# Overview of Models for Automated Process Control

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Baltimore, MD

# Outline

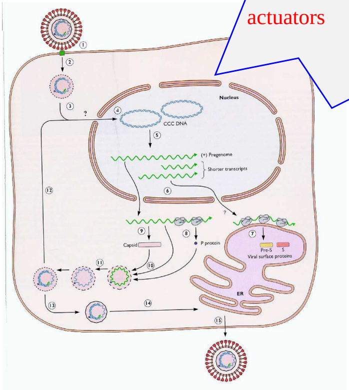
process

$$\frac{dx}{dt} = f(x, u)$$

$$y = g(x, u)$$

actuators

sensors




# Large industrial success story!

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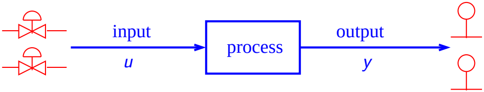
# Broader industrial impact (Qin and Badgwell, 2003)

| Area | Aspen Technology | Honeywell Hi-Spec | Adersa | PCL | MDC | Total |
|---|---|---|---|---|---|---|
| Refining | 1200 | 480 | 280 | 25 | | 1985 |
| Petrochemicals | 450 | 80 | - | 20 | | 550 |
| Chemicals | 100 | 20 | 3 | 21 | | 144 |
| Pulp and Paper | 18 | 50 | - | - | | 68 |
| Air & Gas | - | 10 | - | - | | 10 |
| Utility | - | 10 | - | 4 | | 14 |
| Mining/Metallurgy | 8 | 6 | 7 | 16 | | 37 |
| Food Processing | - | - | 41 | 10 | | 51 |
| Polymer | 17 | - | - | - | | 17 |
| Furnaces | - | - | 42 | 3 | | 45 |
| Aerospace/Defense | - | - | 13 | - | | 13 |
| Automotive | - | - | 7 | - | | 7 |
| Unclassified | 40 | 40 | 1045 | 26 | 450 | 1601 |
| Total | 1833 | 696 | 1438 | 125 | 450 | 4542 |
| First App. | DMC:1985 IDCOM-M:1987 OPC:1987 | PCT:1984 RMPCT:1991 | IDCOM:1973 HIECON:1986 | PCL: 1984 | SMOC: 1988 | |
| Largest App | 603x283 | 225x85 | - | 31x12 | - | |

# Input, output, and state variables




Input/output description

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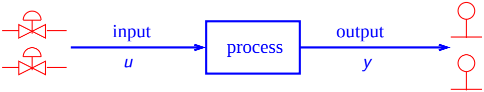
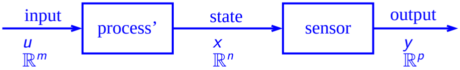



Input/output description




State description

# Nonlinear models

## Nonlinear differential equations

$$\frac{dx}{dt} = f(x, u, t)$$
$$y = h(x, u, t)$$
$$x(t_0) = x_0$$

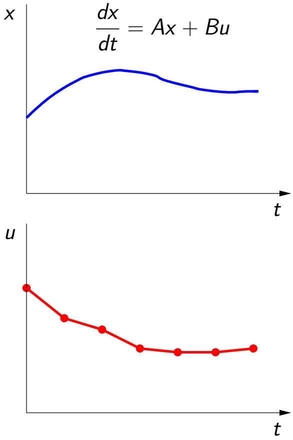
- $x$ is the state
- $u$ is the input
- $y$ is the output
- $t$ is time

# Linear time invariant models

## Linear differential equations

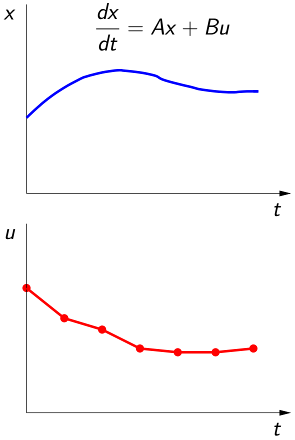
$$\frac{dx}{dt} = Ax + Bu$$
$$y = Cx + Du$$
$$x(0) = x_0$$

Continuous time

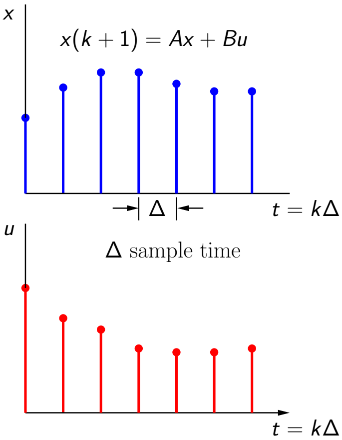


# Continuous time and discrete time models

Continuous time




Discrete time



# Discrete time models

## Linear difference equations

$$
\begin{aligned}
x(k+1) &= Ax(k) + Bu(k) \\
y(k) &= Cx(k) + Du(k) \\
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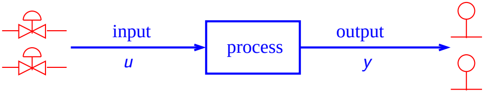
Easier notation

## Linear difference equations

$$
\begin{aligned}
x^+ &= Ax + Bu \\
y &= Cx + Du \\
x(0) &= x_0
\end{aligned}
$$

in which $x(k)^+$ denotes $x(k+1)$.

