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

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Outline

Motivation, challenges and objective

Consider a first-order reaction system:

$$v_A A \Longrightarrow v_B B$$

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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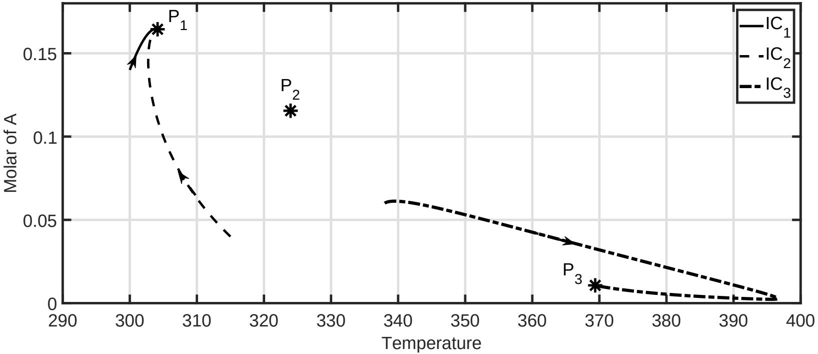

Representation of open-loop phase plan

Objective

Stabilization of the first-order reaction system at desired set point (including unstable-middle steady state)

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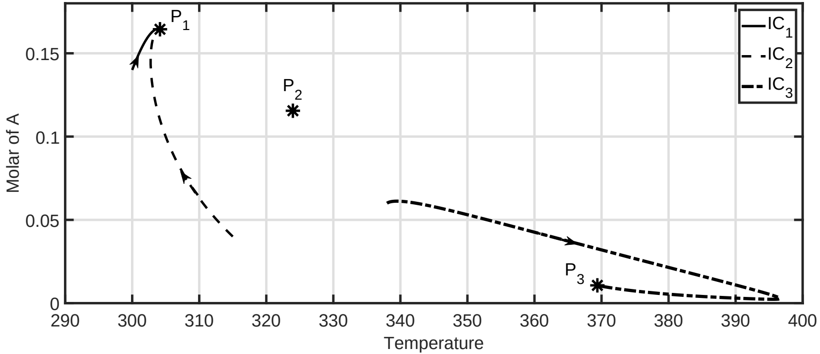

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Concepts of Reaction Variant/Invariants

- 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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Control Scheme

- The variants/invariants-based model is derived by a suitable linear transformation
- The transformed model is then formulated into the quadratic affine PH representation
- The tracking-error-based method is applied to obtain the controllers

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Port Hamiltonian (PH) Formulation With Dissipation

Let consider a lumped multivarible 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 separability condition, this system can be formulated into PH representation:

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

where

- $J(x) = -J^\top(x)$ is the interconnection matrix
- $R(x) = R^\top(x) \geq 0$ is the damping matrix
- The Hamiltonian $\mathscr{H}(x) : \mathbb{R}^n \longrightarrow \mathbb{R}$ is the storage function

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Power-Balance Equation or Dissipation Inequality

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

$$\frac{d\mathcal{H}(x)}{dt} = -\left[\frac{\partial \mathcal{H}(x)}{\partial x}\right]^\top R(x)\frac{\partial \mathcal{H}(x)}{\partial x} + u^\top y \le u^\top y$$

The quadratic affine PH Representation

Assume that

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

$$\mathscr{H}(x) := \frac{1}{2}x^\top R_{di} x$$

- x_d is a reference trajectory passing through a set-point or containing the desired profile

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Tracking-error-based control via PH representation

Proposition 1

If the dynamics of x_d is governed by

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

where

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

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

then x *converge exponentially to* x_d

Mathematical model

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

Under some modeling assumptions, the mathematical model is given

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

- 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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The decoupled model of CSTR

Proposition 2

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

$$\begin{cases} \dfrac{dH}{dt} &= d(H_I - H) + \dot{Q}_J \\ \dfrac{d\overline{\mathscr{M}}}{dt} &= d(\overline{\mathscr{M}}_I - \overline{\mathscr{M}}) - k(T)\overline{\mathscr{M}} \\ \dfrac{d\underline{\mathscr{M}}}{dt} &= d(\underline{\mathscr{M}}_I - \underline{\mathscr{M}}) \end{cases}$$

where the temperature in the reaction kinetics $k(T)$ *is now a nonlinear function of* $(H, \overline{\mathscr{M}}, \underline{\mathscr{M}})$

The decoupled model of CSTR

Proposition 2

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

$$\frac{dx}{dt} = \Big[J(x) - R(x)\Big]\frac{\partial \mathscr{H}}{\partial x} + g(x,u)$$

- *The storage function* $\mathscr{H}(x) = \frac{1}{2}x^\top x$ *and* $g(x,u) = \begin{pmatrix} dH_I + \dot{Q}_J \\ d\overline{\mathscr{M}}_I \\ d\underline{\mathscr{M}}_I \end{pmatrix}$
- *Structured matrices:* $R(x) = diag\Big(d, d + k(T), d\Big)$ *and* $J(x) = \mathbf{0}_{3\times 3}$

