TI0153 - Trabalho de Conclusão de Curso II Department of Teleinformatics Engineering Federal University of Ceará - UFC

Optimal Control: An application to a non-isothermal continuous reactor

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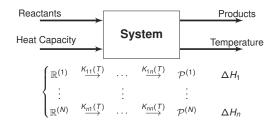
Conclusion



Introduction



- ► We are discussing the automatic control of dynamical systems;
- ▶ We are discussing **chemical reactor network systems**, for processes described as:

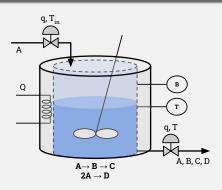


Optimal control theory has been revisited from several innovative fields in the last years [Cairano et al., 2014, Tang et al., 2016, Eren et al., 2017]. Furthermore, reactor systems are subject of active research, with several open challenges [Gupta et al., 2012, Mulas et al., 2015].



The system used for the experiments was the non-isothermal Continuous Stirred Tank Reactor (CSTR) presented by [Klatt and Engell, 1998].

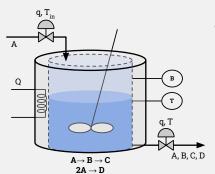
Non-isothermal CSTR





The system used for the experiments was the non-isothermal Continuous Stirred Tank Reactor (CSTR) presented by [Klatt and Engell, 1998].

Non-isothermal CSTR



This system...

- characterizes a wide range of industrial applications;
- is a classical benchmark for multiple-input multiple-output (MIMO) control systems;
- is highly nonlinear, with non-minimum phase behavior and unmeasurable states;



Dynamical System Analysis



Dynamical systems are modelled through the Conservation Laws from physics;

Mass Balance for Chemical Reactors

$$\begin{pmatrix} \text{Accumulation} \\ \text{of mass} \\ \text{in the system} \end{pmatrix} = \begin{bmatrix} \begin{pmatrix} \text{Mass flow} \\ \text{entering} \\ \text{system} \end{pmatrix} + \begin{pmatrix} \text{Mass} \\ \text{produced} \\ \text{by reactions} \end{pmatrix} \end{bmatrix}$$

$$- \begin{bmatrix} \begin{pmatrix} \text{Mass flow} \\ \text{leaving} \\ \text{system} \end{pmatrix} + \begin{pmatrix} \text{Mass} \\ \text{consumed} \\ \text{by reactions} \end{pmatrix} \end{bmatrix}$$

$$(1)$$

Conservation of Energy for Chemical Reactors

$$\begin{pmatrix} \text{Accumulation} \\ \text{of thermal energy} \\ \text{in the system} \end{pmatrix} = \begin{pmatrix} \text{Heat flow} \\ \text{entering} \\ \text{the system} \end{pmatrix} - \begin{pmatrix} \text{Heat flow} \\ \text{leaving} \\ \text{the system} \end{pmatrix} + \begin{pmatrix} \text{Entropy} \\ \text{contribution} \\ \text{from reactions} \end{pmatrix}$$
 (2)



Assuming a continuous reactor of constant volume, comprised by a dilute solution of reactant and products...

Mass Balance for Chemical Reactors

$$\frac{d(\rho_A)}{dt} = q(\rho_{in}^{(A)} - \rho_{out}^{(A)}) + \left(\sum_{\alpha X \to \beta A} \frac{1}{\beta} K_{XA}(T)(\rho_X)^{\alpha}\right) - \left(\sum_{\alpha A \to \beta X} \frac{1}{\beta} K_{AX}(T)(\rho_A)^{\alpha}\right)$$
(3)

Conservation of Energy for Chemical Reactors

$$\begin{cases}
\frac{d(T)}{dt} = q(T_{in} - T_{out}) + \eta(T_C - T) + \delta \sum_{\alpha A \to \beta X} K_{AX}(T)(\rho_A)^{\alpha} \Delta H_{AX} \\
\frac{d(T_C)}{dt} = \gamma Q + \beta (T - T_C)
\end{cases}$$
(4)

► Remark: this model is highly nonlinear!



