Optimization with Differential Algebraic Equations:

Parameter Estimation and Optimal Control

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Outline

- Review: Differential Equations
- Optimization with DAEs
- Orthogonal Collocation
    - **Parameter Estimation**
    - Optimal Control

PARAMETER ESTIMATION

Given a real data set of $\boldsymbol{u}(t)$ and $\boldsymbol{y}(t)$, *find all parameter values* within $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$ that fits the data.

OPTIMAL CONTROL

Given a fully known $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$, *find* $\boldsymbol{u}(t)$ that achieves *a desired trajectory* in $\boldsymbol{y}(t)$ while satisfying other constraints.

Parameter Estimation

Optimization with DAE

Minimize: $\Psi(t, \boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{u}(t))$

Subject to: $\dot{\boldsymbol{x}} = \boldsymbol{f}\big(t, \boldsymbol{x}(t), \boldsymbol{u}(t)\big)$ States

$\boldsymbol{y} = \boldsymbol{g}(t, \boldsymbol{x}(t), \boldsymbol{u}(t))$ Outputs

and $h_i(\boldsymbol{t}, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{y}) \leq 0 \qquad i = 1, 2, \ldots, m$

Parameter Estimation

$$\min \Psi = \sum_{i=1}^{N} \left(\boldsymbol{y}_{\text{actual},i} - \boldsymbol{y}_{\text{sim},i}\right)^2$$

- Must have a data set of $\{t_i, \boldsymbol{y}_{\text{actual},i}\}$, $i = 1, \ldots, N$
- Must ensure that times t_i are included in the ContinuousSet in Pyomo DAE.

Example:

Consider the reaction A → B → C, modeled by the following ODEs:

$$\frac{dA}{dt} = -k_1 A$$

$$\frac{dB}{dt} = k_1 A - k_2 B$$

with initial conditions: $A(0) = 1, B(0) = 0$. Fit the ODEs to the following experimental data set and find k_1 and k_2:

Time	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
A	0.606	0.368	0.223	0.135	0.082	0.050	0.030	0.018	0.011	0.007
B	0.373	0.564	0.647	0.669	0.656	0.624	0.583	0.539	0.494	0.451

Reference: Pyomo Workshop December 2023

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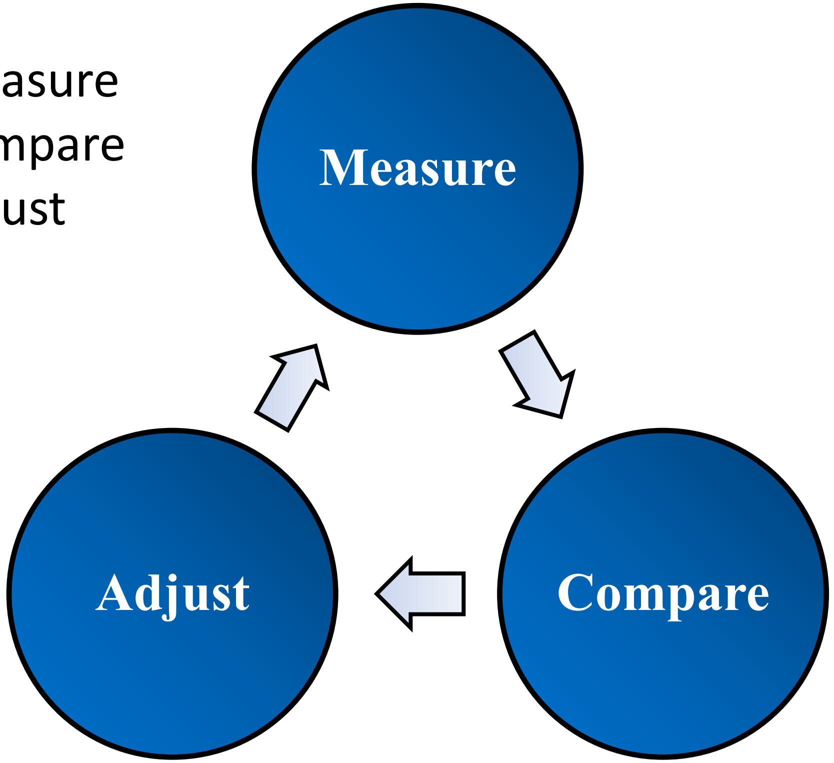
Review: ChemE 182

