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Closed loop optimal experiment design for on-line parameter estimation

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- The OED usually separates parameter identification from the optimal input design (offline identification).
- Most applications of OED are reliable on linear or approximated linearized models.
- Recently, the coupled online OED techniques and parameter estimation has been developed for open loop stable systems without input/output process constraint. (Jayasankar et al. [2010], Zhu and Huang [2011])

Outline of the proposed approach

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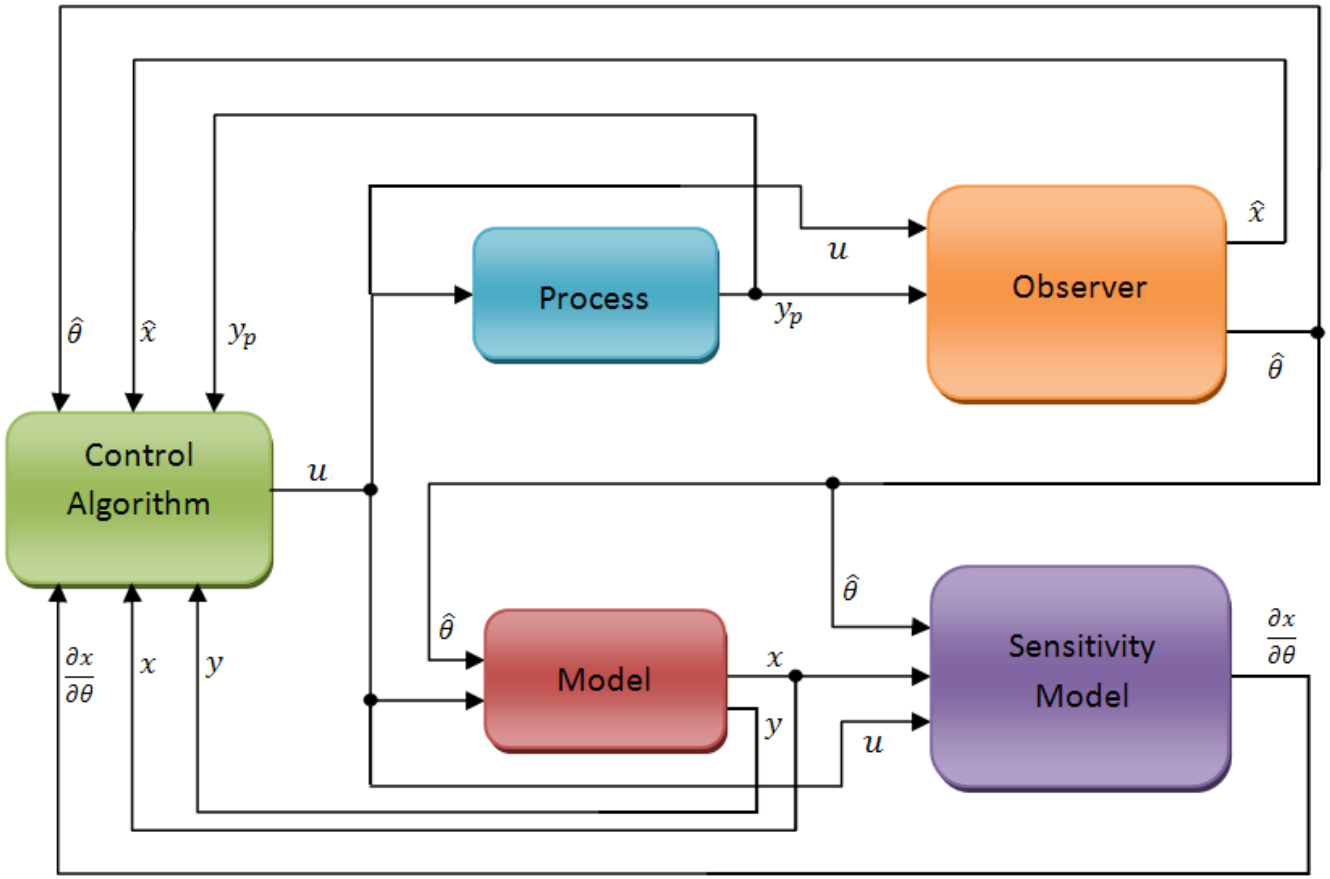
- Input and output constraints may be specified to keep the process in a desired operating zone.

