

Homework 05 – Receding-horizon estimation of process systems

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Problem Setup

An isothermal CSTR implements two reversible reactions in gas phase (Figure 1). Using mass balance, the dynamics of the concentrations c_A , c_B , and c_C [mol/L] are modelled according to the nonlinear state-space

$$\frac{d}{dt}c_A(t) = -\kappa_1 c_A(t) + \kappa_{-1} c_B(t) c_C(t) \quad (1a)$$

$$\frac{d}{dt}c_B(t) = \kappa_1 c_A(t) - \kappa_{-1} c_B(t) c_C(t) - 2\kappa_2 c_B(t)^2 + 2\kappa_{-2} c_C(t) \quad (1b)$$

$$\frac{d}{dt}c_C(t) = \kappa_1 c_A(t) - \kappa_{-1} c_B(t) c_C(t) + \kappa_2 c_B(t)^2 - \kappa_{-2} c_C(t) \quad (1c)$$

with kinetic rates $\kappa_1 = 0.50$, $\kappa_{-1} = 0.05$, $\kappa_2 = 0.20$, and $\kappa_{-2} = 0.01$. The reactor is assumed to be equipped with a pressure sensor measuring the pressure y [mol] as

$$y = RT(c_A + c_B + c_C) \quad (2)$$

in which R is the gas constant and T is the temperature of the reactor, with $RT = 32.84$ mol atm/L. Note that the reactor has no influent feedstock.

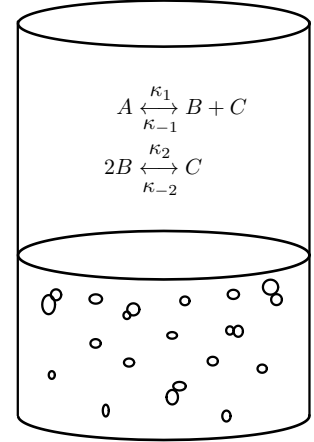


Figure 1. Process layout.

Using control notation, the state signal is $x = (x_1, x_2, x_3) = (c_A, c_B, c_C)$ and there are no controls, that is, $u(t) = 0$. In this homework, you will estimate the state of the system in real-time. Rewrite the model in Eq. (1a)-(1b) using the control notation to have it in the form $\frac{d}{dt}x(t) = f(x(t), u(t))$, then solve the following tasks:

Task 1. (10 points) Design a receding-horizon estimation policy based on the linearization of the model (Eq. 1–2) around the steady-state $x_{\text{ref}} = (0.0121, 0.1824, 0.6656)$. The disturbances/noise are modelled as

$$w[k] \sim \mathcal{N}(0, \Delta t \cdot \sigma_w^2 I), \quad v[k] \sim \mathcal{N}(0, \sigma_v^2)$$

with standard deviations $\sigma_w = 0.002$ and $\sigma_v = 0.25$. Consider a measurement frequency of $1/\Delta t = 4$ Hz and the estimation horizon $T_e = 15$ s (meaning that the estimator uses $N_e = T_e/\Delta t = 60$ data points).

Task 2. (10 points) Simulate the process under the estimation policy $\hat{x}[n] = x_{\text{ref}} + K_{\text{RHE}}(\mathbf{y}_n^{\text{data}} - y_{\text{ref}})$ for a simulation horizon $T_{\text{sim}} = 50$ s, given initial state $x[0] = (0.50, 0.05, 0.00)$. **Comment on the results.** Do the estimates converge to the true state? What happens if $\sigma_w = 0.01$? What component is the easiest/hardest to estimate?

Hint: Initialize the measurement data batch as $\mathbf{y}^{\text{data}} = (x_{\text{ref}}, \dots, x_{\text{ref}})$. It is normal to get poor estimation for $t < T_e$.