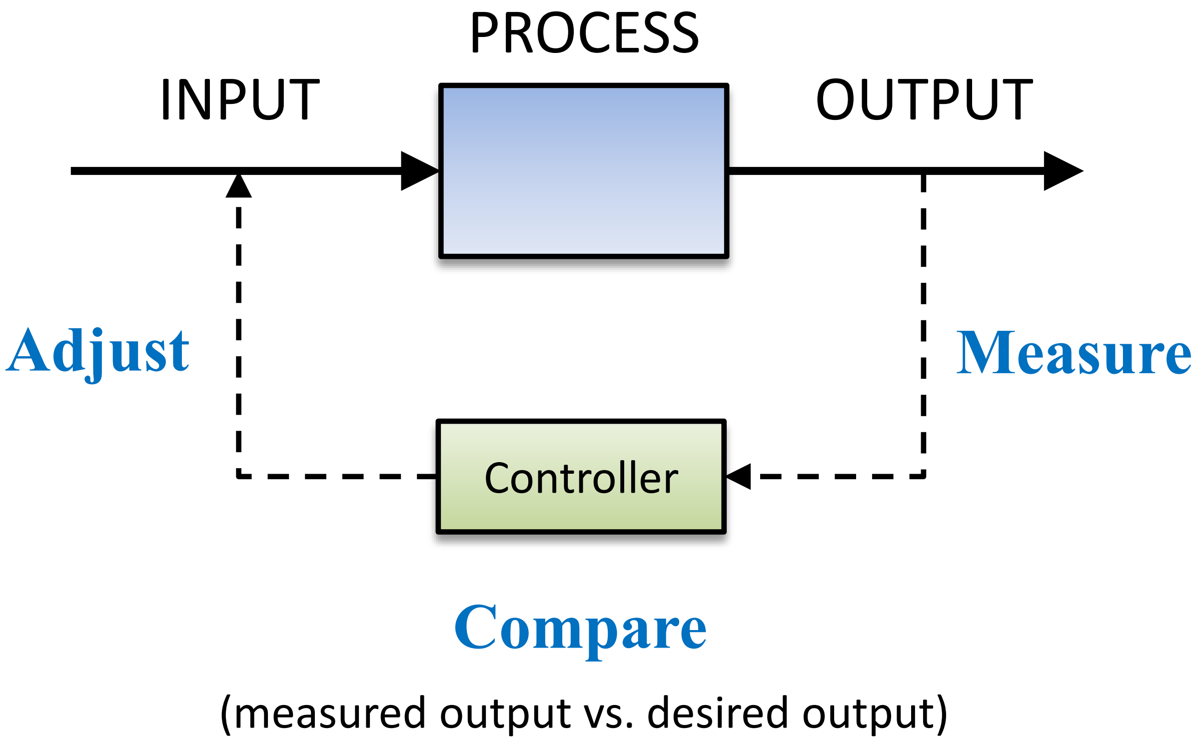
What is a basic process control system?

The key elements needed for process control to occur are:

- Measure
- Compare
- Adjust



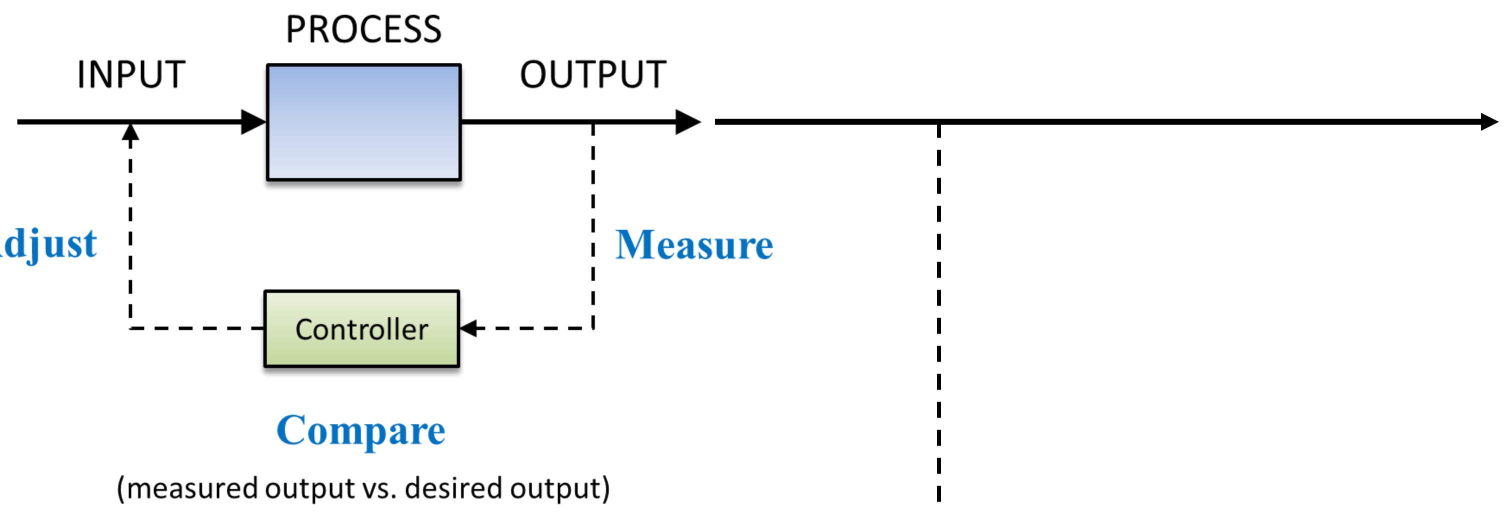
A basic illustration of process control:

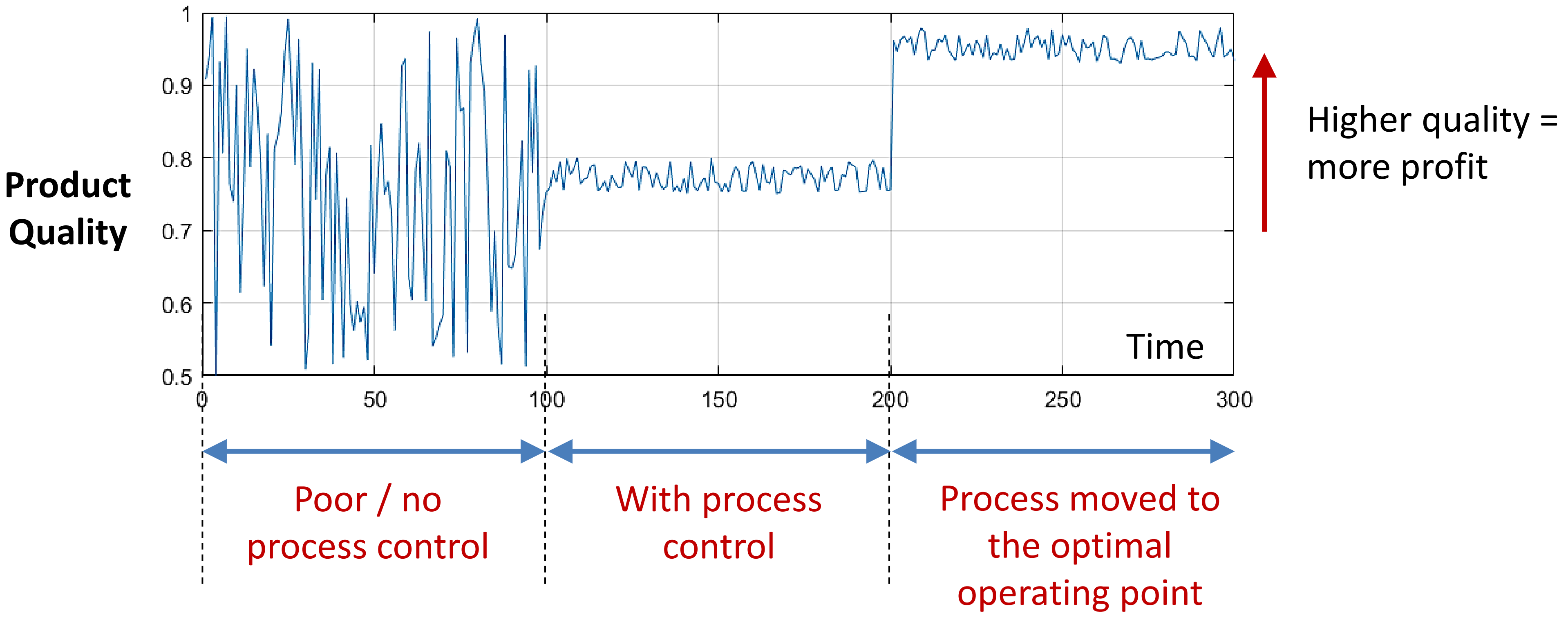


Review: ChemE 182

Why do we need process control?

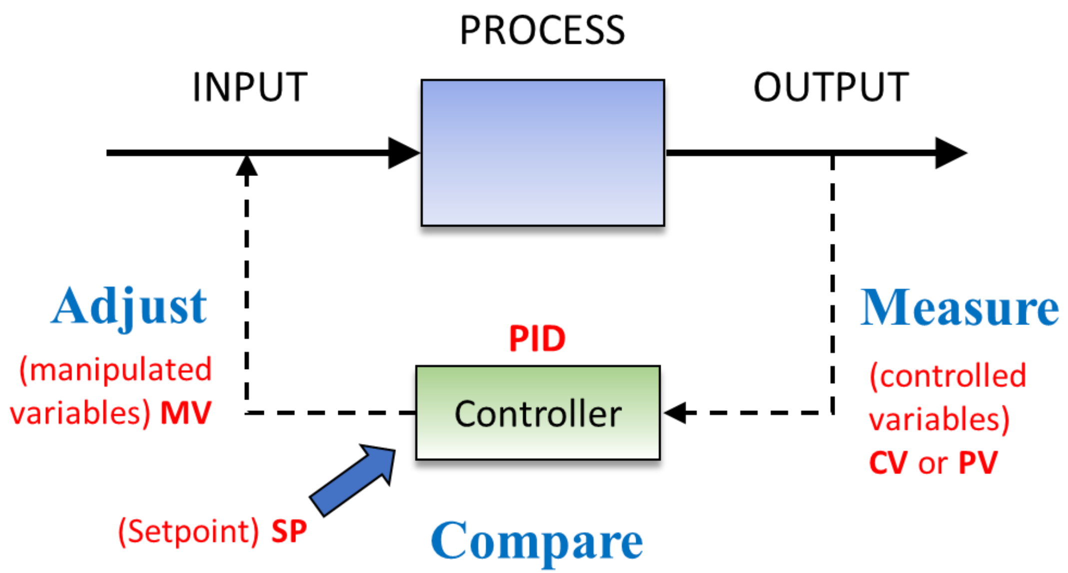
- Reduce variability in the output
  - Higher profit
- Plant safety
- Environmental Compliance