Linearization by Taylor Series Expansion

Consider a nonlinear time-invariant system:

$$\begin{cases} \dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{u}(t)) \\ \boldsymbol{y}(t) = \boldsymbol{g}(\boldsymbol{x}(t), \boldsymbol{u}(t)) \end{cases}$$
(5)

Given steady-state operating points x_0 , y_0 and u_0 , the dynamics of the system in the neighborhood of these points can be represented by the linear model:

$$\begin{cases} \Delta \dot{\mathbf{x}}(t) = \mathbf{A} \Delta \mathbf{x}(t) + \mathbf{B} \Delta \mathbf{u}(t) \\ \mathbf{y}(t) = \mathbf{C} \Delta \mathbf{x}(t) + \mathbf{D} \Delta \mathbf{u}(t) \end{cases}, \tag{6}$$

where

$$\mathbf{A} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right|_{\mathbf{x}_o, \mathbf{u}_o}; \quad \mathbf{B} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right|_{\mathbf{x}_o, \mathbf{u}_o}; \quad \mathbf{C} = \left. \frac{\partial \mathbf{g}}{\partial \mathbf{x}} \right|_{\mathbf{x}_o, \mathbf{u}_o}; \quad \mathbf{D} = \left. \frac{\partial \mathbf{g}}{\partial \mathbf{u}} \right|_{\mathbf{x}_o, \mathbf{u}_o}$$
(7)

and

$$\Delta \mathbf{x}(t) = \mathbf{x}(t) - \mathbf{x}_{o}; \qquad \Delta \mathbf{u}(t) = \mathbf{u}(t) - \mathbf{u}_{o}. \tag{8}$$



► A linear and time-invariant model in State-Space representation has the form:

$$\begin{cases} \dot{x} = Ax + Bu \\ y = Cx + Du \end{cases} \tag{9}$$

This representation has several analysis and control design advantages...

▶ The response of the system has a practical analytical solution:

$$\begin{cases} \mathbf{x}(t) = \mathbf{e}^{\mathbf{A}(t-t_0)}\mathbf{x}(t) + \int_{t_0}^t \mathbf{e}^{\mathbf{A}(t-\tau)}\mathbf{B}\mathbf{u}(\tau)d\tau \\ \mathbf{y}(t) = \mathbf{C}\mathbf{e}^{\mathbf{A}(t-t_0)}\mathbf{x}(t) + \mathbf{C}\int_{t_0}^t \mathbf{e}^{\mathbf{A}(t-\tau)}\mathbf{B}\mathbf{u}(\tau)d\tau + \mathbf{D}\mathbf{u}(t) \end{cases};$$
(10)

► The controllability property is directly related to the *Controllability Matrix*:

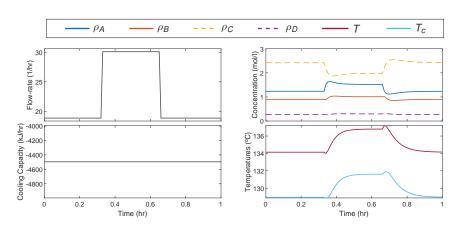
$$C = \begin{bmatrix} \mathbf{B} & \mathbf{A}\mathbf{B} & \mathbf{A}^2\mathbf{B} & \cdots & \mathbf{A}^{n-1}\mathbf{B} \end{bmatrix}; \tag{11}$$

▶ The observability property is directly related to the *Observability Matrix*:

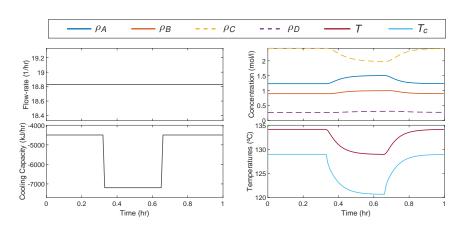
$$\mathcal{O} = \begin{bmatrix} \mathbf{C} & \mathbf{C}\mathbf{A} & \mathbf{C}\mathbf{A}^2 & \cdots & \mathbf{C}\mathbf{A}^{n-1} \end{bmatrix}^T; \tag{12}$$

► The stability of the system is directly related to the eigenvalues of **A**;