# Input-output models

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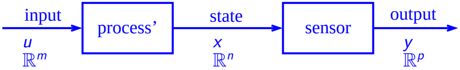


State description

# Input-output to state space

- Current output $y(t)$ is modeled as a time series in past *inputs* and *outputs*, and noise

$$y(t) = \underbrace{a_1 y(t-1) + a_2 y(t-2)}_{\text{past outputs}} + \underbrace{b_1 u(t-1) + b_2 u(t-2)}_{\text{past inputs}} + v(t)$$

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- We estimate the model parameters from $(u, y)$ data (Ljung, 2000)

$$\theta = \begin{bmatrix} a_1 & a_2 & b_1 & b_2 \end{bmatrix}$$

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- Given $\widehat{\theta}$ we can obtain $A, B, C$

# Converting input-output to state space

- Define $x(t)$ to hold the past inputs and outputs.

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- The time series model is

$$\underbrace{\begin{bmatrix} y(t+1) \\ y(t) \\ u(t) \end{bmatrix}}_{x^+} = \underbrace{\begin{bmatrix} a_1 & a_2 & b_2 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} y(t) \\ y(t-1) \\ u(t-1) \end{bmatrix}}_{x} + \underbrace{\begin{bmatrix} b_1 \\ 0 \\ 1 \end{bmatrix}}_{B} u(t)$$

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- The equivalent state space model is

$$x^+ = Ax + Bu$$
$$y = Cx$$

# Constraints

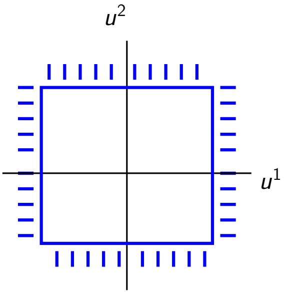
- Physical bounds on inputs (valves full open, full closed)

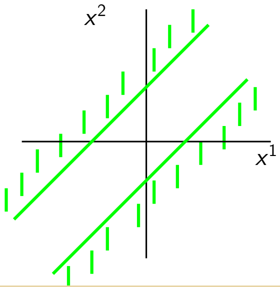
$$\underline{u} \le u(k) \le \overline{u} \qquad k \ge 0$$

$$Eu(k) \le e \qquad k \ge 0$$

in which

$$E = \begin{bmatrix} I \\ -I \end{bmatrix} \qquad e = \begin{bmatrix} \overline{u} \\ -\underline{u} \end{bmatrix}$$



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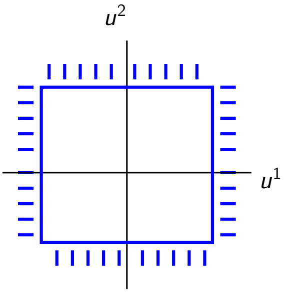
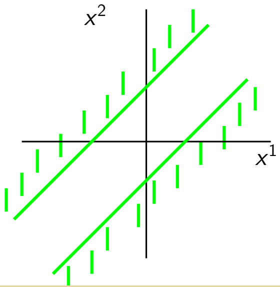



- Constraints on states or outputs for reasons of safety, operability, product quality, etc.

$$Fx(k) \leq f \qquad k \geq 0$$



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- Augmented system model

$$\underbrace{\begin{bmatrix} x(k+1) \\ u(k) \end{bmatrix}}_{\widetilde{x}(k+1)} = \underbrace{\begin{bmatrix} A & 0 \\ 0 & 0 \end{bmatrix}}_{\widetilde{A}} \underbrace{\begin{bmatrix} x(k) \\ u(k-1) \end{bmatrix}}_{\widetilde{x}(k)} + \underbrace{\begin{bmatrix} B \\ I \end{bmatrix}}_{\widetilde{B}} u(k)$$

$$y(k) = \underbrace{\begin{bmatrix} C & 0 \end{bmatrix}}_{\widetilde{C}} \underbrace{\begin{bmatrix} x(k) \\ u(k-1) \end{bmatrix}}_{\widetilde{x}(k)}$$

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is stated as

$$F\widetilde{x}(k) + Eu(k) \leq e \qquad F = \begin{bmatrix} 0 & -I \\ 0 & I \end{bmatrix} \qquad E = \begin{bmatrix} I \\ -I \end{bmatrix} \qquad e = \begin{bmatrix} \overline{\Delta} \\ -\underline{\Delta} \end{bmatrix}$$

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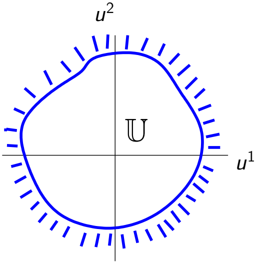
- General *linear* constraints