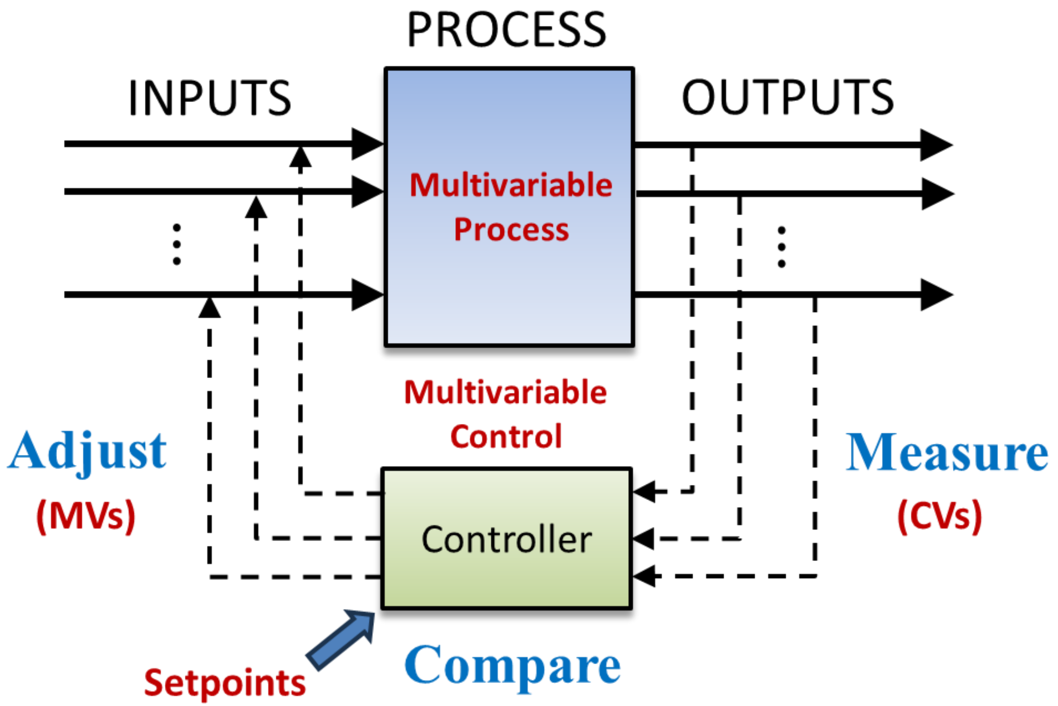
Review: ChemE 182

SISO control versus MIMO control



(measured output vs. desired output)

***ChemE 182 only deals with SISO control and linear ODEs.**



***Can deal with a system of nonlinear ODEs/PDEs.**

- **This can be done using either:**
  - Multi-loop PID control
  - Model Predictive Control

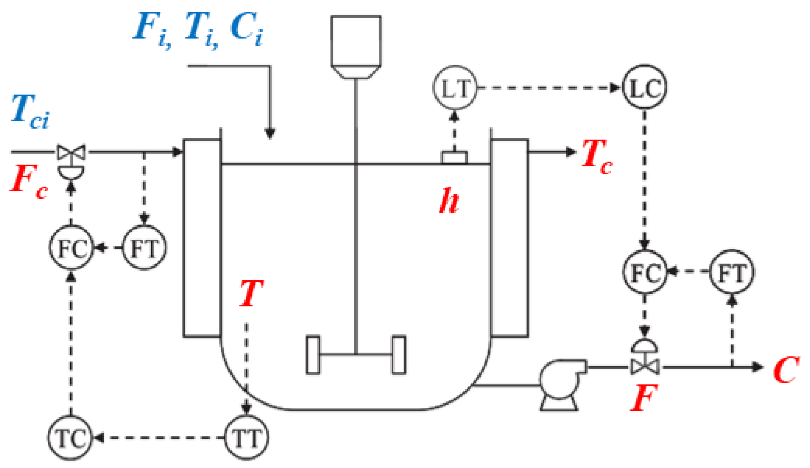
Controlled Variables (CVs)
the <u>outputs</u> that we desire to control (keep constant or follow a setpoint)

Manipulated Variables (MVs)
the <u>inputs</u> that we adjust to achieve desired CV trajectories.

Disturbance Variables (DVs)
other <u>inputs</u> that cause the CVs to deviate from their setpoint.