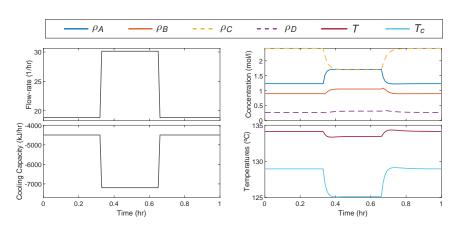




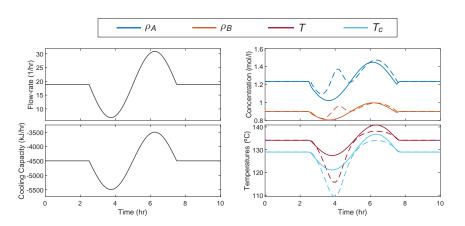














State-Feedback Controllers



Full State-Feedback Controller

Given a linear system in State-Space representation, an input action u(t) is calculated by the linear control law $\pi(\cdot)$ through state-feedback as:

$$\mathbf{u}(t) = \pi(\mathbf{r}(t), \mathbf{x}(t)) = \mathbf{r}(t) - \mathbf{K}\mathbf{x}(t), \tag{13}$$

where $r : \mathbb{R} \to \mathbb{R}^n$ is a state reference signal that the system must follows and $K \in \mathbb{R}^{r \times n}$ is the feedback gain matrix.



Full State-Feedback Controller

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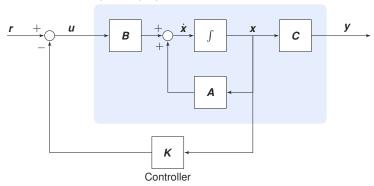
where $r : \mathbb{R} \to \mathbb{R}^n$ is a state reference signal that the system must follows and $K \in \mathbb{R}^{r \times n}$ is the feedback gain matrix.

Pole-Placement Property

If a system in State-Space representation is controllable, then by state feedback using a gain matrix $K \in \mathbb{R}^{r \times n}$ the eigenvalues of $A_{cl} = A - BK$, the poles of the closed-loop system, can be placed arbitrarily in the complex plane, as long as complex conjugate eigenvalues are assigned in pairs.



Open-Loop System



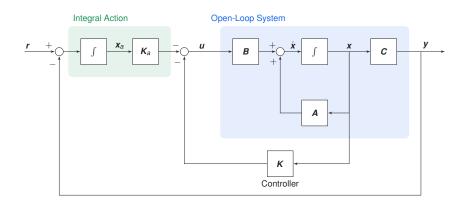


During the semester, we have discussed Conservation Laws of fluid elements...

Conservation of Mass

$$\begin{pmatrix} \text{Time rate of} \\ \text{change of mass} \\ \text{in the system} \end{pmatrix} = \begin{pmatrix} \text{Mass} \\ \text{entering} \\ \text{the system} \end{pmatrix} - \begin{pmatrix} \text{Mass} \\ \text{leaving} \\ \text{the system} \end{pmatrix}$$







Optimal Control



Optimal Controller

Given a system in State-Space formulation, with state signal $\mathbf{x}: \mathbb{R} \to \mathbb{R}^n$, and a reference signal $\mathbf{r}: \mathbb{R} \to \mathbb{R}^n$, the input signal $\mathbf{u}(t) \in \mathbb{R}^r$, for any time t, is optimal if an optimal control law $\pi^*: \mathbb{R}^{n \times n \times 1} \to \mathbb{R}^r$ can be found as:

$$\boldsymbol{u}(t) = \pi^*(\boldsymbol{x}, \boldsymbol{r}, t) = \min_{\boldsymbol{u}} J(\boldsymbol{x}, \boldsymbol{r}, t), \tag{15}$$

where $J: \mathbb{R}^{n \times n \times 1} \to \mathbb{R}$ is known as a *cost function* of the states and reference signals.



Optimal Controller

Given a system in State-Space formulation, with state signal $\mathbf{x}: \mathbb{R} \to \mathbb{R}^n$, and a reference signal $\mathbf{r}: \mathbb{R} \to \mathbb{R}^n$, the input signal $\mathbf{u}(t) \in \mathbb{R}^r$, for any time t, is optimal if an optimal control law $\pi^*: \mathbb{R}^{n \times n \times 1} \to \mathbb{R}^r$ can be found as:

$$\boldsymbol{u}(t) = \pi^*(\boldsymbol{x}, \boldsymbol{r}, t) = \min_{\boldsymbol{u}} J(\boldsymbol{x}, \boldsymbol{r}, t), \tag{16}$$

where $J: \mathbb{R}^{n \times n \times 1} \to \mathbb{R}$ is known as a *cost function* of the states and reference signals.