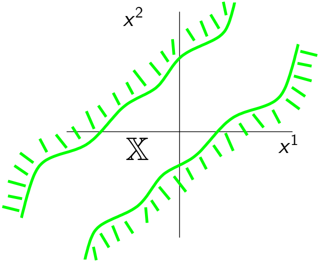
$$Fx(k) + Eu(k) \leq e \qquad k \geq 0$$

subsumes all previous forms

- For nonlinear models, linear constraints are not required

$$u(k) \in \mathbb{U} \qquad x(k) \in \mathbb{X} \qquad k \geq 0$$



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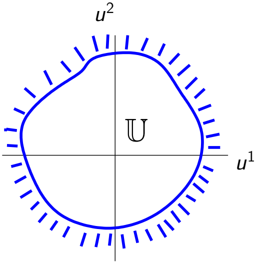
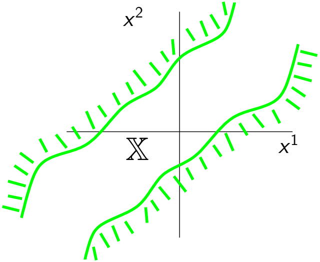
$$u(k) \in \mathbb{U} \qquad x(k) \in \mathbb{X} \qquad k \geq 0$$

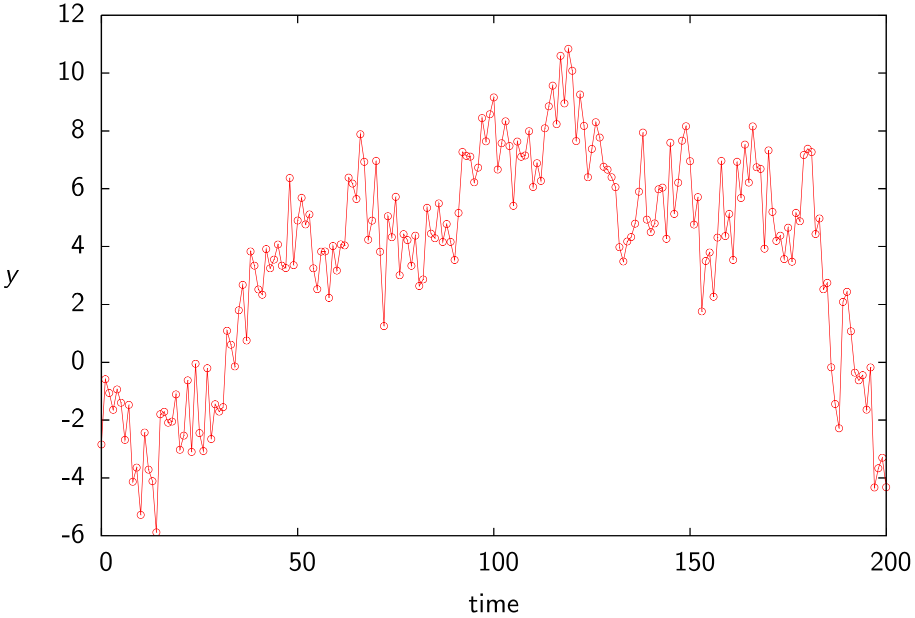
- Even more general

$$(u(k), x(k)) \in \mathbb{Z} \qquad k \geq 0$$



# Typical process data



# Modeling the noise

## Random disturbances

$$
\begin{aligned}
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- So $v$ models measurement noise and $w$ models process disturbance

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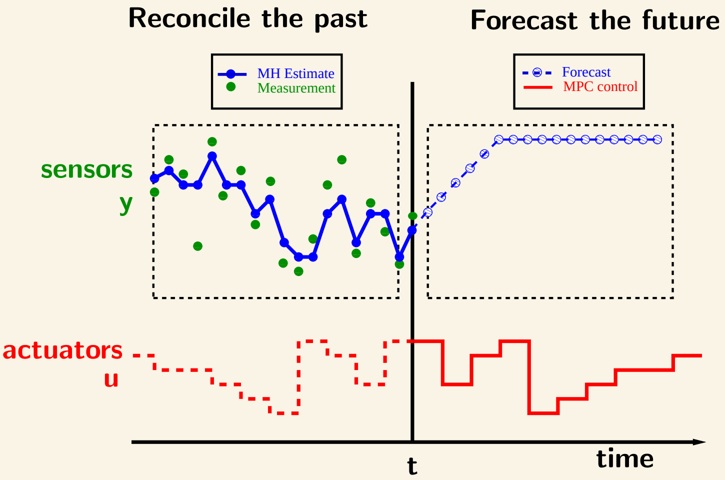
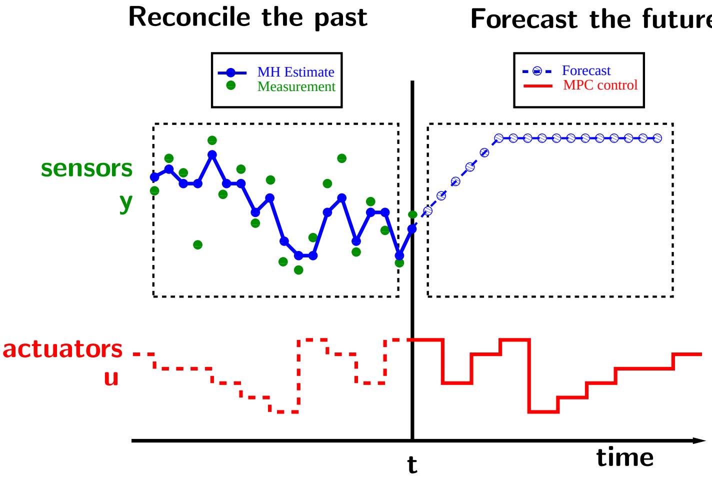
- $w$ is the *random variable* affecting the process
- $v$ is the *random variable* affecting the measurement
- So $v$ models measurement noise and $w$ models process disturbance
- The controller needs to know the *relative amounts of each disturbance*