Optimal Control

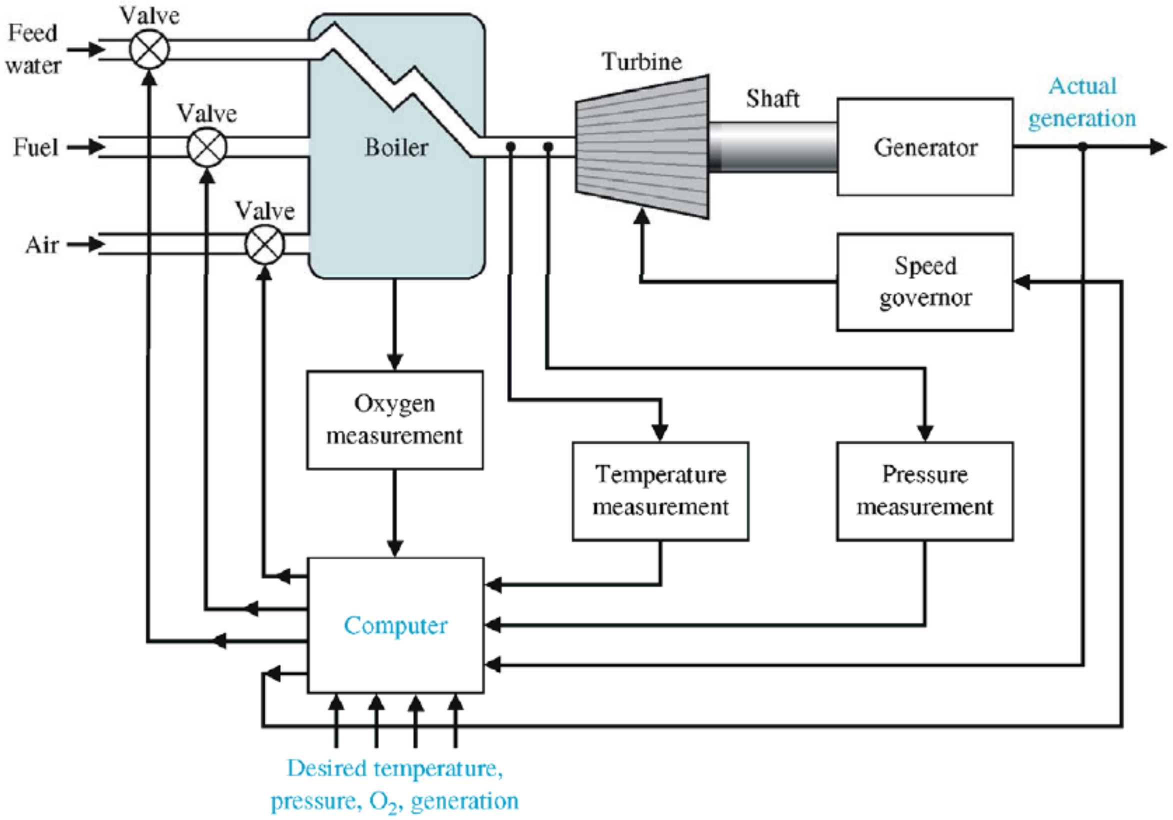
Multi-loop PID control



- 2 cascade control loops = **4 PID controllers**
- 10 variables: **4 inputs** (Fi, Ti, Ci, Tci) + **6 outputs** (Fc, T, Tc, h, F, C)
- PID is still SISO, so we must select **pairs of CV-MVs** to connect.
- Download Link: https://www.mathworks.com/matlabcentral/fileexchange/65091-cascade-controlled-cstr-for-fault-simulation

Model Predictive Control

- Control can be centralized or decentralized to subsystems.
- Solve a big optimization problem to get control actions.
- Requires a computer model of the actual system.



Optimal Control

Optimization with DAE

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and $h_i(\boldsymbol{t}, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{y}) \leq 0 \qquad i = 1, 2, \ldots, m$

Model Predictive Control

Minimize: $\sum_{k=0}^{P} \left[\Delta \boldsymbol{y}_{k+1}^T \boldsymbol{Q} \Delta \boldsymbol{y}_{k+1} + \Delta \boldsymbol{u}_k^T \boldsymbol{R} \Delta \boldsymbol{u}_k\right]$

Weighted sum of squares: $\boldsymbol{v}^T \boldsymbol{W} \boldsymbol{v}$

Subject to: $\dot{\boldsymbol{x}} = \boldsymbol{f}(t, \boldsymbol{x}(t), \boldsymbol{u}(t))$ States