Finite-Horizon Optimal Regulators

A Finite-Horizon Optimal Regulator is defined as any controller whose optimal policy over a time interval $t \in [t_0, T]$ minimizes the cost functional:

$$J(\boldsymbol{x}, \boldsymbol{u}, t_0) = \int_{t_0}^{T} I(\boldsymbol{x}, \boldsymbol{u}, \tau) d\tau + I_f(\boldsymbol{x}, T),$$
(17)

where $I(\cdot): \mathbb{R}^{n \times r \times 1} \to \mathbb{R}$ and $I_f(\cdot): \mathbb{R}^n \to \mathbb{R}$ are, respectively, the *trajectory* and *terminal loss functions*. In the case that $I_0 = 0$, T is also known as the *control horizon*.



Hamilton-Jacobi-Bellman Equation

Consider a finite-horizon cost function for a system described by $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}, t)$:

$$V(\mathbf{x}, \mathbf{u}, t_0) = \int_{t_0}^{T} l(\mathbf{x}, \mathbf{u}, \tau) d\tau + l_f(\mathbf{x}(T))$$
(18)

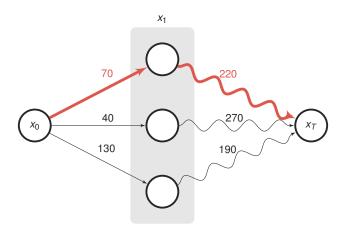
Consider also that the loss $I(\cdot)$ and state function f are smooth on their parameters. Then, minimizing any functional in the form of $V(\cdot)$ is equivalent to determining the solution of the *Hamilton-Jacobi equation*, which is given by the partial differential equation:

$$\frac{\partial V^*}{\partial t} = -\min_{u(t)} \left[I(\mathbf{x}, \mathbf{u}, t) + \left[\frac{\partial V^*}{\partial x} \right]^T \mathbf{f}(\mathbf{x}, \mathbf{u}, t) \right]$$
(19)

and the boundary condition:

$$V^*(\mathbf{x},T) = I_f(\mathbf{x}(T)). \tag{20}$$







Linear Quadratic Regulator (LQR)

Given a linear State-Space system in the form:

$$\begin{cases} \dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \\ \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t) \end{cases}$$
(21)

A *Linear Quadratic Regulator* (LQR) for this system is an optimal controller defined by the quadratic cost function:

$$J(\mathbf{x}, \mathbf{u}, t_0) = \int_{t_0}^{T} \left(\mathbf{x}^{T} \mathbf{Q} \mathbf{x} + \mathbf{u}^{T} \mathbf{R} \mathbf{u} \right) dt + \mathbf{x}^{T} (T) \mathbf{Q}_{f} \mathbf{x} (T),$$
(22)

where is assumed that $\mathbf{Q}, \mathbf{Q}_f \succ 0$ and $\mathbf{R} \succ 0$ are matrices penalizing, respectively, the state-vector magnitude and the control effort.



LQR Control Action from Dynamic Programming

Given a Linear Quadratic Regulator, the optimal action produced by this optimal controller at any time $t \in [t_0, T]$ is given by:

$$\mathbf{u}^*(t) = -\mathbf{R}^{-1}\mathbf{B}^T\mathbf{P}(t)\mathbf{x}(t), \tag{23}$$

where P(t) is the solution of the matrix Riccati differential equation:

$$-\dot{\mathbf{P}}(t) = \mathbf{A}^T \mathbf{P}(t) + \mathbf{P}(t)\mathbf{A} - \mathbf{P}(t)\mathbf{B}\mathbf{R}^{-1}\mathbf{B}^T \mathbf{P}(t) + \mathbf{Q},$$
 (24)

with terminal condition $P(T) = Q_f$.