Closed loop control structure



The components

Process

Must have:

- a dynamic behaviour;
- at least one on-line output measure $y_p(t)$;
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Model (linear or nonlinear)

$$(M)\begin{cases} \dot{x}(t) &= f(x(t),\theta,u(t)) \\ y(t) &= h(x(t),\theta,u(t)) \end{cases} \quad (1)$$

where $x \in \mathbb{R}^n$ is the state vector, $y \in \mathbb{R}^p$ is the output vector, $u \in \mathcal{U} \subset \mathbb{R}^m$ is the input vector, $\theta \in \mathbb{R}^q$ is the unknown constant parameters vector. f and h are nonlinear functions of suitable dimensions.

Assumptions

1. In this study, the unknown model parameters are all constant.
2. In the system (1), f and h are C^∞ w.r.t. their arguments.

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Observer design for augmented system

System augmented with the unknown constant model parameters.

$$(M_a)\begin{cases} \dot{x}(t) &= f(x(t),\theta(t),u(t)) \\ \dot{\theta} &= 0 \\ y(t) &= h(x(t),\theta(t),u(t)) \end{cases} \tag{2}$$

The augmented state vector $x_a = [x\ \theta]^T$ and the vector function $f_a = [f\ 0]^T$

Observer definition

A global observer for system (13) can be given by

$$(O)\begin{cases} \dot{\hat{x}}_a(t) = f_a(\hat{x}_a(t),u(t)) + g_a(t, h(\hat{x}_a(t),u(t)) - y_p(t)) \\ \text{with: } g_a(t,0) = 0, \end{cases} \tag{3}$$

such that
i) if $\hat{x}_a(0) = x_a(0)$, then $\hat{x}_a(t) = x_a(t), \quad \forall t \geq 0$;
ii) if $\forall x_a(0),\ \forall \hat{x}_a(0)$, then $\lim_{t\to+\infty} \|\hat{x}_a(t) - x_a(t)\| = 0$,
where g_a is a function of the output estimation error to be designed.

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Sensitivity model

Using the definition of the sensitivity function $(\cdot)_\theta = \frac{\partial(\cdot)}{\partial\theta}$ of a variable $(\cdot)$ with respect to the parameters θ, and the dynamical model (M), we give the sensitivity model as follows

$$(M_\theta)\begin{cases} \dot{x}_\theta(t) &= \dfrac{\partial f(x(t),\theta,u(t))}{\partial x}x_\theta + \dfrac{\partial f(x(t),\theta,u(t))}{\partial\theta} \\ y_\theta(t) &= x_\theta(t), \end{cases} \tag{4}$$

where $x_\theta \in R^{n\times q}$ and $y_\theta \in R^{n\times q}$ are the matrices of sensitivities of the states (the outputs) with respect to the parameters.

The relative-sensitivity function

$$\begin{cases} \bar{x}_\theta(i,j) &= \dfrac{\theta_j}{x_i}x_\theta(i,j); \quad i=1,\cdots,n; j=1,\cdots,q \\ \bar{y}_\theta(i,j) &= \dfrac{\theta_j}{y_i}y_\theta(i,j); \quad i=1,\cdots,p; j=1,\cdots,q. \end{cases} \tag{5}$$

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  - many theoretical papers published
  - +4000 applications in the world (Qin and Badgwell [2003])
- Idea:
  - use the model to predict the future process behavior
  - optimize any specified criteria
  - take account for constrains on measures/estimations
  - closed loop control approach

Optimal control law design

- Time discretization: $t = k \times T_s$ (k =current time index)
- At each k, over the prediction horizon N_p: maximize the norm of the sensitivity $\frac{\partial y_p}{\partial \theta}$ to get "rich" data for parameter identification.