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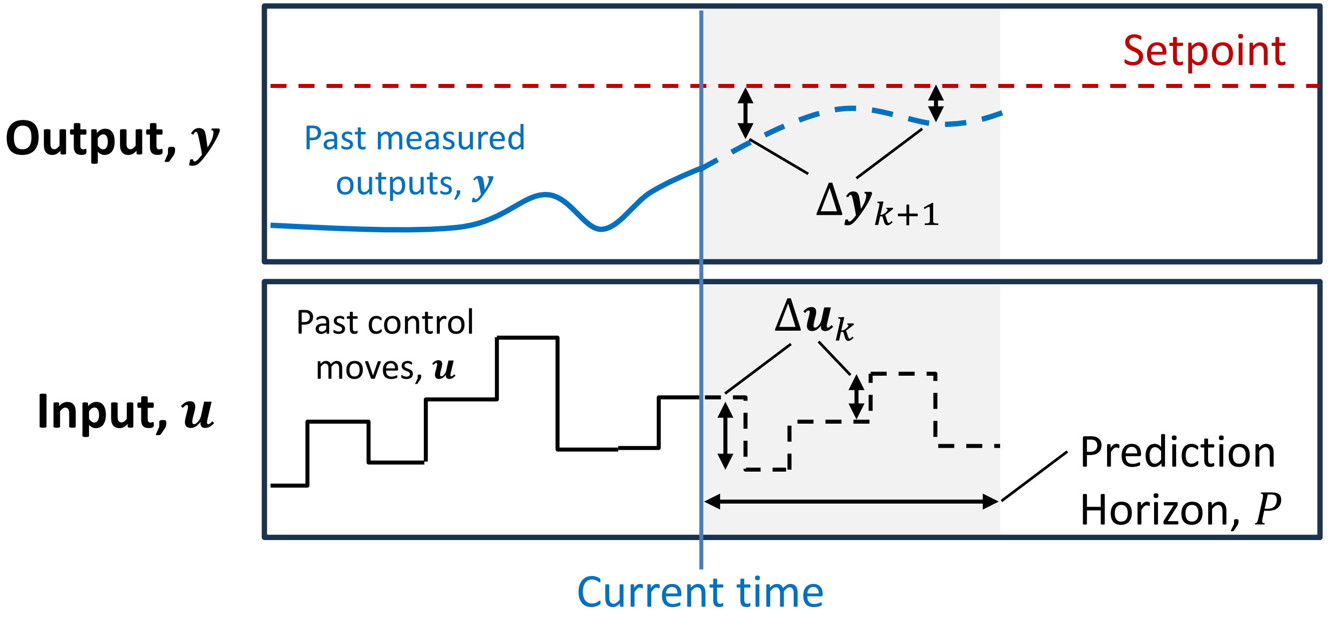
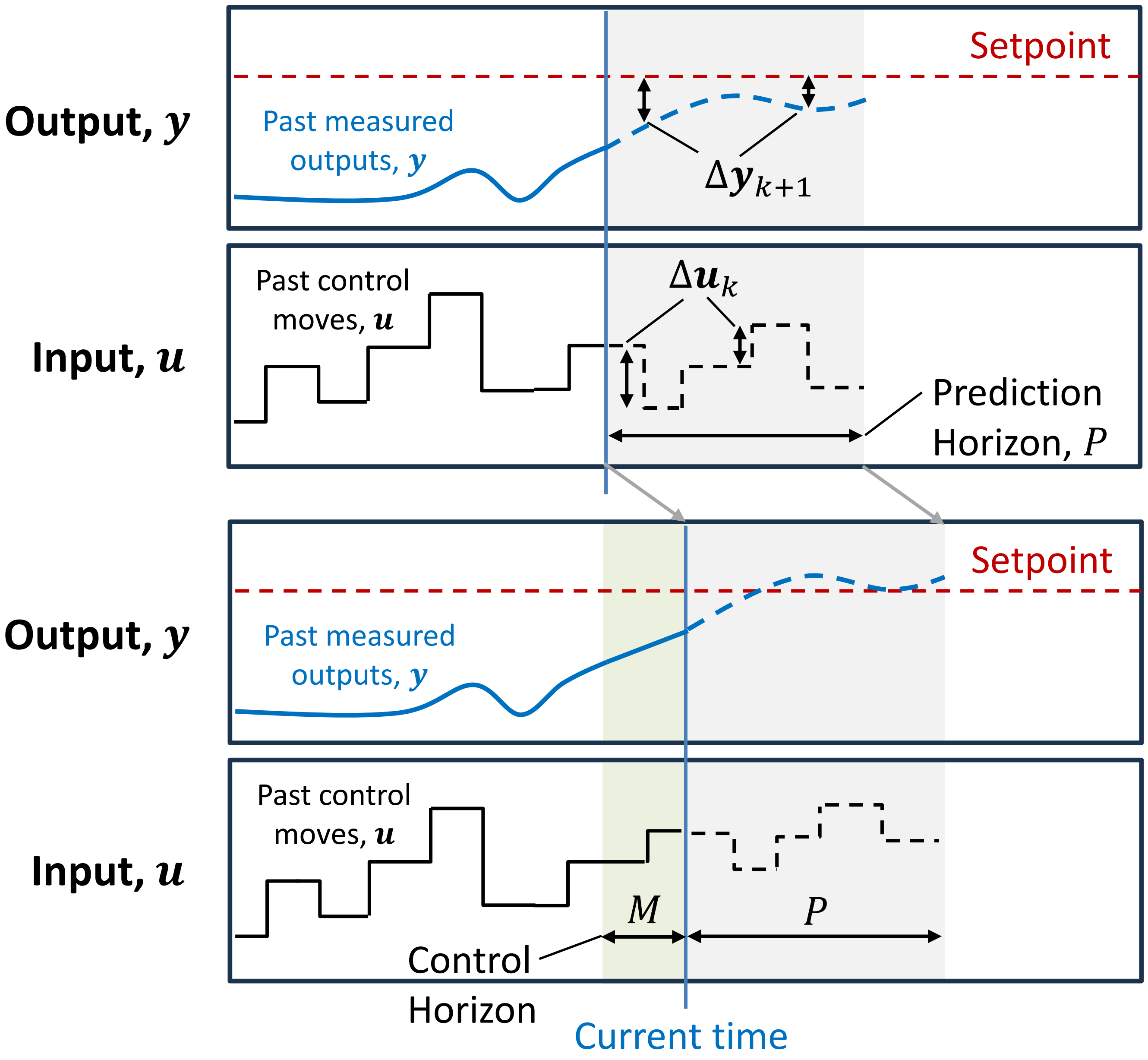
Notation:

$\Delta \boldsymbol{y}_{k+1}$	Deviation from setpoint at time $k+1$
$\Delta \boldsymbol{u}_k$	Amount of control effort at time k
$\boldsymbol{Q}$	State weight matrix
$\boldsymbol{R}$	Control input weight matrix
P	Prediction horizon
M	Control horizon



Optimal Control



Model Predictive Control

Minimize: $$\sum_{k=0}^{P} \left[\Delta \boldsymbol{y}_{k+1}^T \boldsymbol{Q} \Delta \boldsymbol{y}_{k+1} + \Delta \boldsymbol{u}_k^T \boldsymbol{R} \Delta \boldsymbol{u}_k\right]$$

Subject to: $\dot{\boldsymbol{x}} = \boldsymbol{f}\big(t, \boldsymbol{x}(t), \boldsymbol{u}(t)\big)$ States

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MPC Algorithm

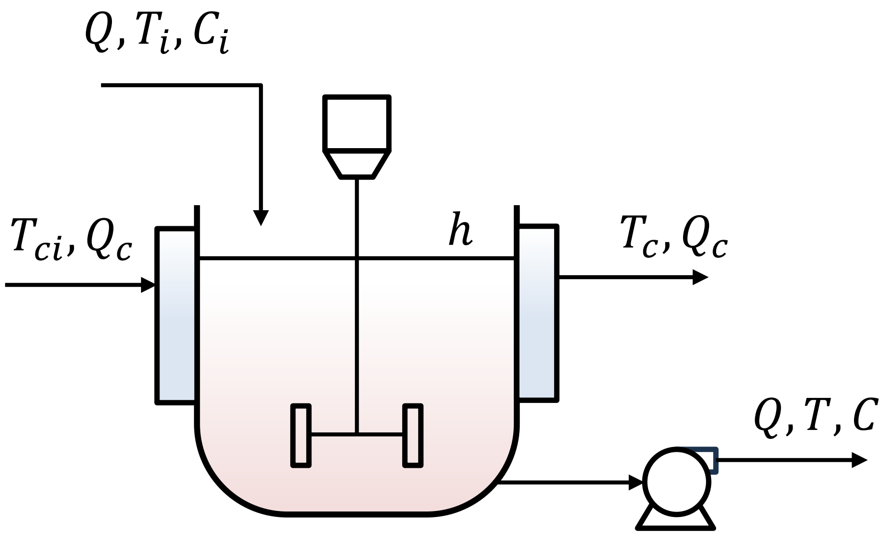
Set: Prediction Horizon, Control Horizon, Process Model, Setpoints and Constraints, $\boldsymbol{R}$ and $\boldsymbol{Q}$.

Steps:

1. Solve NLP for $\boldsymbol{u}$ within the prediction horizon, P.
2. Apply the $\boldsymbol{u}$ within the control horizon, M, only.
3. Roll the horizon M steps forward: $k \leftarrow k + M$.

Optimal Control: Example

Optimal Control of a Jacketed CSTR



$$\frac{dC}{dt} = \frac{Q}{V}(C_i - C) - akC$$

$$\frac{dT}{dt} = \frac{Q}{V}(T_i - T) - \frac{\Delta H_r akC}{\rho C_p} - b\frac{UA}{\rho C_p V}(T - T_c)$$

$$\frac{dT_c}{dt} = \frac{Q_c}{V_c}(T_{ci} - T_c) + b\frac{UA}{\rho C_{pc} V_c}(T - T_c)$$

The model of a constant hold-up, jacketed CSTR carrying out an exothermic first-order reaction A → B is given. Simulate an MPC for a single prediction horizon of $P = 10$ min that aims to decrease C from 0.1 mol/L to 0.05 mol/L by manipulating Q_c under:

a. Normal case
b. Fouling at 5 min (b decreases from 1.00 to 0.05)
c. Catalyst decay at 5 min (a decreases from 1.00 to 0.05)

Parameter	Description	Value	Units
Q	Inlet Flow rate	100.0	L/min
V	Tank Volume	150.0	L
V_c	Jacket Volume	10.0	L
ΔH_r	Heat of reaction	$-2e5$	cal/mol
UA	Heat transfer coefficient	7.0e5	cal/min/K
k_0	Arrhenius factor	7.2e10	1/min
E/R	Activation Energy	1e4	K
ρ, ρ_c	Density	1000	g/L
C_p, C_{pc}	Heat capacity	1.0	cal/g/K

Inputs:
C_i = inlet concentration of A
T_i = inlet temperature
T_{ci} = inlet coolant temp.
Q_c = coolant flow rate

Outputs:
C = outlet concentration of A
T = outlet temperature
T_c = outlet coolant temp.