LQR with Integral Action

Given a linear State-Space system represented by matrices $(\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D})$, augmented with state $\dot{\mathbf{x}}_a(t) = \mathbf{r}(t) - \mathbf{C}\mathbf{x}(t)$:

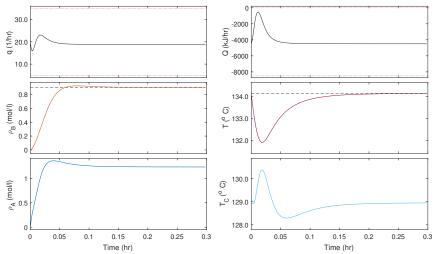
$$\begin{cases}
\begin{bmatrix}
\dot{\mathbf{x}}(t) \\
\dot{\mathbf{x}}_{a}(t)
\end{bmatrix} &= \underbrace{\begin{bmatrix} \mathbf{A} & \mathbf{0} \\ -\mathbf{C} & \mathbf{0} \end{bmatrix}}_{\tilde{\mathbf{A}}} \underbrace{\begin{bmatrix} \mathbf{x}(t) \\ \mathbf{x}_{a}(t) \end{bmatrix}}_{\tilde{\mathbf{x}}(t)} + \underbrace{\begin{bmatrix} \mathbf{B} \\ \mathbf{0} \end{bmatrix}}_{\tilde{\mathbf{B}}} \mathbf{u}(t) + \begin{bmatrix} \mathbf{0} \\ \mathbf{I} \end{bmatrix} \mathbf{r}(t) \\
\mathbf{y}(t) &= \begin{bmatrix} \mathbf{C} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{x}(t) \\ \mathbf{x}_{a}(t) \end{bmatrix}
\end{cases} \tag{25}$$

A *Linear Quadratic Servo* (LQ-Servo) for this system is an optimal controller defined by the quadratic cost function:

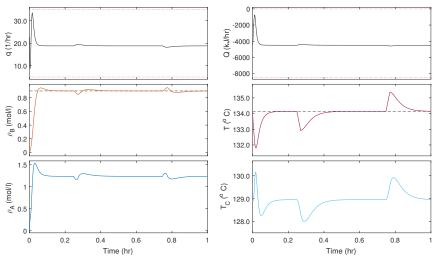
$$J(\mathbf{x}, \mathbf{u}, t_0) = \int_{t_0}^{T} \left(\tilde{\mathbf{x}}^T \tilde{\mathbf{Q}} \tilde{\mathbf{x}} + \mathbf{u}^T \mathbf{R} \mathbf{u} \right) dt + \tilde{\mathbf{x}} \tilde{\mathbf{Q}}_t \tilde{\mathbf{x}}(T),$$
(26)

where is assumed that $\tilde{\mathbf{Q}}$, $\tilde{\mathbf{Q}}_f \succ 0$ and $\mathbf{R} \succ 0$ are matrices penalizing, respectively, the state-vector magnitude and the control effort.

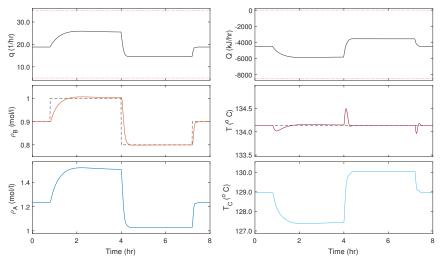




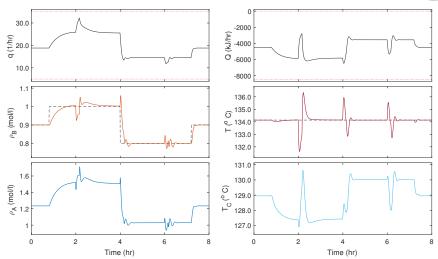














Optimal State Estimation



Closed-Loop Observer

Given a system in State-Space with output signal $y(t): \mathbb{R} \to \mathbb{R}^p$ and an observer gain $L \in \mathbb{R}^{n \times p}$, the estimated state-vector $\hat{x}(t)$ is represented by the system:

$$\dot{\hat{\mathbf{x}}}(t) = \mathbf{A}\hat{\mathbf{x}}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{L}(\mathbf{y}(t) - \mathbf{C}\hat{\mathbf{x}}(t)), \tag{27}$$

or, equivalently:

$$\dot{\hat{\mathbf{x}}}(t) = (\mathbf{A} - \mathbf{LC})\,\hat{\mathbf{x}}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{L}\mathbf{y}(t). \tag{28}$$