Sensitivity matrix

$$\bar{y}_{\theta\, l|k} = \begin{bmatrix} \bar{y}_\theta(1,1)|_{l|k} & \bar{y}_\theta(1,2)|_{l|k} & \dots & \bar{y}_\theta(1,q)|_{l|k} \\ \bar{y}_\theta(2,1)|_{l|k} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \bar{y}_\theta(p,1)|_{l|k} & \dots & \dots & \bar{y}_\theta(p,q)|_{l|k} \end{bmatrix}. \tag{6}$$

which gives at the current instant k the prediction at a future time $l \leq k$ ($l \in [k\ k+N_p]$) of the normalized outputs sensitivity $\bar{y}_\theta$.

Fisher Information Matrix (FIM)

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- Cost function

$$\begin{cases} F(\bar{y}_{\theta l|k}, u_{l|k}, y_p(k), \hat{x}_a(k)) = \frac{1}{N_p} \sum_{l=k+1}^{k+N_p} M_{l|k} \\ u_{l|k} = \{u(k) \dots u(l) \dots u(k+N_p)\}, l \in [k \ k+N_p]. \end{cases} \quad (8)$$

- E-optimality

$$\begin{cases} u^*_{l|k} = & arg\max_{u_{l|k}} \left(J(u_{l|k}) = \frac{\lambda_{min}(F)}{\lambda_{max}(F)} \right) \\ u_{l|k} = & \{u(k) \dots u(l) \dots u(k+N_p)\}, l \in [k \ k+N_p]. \end{cases} \quad (9)$$

- Handling specified constraints:
  - Constraints on the inputs (physical limitations of the actuator):

$$u_{min} \leq u(k) \leq u_{max}, \ \forall k \quad (10)$$

    Velocity constraints may also be added.
  - Constraints on the estimated states and/or the measured outputs (dealing with safety, operating zone, production, ...):

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The nonlinear model of CSTR

The nonlinear dynamic model of the process is:

$$\begin{cases} \dot{c_A}(t) = \frac{q}{V}(c_A^f - c_A(t)) - k_0 exp\left(-\left(\frac{E}{R}\right)/T(t)\right) c_A(t) \\ \dot{T}(t) = \frac{q}{V}(T_f - T(t)) + \frac{\Delta H}{\rho C_p} k_0 exp\left(-\left(\frac{E}{R}\right)/T(t)\right) c_A + \frac{UA}{\rho V C_p}(T_c - T(t)) \end{cases} \tag{12}$$

where:

- The concentration of component A, c_A, and the reactor temperature, T, are the two states x and the two measured outputs y.
- The temperature of cooling jacket T_c is the manipulated input.
- The vector of unknown parameter θ is $[1/\rho,\ k_0]$.
- Input constraints: $250K \leqslant T_c(k) \leqslant 320K$, $\forall k$.
- Output constraints: $c_A(k) \leqslant 0.95 mol/m^3$

Objective: based on (12) online identify the two unknowns parameters.
(more development details on appendix)

Simulation results

- Input applied: $u(t)$
- Process output: $y_{p1}(t)$
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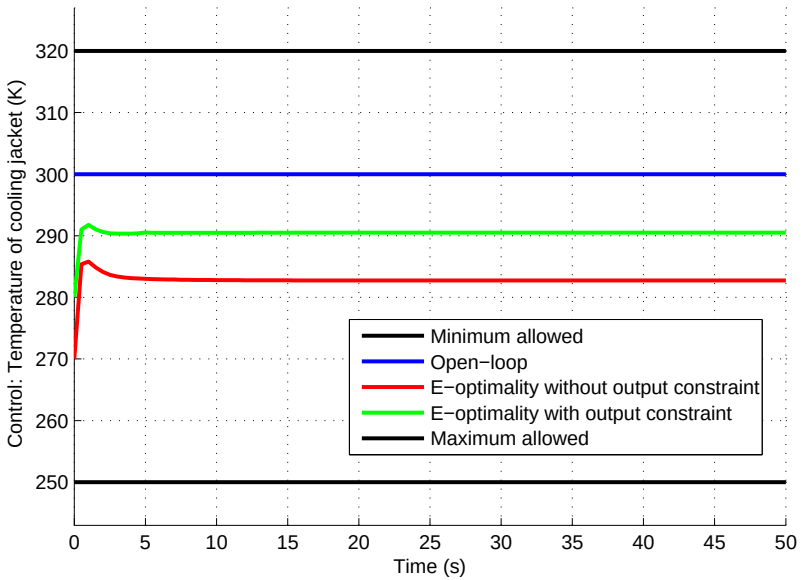

