# Mathematical modeling

# Model

A less complex representation of the system to be studied

## Why making a model?

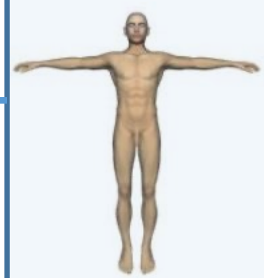
- **Simulation and analysis**
  - gain an understanding of the behavior of the system
  - estimate a quantity or measure an objective
- **Control**
- **Optimization**

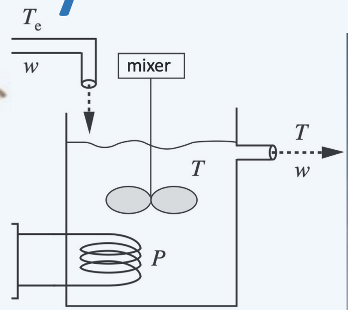
(Control and Optimization:) Evaluate alternative strategies

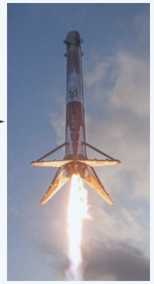
There is a trade-off between model accuracy and complexity and the cost/effort required to develop the model.

# Classes of models

## System





Known physical laws
Limited complexity

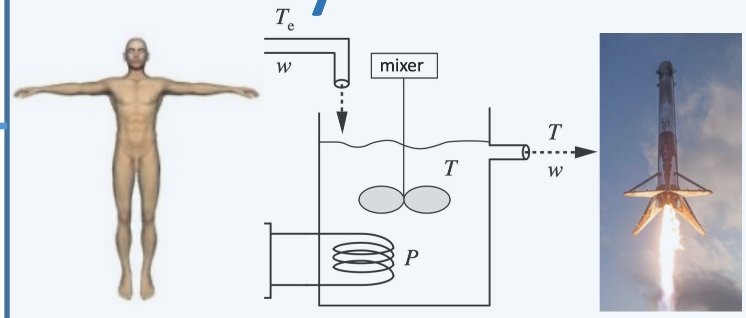
Analytically derived
KNOWLEDGE-BASED models

**Molar balance**

$$\frac{dC_A}{dt} = -kC_A$$
$$C_A\,(t_0) = C_{A0}$$

# Classes of models

## System




Known physical laws
Limited complexity

Analytically derived
KNOWLEDGE-BASED models

**Molar balance**

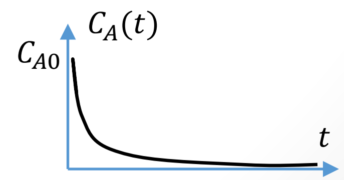
$$\frac{dC_A}{dt} = -kC_A$$

$$C_A(t_0) = C_{A0}$$

Observed behavior
(dominant or specific)

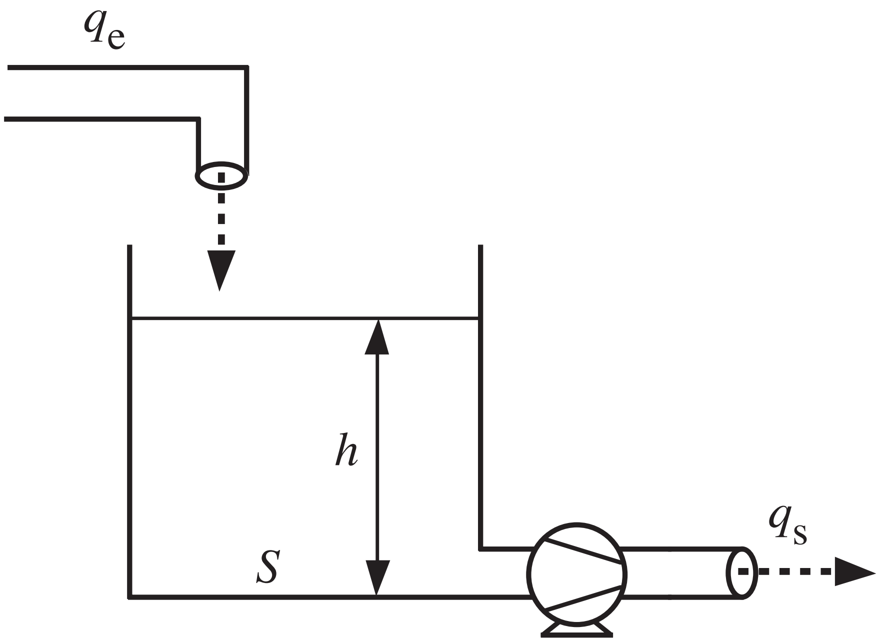
Experimentally derived
REPRESENTATION models