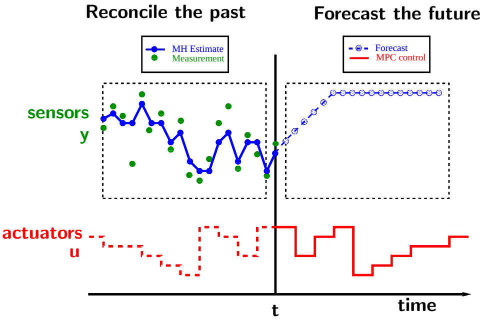
# The model predictive control framework



The future influences the present just as much as the past does.



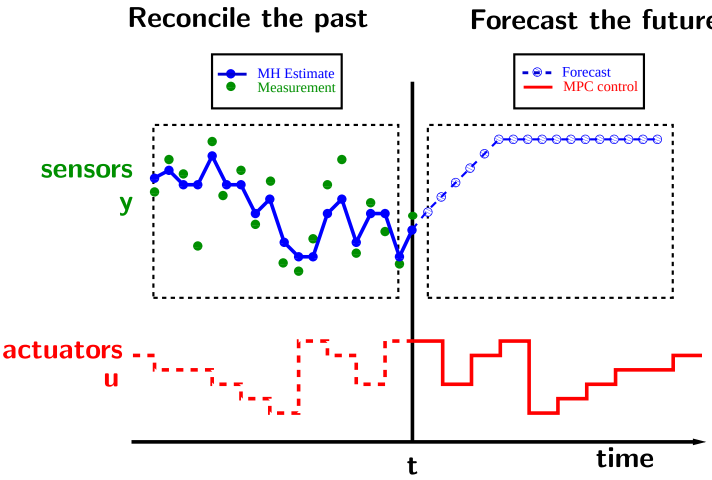
# Predictive control



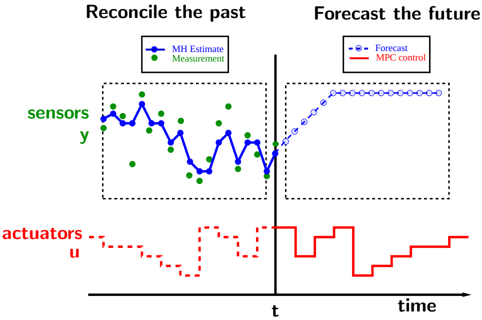

$$\min_{u(t)} \int_0^T |y_{sp} - g(x,u)|_Q^2 + |u_{sp} - u|_R^2 \, dt$$

$$\dot{x} = f(x,u)$$
$$x(0) = x_0 \quad \text{(given)}$$
$$y = g(x,u)$$

When I want to understand what is happening today or try to decide what will happen tomorrow, I look back.



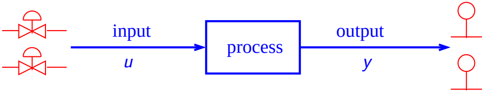
# State estimation




$$\min_{x_0, w(t)} \int_{-T}^{0} |y - g(x,u)|_R^2 + |\dot{x} - f(x,u)|_Q^2 \, dt$$

$$\dot{x} = f(x,u) + w \quad \text{(process noise)}$$
$$y = g(x,u) + v \quad \text{(measurement noise)}$$

# Separation of the control problem




Input/output description

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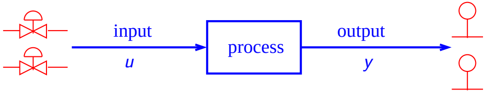


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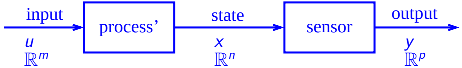


State description

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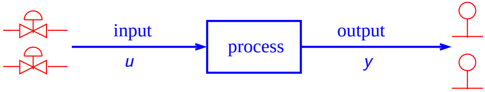


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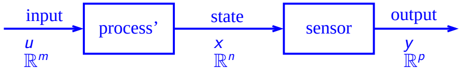
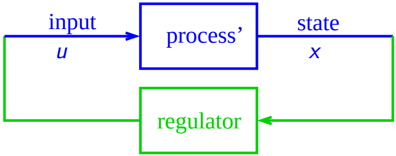
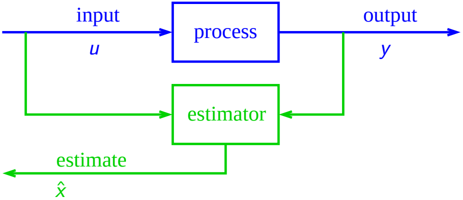