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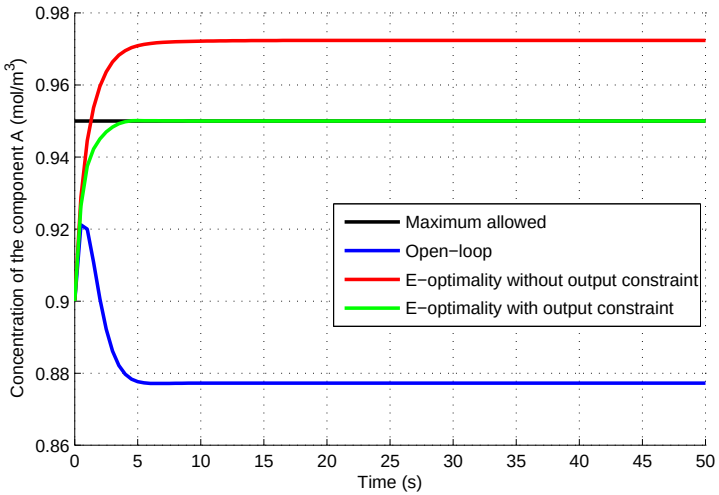

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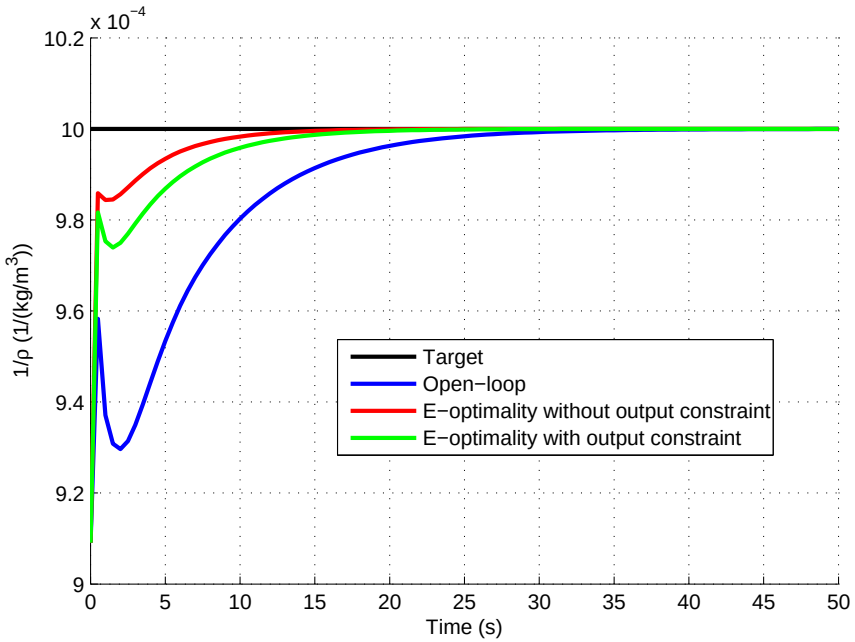