**Observation**



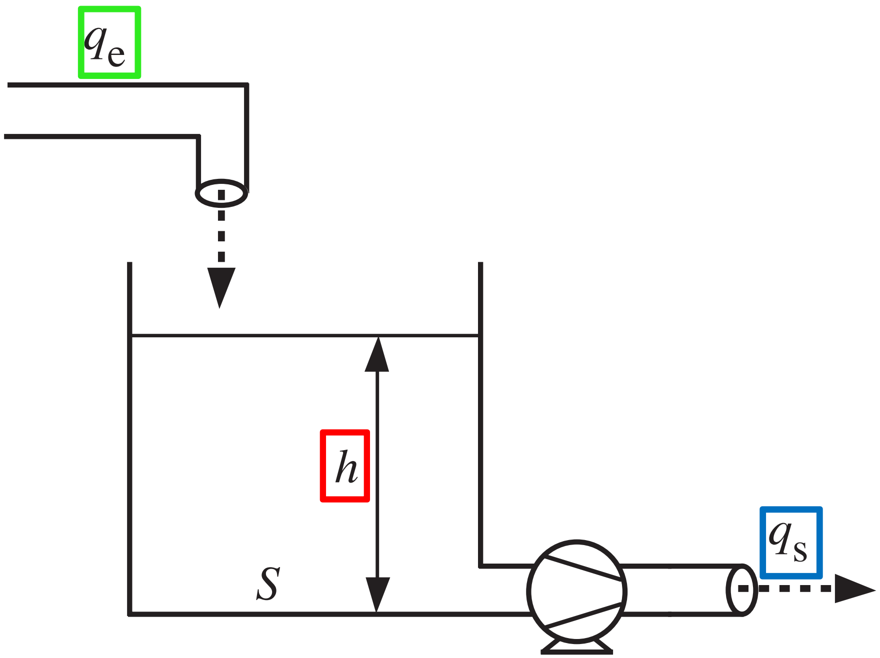

$C_A(t) = C_{A0}e^{-kt}$

# Input/output




$q_e$ **Physical input** (input flow) → Physical process (chemical reactor, heat exchanger…) → **Physical output** (output flow) $q_s$