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

$$\begin{cases} \frac{dH_d}{dt} & = -dH_d + R_{I1}(H - H_d) + dH_I + \dot{Q}_J \\ \frac{d\overline{\mathscr{M}}_d}{dt} & = -(d+k)\overline{\mathscr{M}}_d + R_{I2}(\overline{\mathscr{M}} - \overline{\mathscr{M}}_d) + d\overline{\mathscr{M}}_I \\ \frac{d\underline{\mathscr{M}}_d}{dt} & = -d\underline{\mathscr{M}}_d + R_{I3}(\underline{\mathscr{M}} - \underline{\mathscr{M}}_d) + d\underline{\mathscr{M}}_I \end{cases}$$

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Internal dynamics of feedback laws

- Secondly, desirable reference trajectories are assigned

$$\frac{dH_d}{dt} = k_1(H^e - H_d), \frac{d\overline{\mathscr{M}}_d}{dt} = k_2(\overline{\mathscr{M}}^e - \overline{\mathscr{M}}_d), \frac{d\underline{\mathscr{M}}_d}{dt} = k_3(\underline{\mathscr{M}}^e - \underline{\mathscr{M}}_d)$$

where
  - k_1, k_2 and k_3 are the gains of controller
  - $\mathscr{M}^e = \left(\overline{\mathscr{M}}^e, \underline{\mathscr{M}}^e\right) = \mathscr{T}(N_A^e, N_B^e)$ and (H^e, N_A^e, N_B^e) are the desired steady states

- Thirdly, internal dynamics of feedback laws are obtained

$$\dot{Q}_J = k_1(H^e - H_d) + dH_d - R_{I1}(H - H_d) - dH_I$$

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The actual control input

- Fourthly, the actual controllers (or the physical input): T_J, N_{AI} and N_{BI} can be derived by

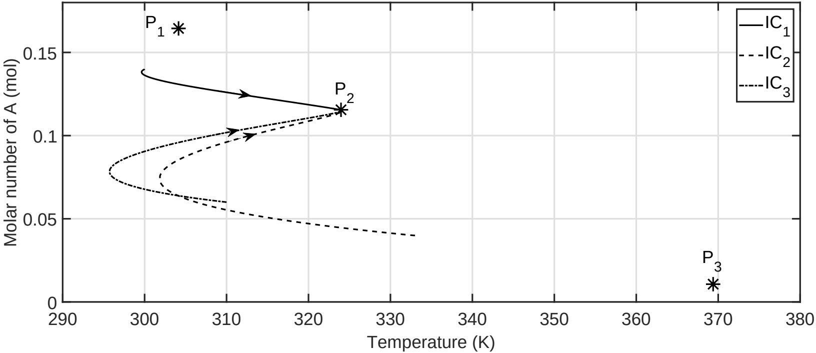
$$T_J = T + \frac{1}{\lambda}\dot{Q}_J$$

$$N_I = \mathscr{T}^{-1}\mathscr{M}_I$$

where

- $\mathscr{T}^{-1} = \begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix}$
- $\mathscr{M}_I = \left(\overline{\mathscr{M}}_I, \underline{\mathscr{M}}_I\right)$

The phase plane of closed-loop system



- All of system trajectories converge exponentially to the point $x^e \equiv P_2$

$\Longrightarrow$ The system is stabilized in the desired equilibrium point P_2

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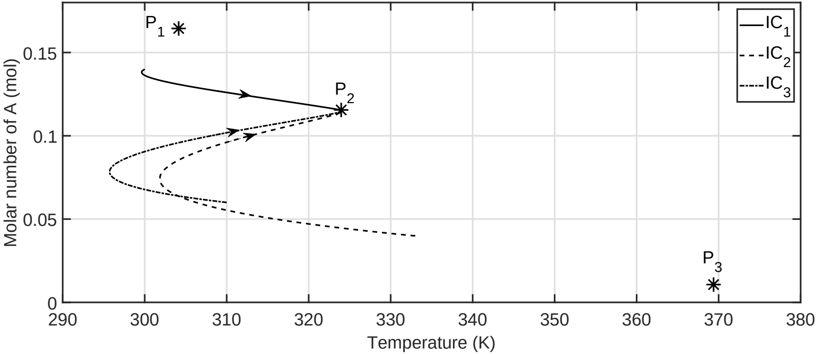

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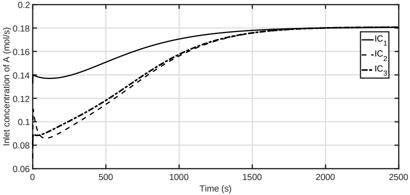
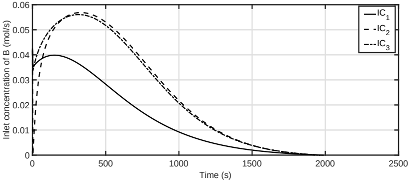
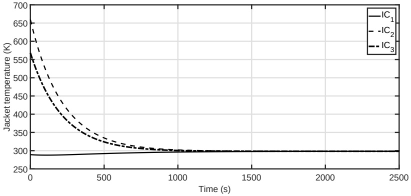
Time variation of manipulated control input



N_{AI}



N_{BI}



T_J

- 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