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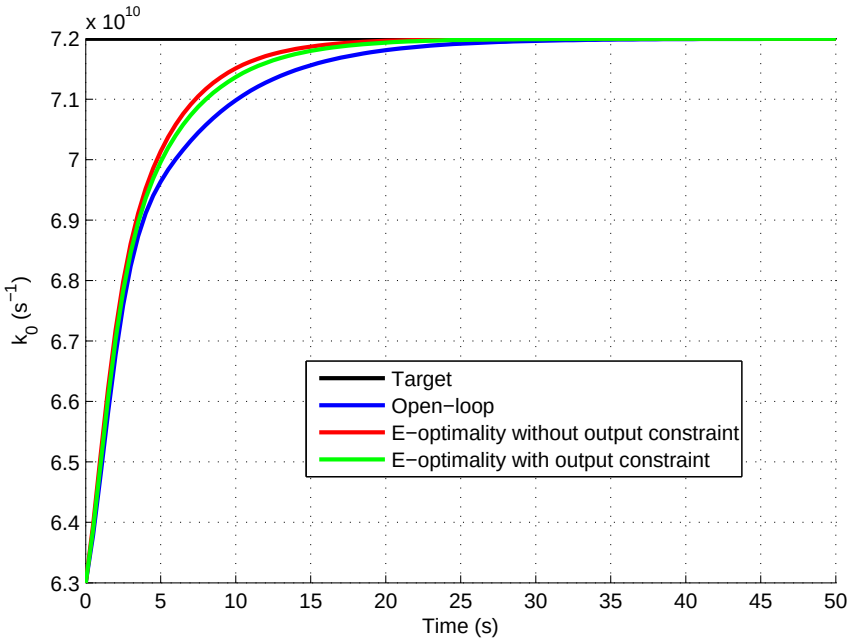

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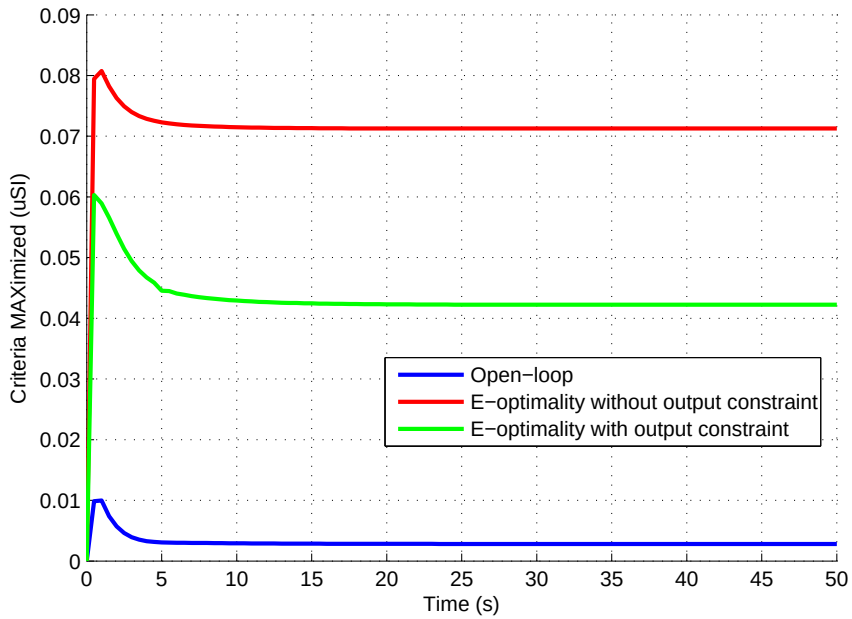

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- The proposed approach may be adapted and tuned for any user defined dynamic model.

Contacts and discussion

Software

- MPC@CB (Model Predictive Control)
  Email: MPCatCB@univ-lyon1.fr; Website: http://mpcatcb.univ-lyon1.fr/
- ODOE4OPE (Optimal Design Of Experiments for Online Parameter Estimation)
  Email: odoe4ope@univ-lyon1.fr; Website: http://odoe4ope.univ-lyon1.fr/

Business contacts

- Acsysteme: Expertise in automation, signal processing, optimization, software developing, ...
  Website: http://www.acsysteme.com/en/
- LAGEP: Laboratory of Process Control and Chemical Engineering
  Website: http://www-lagep.univ-lyon1.fr

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Annex: CSTR

Table : CSTR: known model parameters.