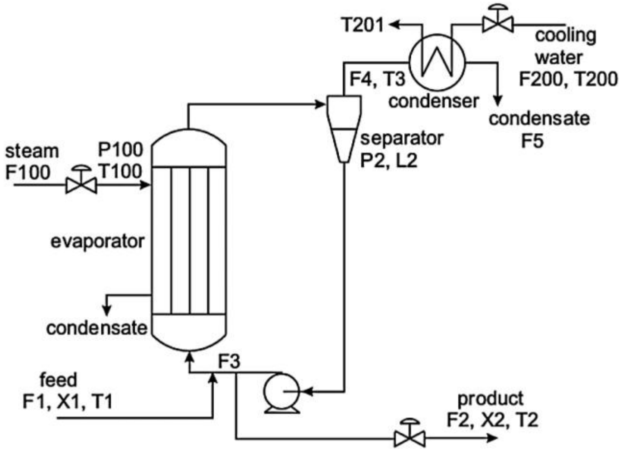
Optimal Control: Example

Optimal Control of an Evaporator

$$\frac{dL_2}{dt} = \frac{F_1 - F_4 - F_2}{20}$$

$$\frac{dX_2}{dt} = \frac{F_1X_1 - F_2X_2}{20}$$

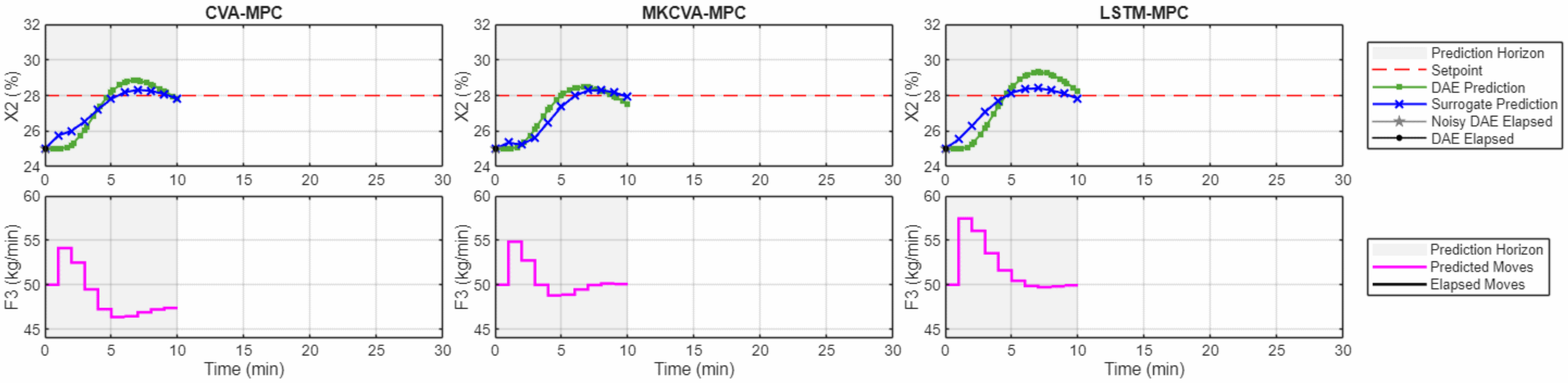
$$\frac{dP_2}{dt} = \frac{F_4 - F_5}{4}$$



Ref: Pilario and Wu (2025). "Fast Mixed Kernel Canonical Variate Analysis for Learning based Nonlinear Model Predictive Control." *Chemical Engineering Research and Design*.

- Control X2 by manipulating F3, P100, F200 simultaneously.
- Use a surrogate machine learning (ML) model instead of DAEs.
- The proposed method (middle) has the best control performance among the three ML models being compared.

$$T_2 = 0.5616P_2 + 0.3126X_2 + 48.43$$
$$T_3 = 0.507P_2 + 55.0$$
$$F_4 = \frac{Q_{100} - 0.07F_1(T_2 - T_1)}{38.5}$$
$$T_{100} = 0.1538P_{100} + 90.0$$
$$Q_{100} = 0.16(F_1 + F_3)(T_{100} - T_2)$$
$$F_{100} = Q_{100}/36.6$$
$$Q_{200} = \frac{0.9576F_{200}(T_3 - T_{200})}{0.14F_{200} + 6.84}$$
$$T_{201} = T_{200} + Q_{200}/0.07F_{200}$$
$$F_5 = Q_{200}/38.5$$



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