- The observer system works as a parallel system that is simulated alongside the actual system;
- ► Alternatively, it is possible to create a variable $\mathbf{e}(t) = \mathbf{x}(t) \hat{\mathbf{x}}(t)$ such that:

$$\dot{\mathbf{e}} = \mathbf{x} - \hat{\mathbf{x}}
= (\mathbf{A} - \mathbf{LC})(\mathbf{x} - \hat{\mathbf{x}})
= (\mathbf{A} - \mathbf{LC})\mathbf{e},$$
(29)

implying that the observer tracks the actual state-vector if $\mathbf{e}(t) = \mathbf{0}$ as $t \to \infty$.

Formulation
Kalman Filter and LQG Controllers
Simulations



Pole-Placement Property of Observers

If a system in State-Space representation is observable, then by a closed-loop observer with gain matrix $\boldsymbol{L} \in \mathbb{R}^{n \times p}$ the eigenvalues of $\boldsymbol{A}_{obs} = \boldsymbol{A} - \boldsymbol{L}\boldsymbol{C}$ can arbitrarily be assigned anywhere in the complex plane, as long as that complex conjugate eigenvalues are assigned in pairs.

▶ a

Optimal State Estimation

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The Separation Principle

Given a system in State-Space with a Luenberger observer of gain L and state-feedback controller of gain K, the closed-loop eigenvalues contributions of (A - BK) are independent from those of (A - LC).

▶ a



Kalman-Bucy Optimal Filter

Consider a continuous-time State-Space linear system subject to additive process noise variable $\mathbf{w}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}_{kf})$ and measurement noise variable $\mathbf{v}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{R}_{kf})$, where the covariances $\mathbf{Q}_{kf} \in \mathbb{R}^{n \times n}$ and $\mathbf{R}_{kf} \in \mathbb{R}^{p \times p}$ represents the *power spectral density* of the noises. In this case, for an estimated state $\bar{\mathbf{x}}(t)$ at time t, the error covariance:

$$\boldsymbol{J}(\boldsymbol{x}, \bar{\boldsymbol{x}}, t) = \mathbb{E}\left\{ [\boldsymbol{x}(t) - \bar{\boldsymbol{x}}(t)][\boldsymbol{x}(t) - \bar{\boldsymbol{x}}(t)]^{T} \right\}$$
(30)

is minimized by $\bar{x}(t)$ obtained through the system:

$$\dot{\bar{\mathbf{x}}}(t) = \mathbf{A}\bar{\mathbf{x}}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{K}_{\theta}(t)\left(\mathbf{y}(t) - \mathbf{C}\bar{\mathbf{x}}(t)\right),\tag{31}$$

where $K_e(t) = P_e(t)CR^{-1}$, being $P_e(t)$ the solution of the Riccati differential matrix equation:

$$\dot{\boldsymbol{P}}_{e}(t) = \boldsymbol{A}\boldsymbol{P}_{e}(t) + \boldsymbol{P}_{e}(t)\boldsymbol{A}^{T} - \boldsymbol{P}_{e}(t)\boldsymbol{C}^{T}\boldsymbol{R}_{kf}^{-1}\boldsymbol{C}\boldsymbol{P}_{e}(t) + \boldsymbol{Q}_{kf}, \tag{32}$$

with initial condition $P_e(t_0) = \mathbb{E}\left\{ [\boldsymbol{x}(t_0) - \bar{\boldsymbol{x}}(t_0)][\boldsymbol{x}(t_0) - \bar{\boldsymbol{x}}(t_0)]^T \right\}$ for $t_0 > -\infty$.