Parameter (units)	Symbol	Value
Volumetric flowrate (m^3/s)	q	100
Volume of CSTR (m^3)	V	100
Heat capacity of A-B mixture (J/kgK)	C_p	0.239
Heat of reaction for A-B (J/mol)	ΔH	5×10^4
- (W/K) U: overall heat transfer coefficient (W/m^2K)	UA	5×10^4
A: Area, this value is specific for the U calculation (m^2)		
Feed concentration (mol/m^3)	c_a^f	1
Feed temperature (K)	T^f	350
Exponential factor (K), E: Activation energy in the Arrhenius equation (J/mol), R: Universal gas constant $(J/mol/K)$, 8.31451	$\frac{E}{R}$	8750

Table : CSTR: target for the unknown model parameters.

Parameter (units)	Symbol	Initial Value	Target Value
Density of A-B mixture (kg/m^3)	ρ	1100	1000
Pre-exponential factor (s^{-1})	k_0	6.3×10^{10}	7.2×10^{10}

Annex: CSTR

- Augmented system:

$$(M_a)\begin{cases} \dot{x}_1(t) = \alpha_1(\alpha_2 - x_1(t)) - x_4(t)exp(\frac{\alpha_3}{x_2(t)})x_1(t) \\ \dot{x}_2(t) = \alpha_1(\alpha_4 - x_2(t)) + \alpha_5 x_4(t)x_3(t)exp(\frac{\alpha_3}{x_2(t)})x_1(t) + \alpha_6 x_3(t)(u(t) - x_2(t)) \\ \dot{x}_3(t) = 0 \\ \dot{x}_4(t) = 0 \\ y(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} \end{cases} \tag{13}$$

- Two interconnected subsystems:

$$\begin{cases} \dot{x}_1(t) = \alpha_1(\alpha_2 - x_1(t)) - x_4(t)exp(\frac{\alpha_3}{x_2(t)})x_1(t) \\ \dot{x}_4(t) = 0 \\ y_1(t) = x_1(t) \end{cases} \tag{14}$$

$$\begin{cases} \dot{x}_2(t) = \alpha_1(\alpha_4 - x_2(t)) + \alpha_5 x_4(t)x_3(t)exp(\frac{\alpha_3}{x_2(t)})x_1(t) + \alpha_6 x_3(t)(u(t) - x_2(t)) \\ \dot{x_3}(t) = 0 \\ y_2(t) = x_2(t) \end{cases} \tag{15}$$

Annex: CSTR

- Form general of two subsystems:

$$\begin{cases} \dot{X}_1 = A_1(u, y_1, \alpha, X_2)X_1 + \varphi_1(u, y_1, \alpha, X_1, X_2) \\ y_1 = C_1 X_1 \end{cases} \tag{16}$$

$$\begin{cases} \dot{X}_2 = A_2(u, y_2, \alpha, X_1)X_2 + \varphi_2(u, y_2, \alpha, X_1, X_2) \\ y_2 = C_2 X_2 \end{cases} \tag{17}$$

where:

$$A_1(u, y_1, \alpha, X_2) = \begin{bmatrix} 0 & -y_1 exp\left(\frac{\alpha_3}{X_2(1)}\right) \\ 0 & 0 \end{bmatrix}; \quad \varphi_1(u, y_1, \alpha, X_1, X_2) = \begin{bmatrix} \alpha_1\alpha_2 - \alpha_1 y_1 \\ 0 \end{bmatrix};$$

$$A_2(u, y_2, \alpha, X_1) = \begin{bmatrix} 0 & \alpha_5 X_1(2) exp\left(\frac{\alpha_3}{y_2}\right) X_1(1) + \alpha_6(u - y_2) \\ 0 & 0 \end{bmatrix};$$

$$\varphi_2(u, y_2, \alpha, X_1, X_2) = \begin{bmatrix} \alpha_1\alpha_4 - \alpha_1 y_2 \\ 0 \end{bmatrix}; \quad C_2 = [1\ 0].$$

Annex: CSTR

- Observers in cascade:
  - For the subsystem (16), an observer is designed as follows:

$$\dot{Z}_1 = A_1 Z_1 + \varphi_1 - G(C_1 Z_1 - y_p(1)) \tag{18}$$

where:

- estimated state vector: $Z_1 = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_4 \end{bmatrix}$;
- gain of observer: $G = \Delta^{-1} S_\theta^{-1} C_1^T$ with $\Delta = \begin{bmatrix} 1 & 0 \\ 0 & A_{12} \end{bmatrix}$ and

$$S_\theta = \begin{bmatrix} \frac{1}{\theta_{o1}} & -\frac{1}{\theta_{o1}^2} \\ -\frac{1}{\theta_{o1}^2} & \frac{2}{\theta_{o1}^3} \end{bmatrix};$$

  - For the subsystem (17), we design a type of observer for the state-affine system with output injection:

$$\begin{cases} \dot{Z}_2 = A_2 Z_2 + \varphi_2 - S^{-1} C_2^T R(C_2 Z_2 - y_p(2)) \\ \dot{S} = -\theta_{o2} S - A_2^T S - S A_2^T + C_2^T R C_2 \end{cases} \tag{19}$$

where:

- estimated state vector: $Z_2 = \begin{bmatrix} \hat{x}_2 \\ \hat{x}_3 \end{bmatrix}$;
- S: matrix 2×2 S.D.P.;
- R: weight matrix 1×1;
- θ_{o2}: tuning parameter of observer.

Annex: CSTR

- Sensitivity model

$$
(M_\theta)\begin{cases}
\dot{x}_{1\theta 1}(t) = & -\alpha_1 x_{1\theta 1}(t) - \hat{\theta}_2(t) exp\left(\frac{\alpha_3}{x_2(t)}\right) x_{1\theta 1}(t) \\
& +\hat{\theta}_2(t) x_1(t) exp\left(\frac{\alpha_3}{x_2(t)}\right) \frac{\alpha_3}{x_2^2(t)} x_{2\theta 1}(t) \\
\dot{x}_{1\theta 2}(t) = & -exp\left(\frac{\alpha_3}{x_2(t)}\right) x_1(t) - \alpha_1 x_{1\theta 2}(t) - \hat{\theta}_2(t) exp\left(\frac{\alpha_3}{x_2(t)}\right) x_{1\theta 2}(t) \\
& +\hat{\theta}_2(t) x_1(t) exp\left(\frac{\alpha_3}{x_2(t)}\right) \frac{\alpha_3}{x_2^2(t)} x_{2\theta 2}(t) \\
\dot{x}_{2\theta 1}(t) = & -\frac{\left[\alpha_5 \hat{\theta}_2(t) exp\left(\frac{\alpha_3}{x_2(t)}\right) x_1(t) + \alpha_6 (u(t) - x_2(t))\right]}{\hat{\theta}_1^2(t)} \\
& -\left(\alpha_1 + \frac{\alpha_5 \hat{\theta}_2(t)}{\hat{\theta}_1(t)} exp\left(\frac{\alpha_3}{x_2(t)}\right) x_1(t) \frac{\alpha_3}{x_2^2(t)} + \frac{\alpha_6}{\hat{\theta}_1(t)}\right) x_{2\theta 1}(t) \\
& +\frac{\alpha_5 \hat{\theta}_2(t)}{\hat{\theta}_1(t)} exp\left(\frac{\alpha_3}{x_2(t)}\right) x_{1\theta 1}(t); \\
\dot{x}_{2\theta 2}(t) = & \frac{\alpha_5}{\hat{\theta}_1(t)} exp\left(\frac{\alpha_3}{x_2(t)}\right) x_1(t) \\
& -\left(\alpha_1 + \frac{\alpha_5 \hat{\theta}_2(t)}{\hat{\theta}_1(t)} exp\left(\frac{\alpha_3}{x_2(t)}\right) x_1(t) \frac{\alpha_3}{x_2^2(t)} + \frac{\alpha_6}{\hat{\theta}_1(t)}\right) x_{2\theta 2}(t) \\
& +\frac{\alpha_5 \hat{\theta}_2(t)}{\hat{\theta}_1(t)} exp\left(\frac{\alpha_3}{x_2(t)}\right) x_{1\theta 2}(t);
\end{cases}
\tag{20}
$$