### State description



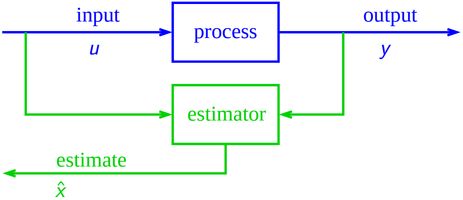

### Regulation problem

# Separation of the control problem

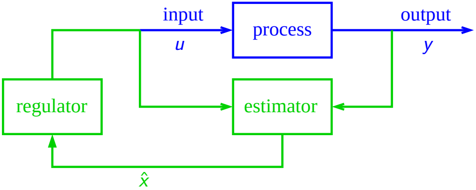



Estimation problem

# Separation of the control problem




Estimation problem




Control problem

# Controller Design for Zero Offset

- Often want *zero tracking error* and rejection of *constant disturbances*

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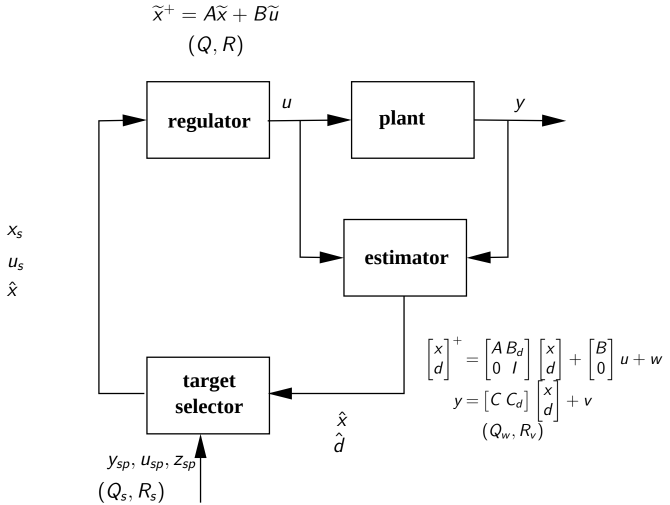
- Augment the model with a constant disturbances (Davison and Smith, 1971, Kwakernaak and Sivan, 1972, p. 278) .

$$\begin{bmatrix} x(k+1) \\ d(k+1) \end{bmatrix} = \begin{bmatrix} A & B_d \\ 0 & I \end{bmatrix} \begin{bmatrix} x(k) \\ d(k) \end{bmatrix} + \begin{bmatrix} B \\ 0 \end{bmatrix} u(k) + w(k)$$

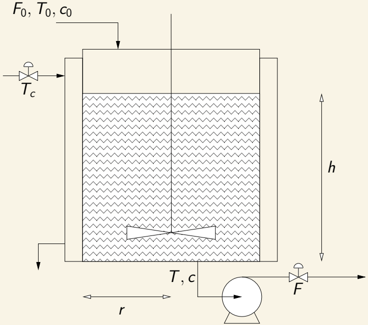
$$y(k) = \begin{bmatrix} C & C_d \end{bmatrix} \begin{bmatrix} x(k) \\ d(k) \end{bmatrix} + v(k)$$

# Offset free control system




MPC controller consisting of: receding horizon regulator, state estimator, and target selector.

# Design example. (Pannocchia and Rawlings, 2003)

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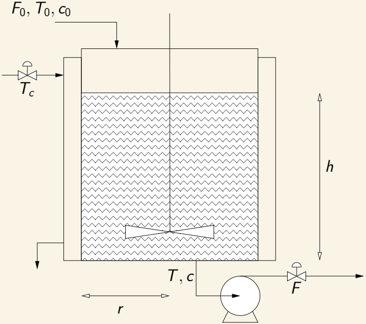


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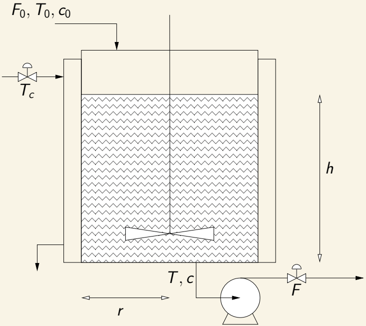
  - level of the tank ($h$)

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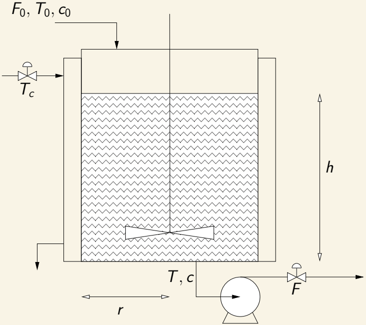


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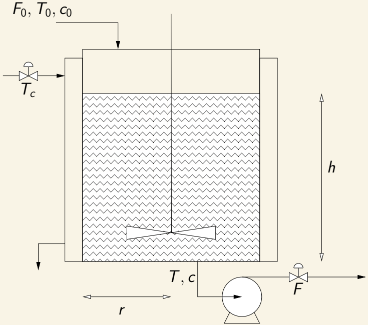


