{align*}
\frac{dH}{dt} &= d(H_I - H) + \dot{Q}_J \\
\frac{dN}{dt} &= d(N_I - N) + \nu r_v V
\end{align*}
\]

- $H$ and $H_I$ are the enthalpy of outlet and inlet, respectively
- $d = \frac{F}{V}$ is the dilution rate and $\dot{Q}_J = \lambda(T_J - T)$ is heat exchange
- $N_I = (N_{AI}, N_{BI})^\top$ and $N = (N_A, N_B)^\top$ are the vectors of inlet and outlet molar numbers, respectively
- $\nu = (\nu_A, \nu_B)^\top = (-1, 1)^\top$ is the vector of stoichiometric coefficients
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Proposition 2

The state transformation $\mathcal{M} = \mathcal{I}N$ transforms the reaction system dynamics into reaction variant and reaction invariant dynamics modes

\[
\begin{align*}
\frac{dH}{dt} &= d(H_I - H) + \dot{Q}_J \\
\frac{d\mathcal{M}}{dt} &= d(\mathcal{M}_I - \mathcal{M}) - k(T)\mathcal{M} \\
\frac{d\mathcal{M}}{dt} &= d(\mathcal{M}_I - \mathcal{M})
\end{align*}
\]

where the temperature in the reaction kinetics $k(T)$ is now a nonlinear function of $(H, \mathcal{M}, \mathcal{M})$.
Proposition 2

The reaction-variant/invariant-based model expresses a **quadratic affine port-Hamiltonian** form with $x = (H, \overline{M}, \underline{M})^\top$ as follows,

\[
\frac{dx}{dt} = \left[ J(x) - R(x) \right] \frac{\partial \mathcal{H}}{\partial x} + g(x, u)
\]

- The storage function $\mathcal{H}(x) = \frac{1}{2} x^\top x$ and $g(x, u) = \begin{pmatrix} dH_1 + \dot{Q}_J \\ d\overline{M}_I \\ d\underline{M}_I \end{pmatrix}$

- **Structured matrices:** $R(x) = \text{diag}(d, d + k(T), d)$ and $J(x) = 0_{3 \times 3}$
Reference trajectory $x_d$

- By using Proposition 2, the control design in Proposition 1 can be applied easily.
- Firstly, the representation of the reference trajectory $x_d = (x_{1d}, x_{2d}, x_{3d})$ is derived.

\[
\begin{align*}
\frac{dH_d}{dt} &= -dH_d + R_{I1}(H - H_d) + dH_I + \dot{Q}_J \\
\frac{dM_d}{dt} &= -(d + k)M_d + R_{I2}(M - M_d) + dM_I \\
\frac{d\dot{M}_d}{dt} &= -d\dot{M}_d + R_{I3}(\dot{M} - \dot{M}_d) + d\dot{M}_I
\end{align*}
\]

where $R_{I1}$, $R_{I2}$ and $R_{I3}$ are the positive element of $R_I(x) = \text{diag}(R_{I1}, R_{I2}, R_{I3})$.
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where $R_{I1}$, $R_{I2}$, and $R_{I3}$ are the positive element of $R_I(x) = \text{diag}(R_{I1}, R_{I2}, R_{I3})$.
Secondly, desirable reference trajectories are assigned

\[
\frac{dH_d}{dt} = k_1(H^e - H_d), \quad \frac{dM_d}{dt} = k_2(M^e - M_d), \quad \frac{dM_d}{dt} = k_3(M^e - M_d)
\]

where

- \(k_1, k_2,\) and \(k_3\) are the gains of controller
- \(M^e = (M^{e_A}, M^{e_B}) = T(N^e_A, N^e_B)\) and \((H^e, N^e_A, N^e_B)\) are the desired steady states

Thirdly, internal dynamics of feedback laws are obtained

\[
\begin{align*}
\dot{Q}_I &= k_1(H^e - H_d) + dH_d - R_{I1}(H - H_d) - dH_1 \\
\overline{M}_1 &= \frac{1}{d} \left[ k_2(M^e - M_d) + (d + k)M_d - R_{I2}(M - M_d) \right] \\
\underline{M}_1 &= \frac{1}{d} \left[ k_3(M^e - M_d) + dM_d - R_{I3}(M - M_d) \right]
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\]

\[
\bar{M}_I = \frac{1}{d} \left[ k_3(\bar{M}^e - \bar{M}_d) + d\bar{M}_d - R_{I3}(\bar{M} - \bar{M}_d) \right]
\]
Fourthly, the actual controllers (or the physical input): $T_J$, $N_{AI}$ and $N_{BI}$ can be derived by

$$T_J = T + \frac{1}{\lambda} \dot{Q}_J$$

$$N_I = \mathcal{F}^{-1} \mathcal{M}_I$$

where

- $\mathcal{F}^{-1} = \begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix}$
- $\mathcal{M}_I = (\overline{M}_I, \overline{M}_I)$
All of system trajectories converge exponentially to the point $x^e \equiv P_2$

$\implies$ The system is stabilized in the desired equilibrium point $P_2$
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The dynamics and amplitude of \((T_J, N_{AI}, N_{BI})\) are physically admissible.
Main contributions

- Obtain the reaction-variant/invariant-based model by a linear transformation
- Formulate this transferred model into a quadratic affine PH representation
- Apply the tracking-error-based method in the framework of passivity theory
Future work

- Exploit the model reduction via the reaction variant/invariant for the control design and state reconstruction.

- Extend the proposed control design method to other nonlinear processes.
Thank You for Your Attention