Linear Quadratic Gaussian (LQG) Controller

Consider a stochastic system in State-Space representation:

$$\begin{cases} \dot{\boldsymbol{x}}(t) &= \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{w}(t) \\ \boldsymbol{y}(t) &= \boldsymbol{C}\boldsymbol{x}(t) + \boldsymbol{v}(t) \end{cases}, \tag{33}$$

whose estimated state-vector $\hat{\boldsymbol{x}}(t)$ is determined by a Kalman-Bucy filter and whose optimal input signal $\boldsymbol{u}(t)$ is calculated through a finite-horizon LQR. The Linear Quadratic Gaussian (LQG) control for the horizon $t \in [t_0, T]$, with $-\infty < t_0 \le T < \infty$, is defined as:

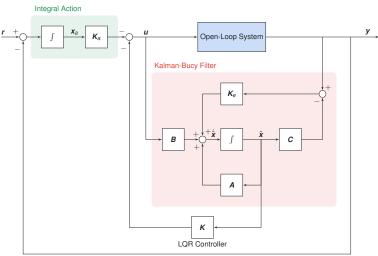
$$\hat{\mathbf{x}}(t) = [\mathbf{A} - \mathbf{K}_{\theta}(t)\mathbf{C} - \mathbf{B}\mathbf{K}(t)]\,\hat{\mathbf{x}}(t) + \mathbf{K}_{\theta}(t)\mathbf{y}(t),\tag{34}$$

where $K(t) = \mathbf{R}^{-1}\mathbf{B}^{T}\mathbf{P}(t)$ and $K_{e}(t) = \mathbf{P}_{e}(t)\mathbf{C}\mathbf{R}^{-1}$ are, respectively, the LQR and Kalman-Bucy gains for matrices $\mathbf{P}(t)$ and $\mathbf{P}_{e}(t)$ that solve the Riccati differential equations:

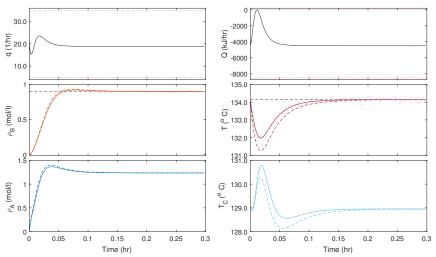
$$\begin{cases} -\dot{\boldsymbol{P}}(t) = \boldsymbol{A}^T \boldsymbol{P}(t) + \boldsymbol{P}(t) \boldsymbol{A} - \boldsymbol{P}(t) \boldsymbol{B} \boldsymbol{R}^{-1} \boldsymbol{B}^T \boldsymbol{P}(t) + \boldsymbol{Q} \\ \dot{\boldsymbol{P}}_{e}(t) = \boldsymbol{A} \boldsymbol{P}_{e}(t) + \boldsymbol{P}_{e}(t) \boldsymbol{A}^T - \boldsymbol{P}_{e}(t) \boldsymbol{C}^T \boldsymbol{R}_{kf}^{-1} \boldsymbol{C} \boldsymbol{P}_{e}(t) + \boldsymbol{Q}_{kf} \end{cases}$$
(35)

for boundary conditions $P(T) = Q_f$ and $P_{\theta}(t_0) = \mathbb{E}\left\{ [\mathbf{x}(t_0) - \bar{\mathbf{x}}(t_0)][\mathbf{x}(t_0) - \bar{\mathbf{x}}(t_0)]^T \right\}$, respectively.

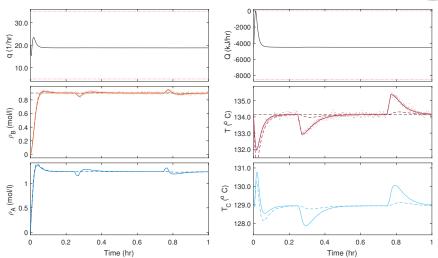




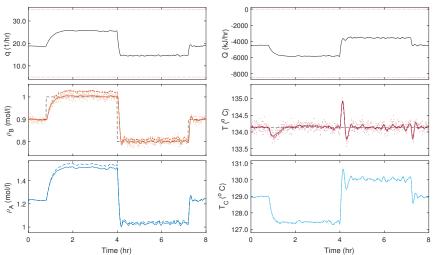




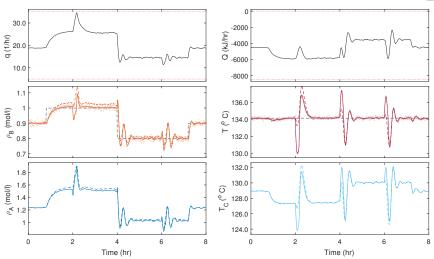
















- ▶ Past;
- ► Present;
- ► Future;

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