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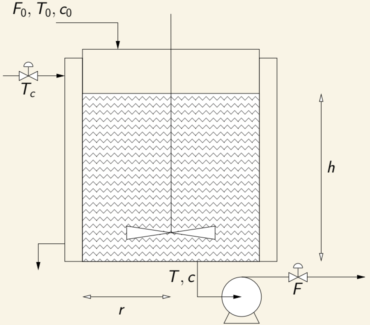


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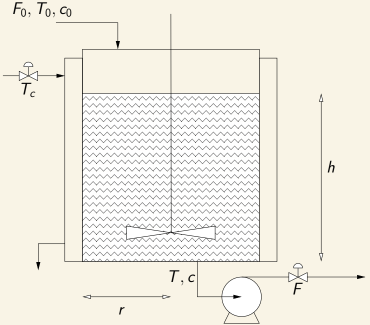


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# More measured outputs than inputs and zero offset

- Component mass and energy balances

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- Nonlinear differential equation model:

$$\frac{dc}{dt} = \frac{F_0(c_0 - c)}{Ur^2 h} - k_0 c \exp\left(-\frac{E}{RT}\right)$$
$$\frac{dT}{dt} = \frac{F_0(T_0 - T)}{Ur^2 h} + \frac{-\Delta H}{\rho C_p} k_0 c \exp\left(-\frac{E}{RT}\right) + \frac{2U}{r\rho C_p}(T_c - T)$$
$$\frac{dh}{dt} = \frac{F_0 - F}{Ur^2}$$

# Well-stirred reactor example: parameters

| Parameter | Nominal value | Units |
|---|---|---|
| $F_0$ | 0.1 | $\mathrm{m^3/min}$ |
| $T_0$ | 350 | K |
| $c_0$ | 1 | $\mathrm{kmol/m^3}$ |
| $r$ | 0.219 | m |
| $k_0$ | $7.2 \times 10^{10}$ | $\mathrm{min^{-1}}$ |
| $E/R$ | 8750 | K |
| $U$ | 54.94 | $\mathrm{kJ/min{\cdot}m^2{\cdot}K}$ |
| $\rho$ | 1000 | $\mathrm{kg/m^3}$ |
| $C_p$ | 0.239 | $\mathrm{kJ/kg{\cdot}K}$ |
| $\Delta H$ | $-5 \times 10^4$ | $\mathrm{kJ/kmol}$ |

# Well-stirred reactor example: linearized model

- Using $\Delta = 1\,\mathrm{min}$, the linearized model is

$$\begin{aligned} x^+ &= Ax + Bu + B_p p \\ y &= Cx \end{aligned}$$

in which all the states are measured

$$x = \begin{bmatrix} c - c^s \\ T - T^s \\ h - h^s \end{bmatrix} \qquad u = \begin{bmatrix} T_c - T_c^s \\ F - F^s \end{bmatrix} \qquad y = \begin{bmatrix} c - c^s \\ T - T^s \\ h - h^s \end{bmatrix} \qquad p = F_0 - F_0^s$$

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and

$$A = \begin{bmatrix} 0.2681 & -0.00338 & -0.00728 \\ 9.703 & 0.3279 & -25.44 \\ 0 & 0 & 1 \end{bmatrix} \qquad C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$B = \begin{bmatrix} -0.00537 & 0.1655 \\ 1.297 & 97.91 \\ 0 & -6.637 \end{bmatrix} \qquad B_p = \begin{bmatrix} -0.1175 \\ 69.74 \\ 6.637 \end{bmatrix}$$

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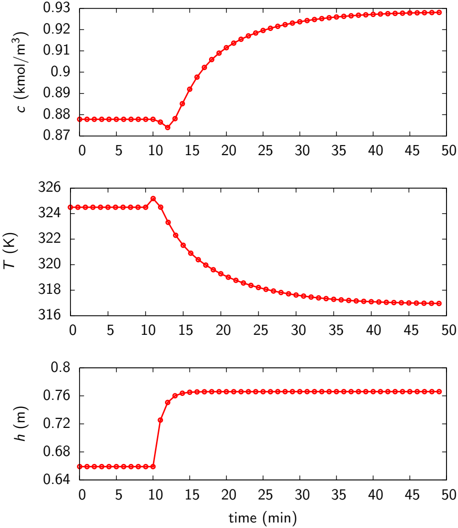
- Is there steady offset in any of the outputs? Which ones?

# Two integrating disturbances: output results




Three measured outputs versus time after a step change in $F_0$ at $t = 10\,\mathrm{min}$

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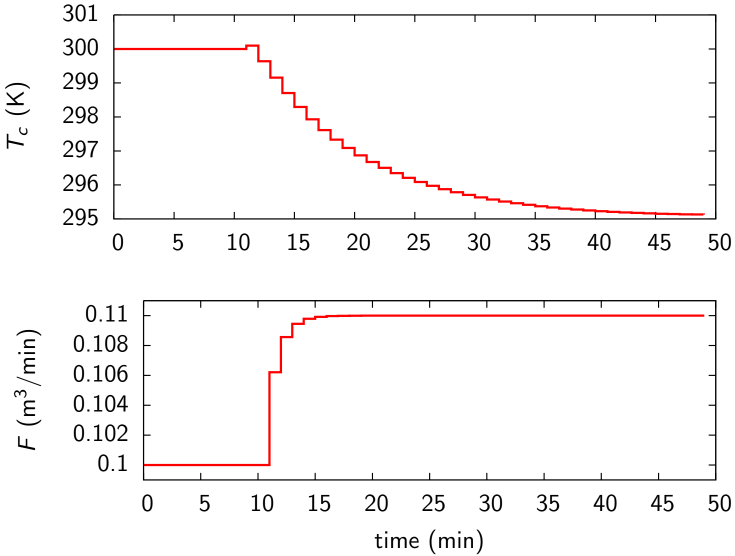


Two manipulated inputs versus time after a step change in $F_0$ at $t = 10\,\mathrm{min}$

# Reactor case studies - two and three integrating disturbances

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- Two integrating disturbances - conclusion:
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- Next we try *three* integrating disturbances:
  - two added to the two controlled variables
  - one added to the second manipulated variable

$$C_d = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \qquad B_d = \begin{bmatrix} 0 & 0 & 0.1655 \\ 0 & 0 & 97.91 \\ 0 & 0 & -6.637 \end{bmatrix}$$

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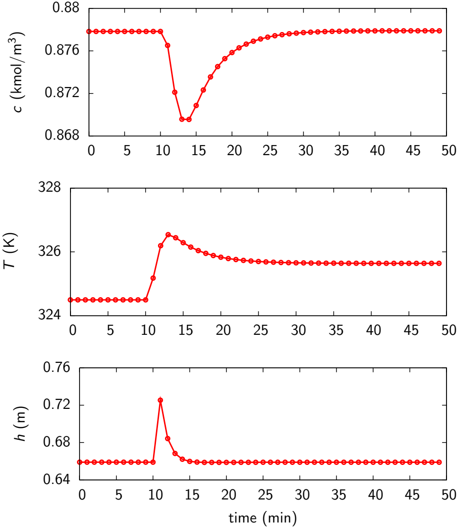


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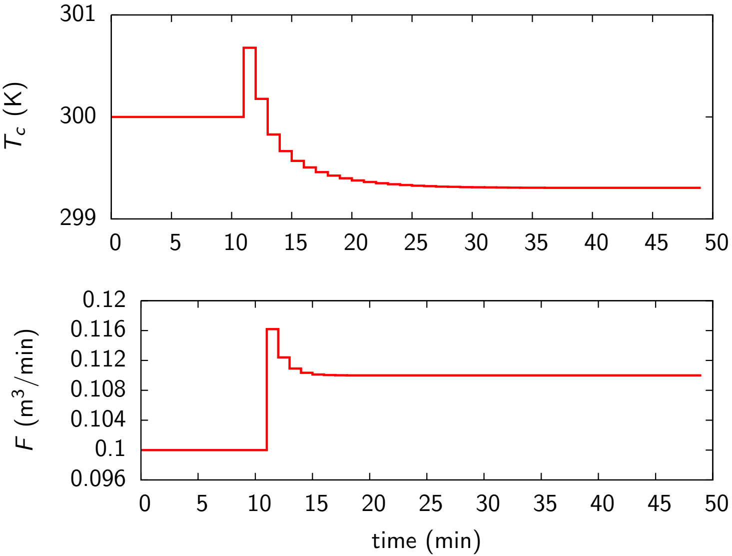


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- With a more accurate disturbance model, better overall control is achieved
  - The controller uses smaller manipulated variable action and also achieves better output variable behavior
  - An added bonus is that steady offset is removed in the maximum possible number of outputs

# Advanced process control and drug manufacturing

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- Small volume, high value-added products
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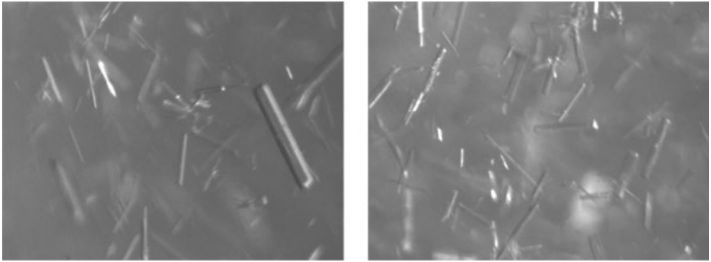
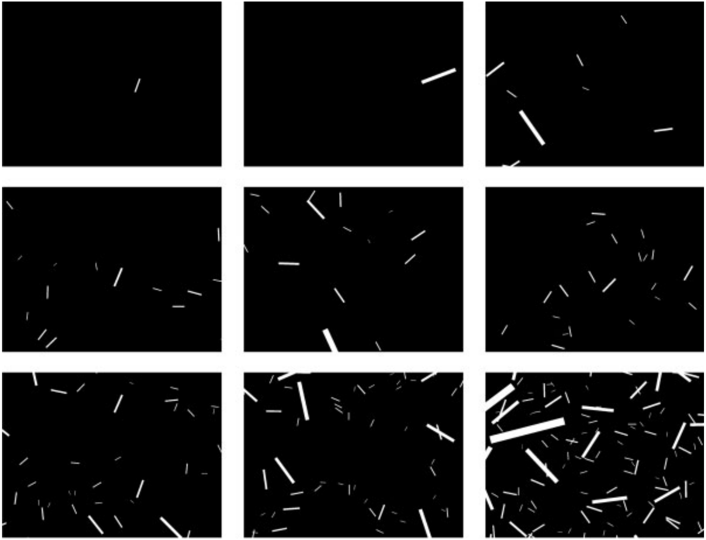
- Importance of the solid phase
- Novel solid-phase sensors (on-line video imaging)

# On-line Video Imaging



In situ images of rod-like crystals from our crystallization lab (Larsen and Rawlings, 2009).

# Idealized data from a batch crystallization



Optimal cooling profile. Images correspond to 60-minute intervals from 0 hours (upper left) to 8 hours (lower right).

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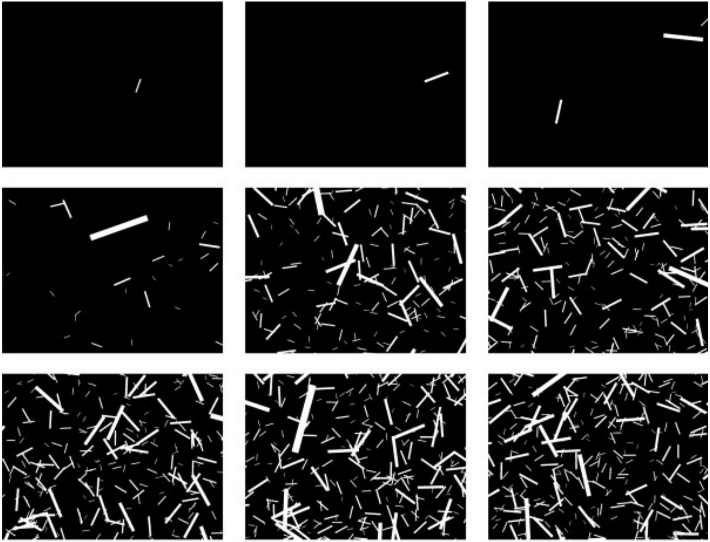
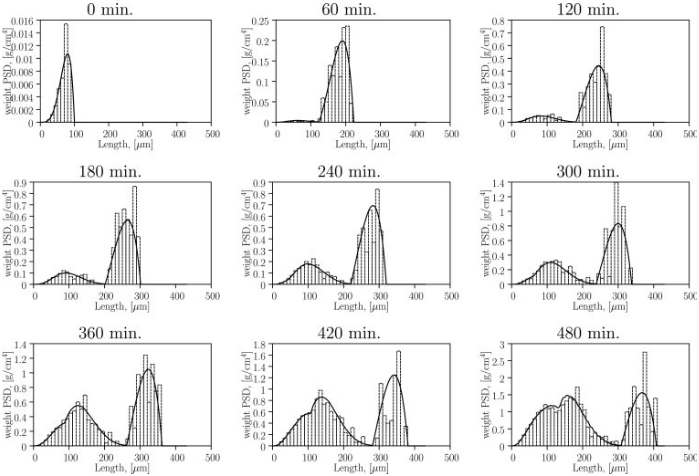


Linear cooling profile. Images correspond to 60-min intervals from 0 h (upper left) to 8 h (lower right).

# Inferring size distribution from video images




Measured and estimated weight PSD for optimal cooling and perfect image analysis. Bin size = 10 $\mu$m and 100 bins.

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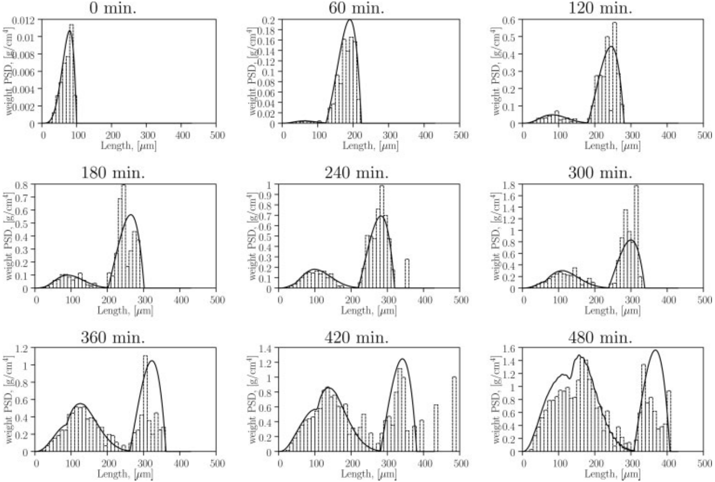


Measured and estimated weight PSD for optimal cooling and image analysis using SHARC. Bin size = 10 $\mu$m and 100 bins.

# Further reading I


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# Further reading II


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