# Input/output



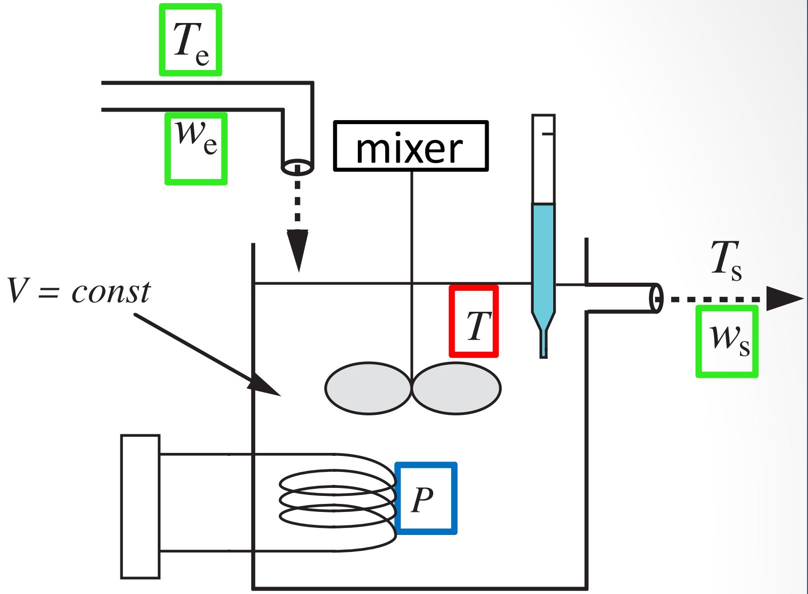

$q_e$ **Physical input** (input flow) → Physical process (chemical reactor, heat exchanger…) → **Physical output** (output flow) $q_s$

$q_s$ $q_e$ **Input variables** (independent) → System (mathematical model) → **Output variables** (dependent) $h$

# Stirred tank with constant volume

**Assumptions**

- V is constant
- No heat loss to the outside
- Well-mixed tank $T_s = T(t)$




**Global mass balance**

$$w(t) \stackrel{\text{def}}{=} w_s(t) = w_e(t)$$

**Global energy balance**

$$\begin{pmatrix}\text{rate of energy} \\ \text{accumulation}\end{pmatrix} = \begin{pmatrix}\text{rate of} \\ \text{input energy}\end{pmatrix} - \begin{pmatrix}\text{rate of} \\ \text{output energy}\end{pmatrix}$$

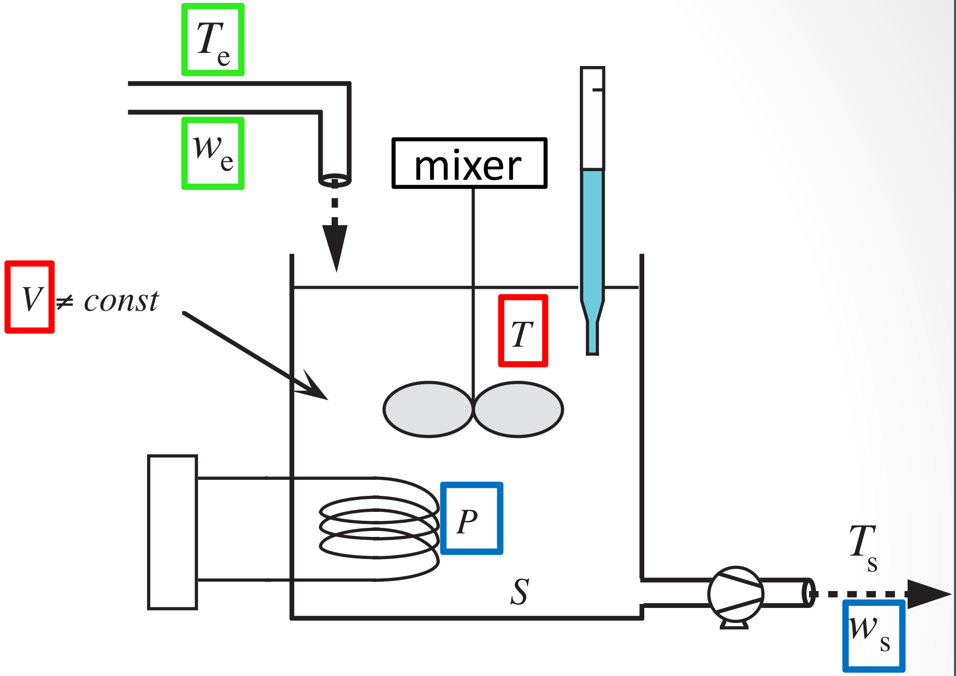
$$\frac{\mathrm{d}}{\mathrm{d}t}\left[V\rho c_\mathrm{p}\left(T(t)-T_\mathrm{ref}\right)\right] = \left[w(t)c_\mathrm{p}\left(T_\mathrm{e}(t)-T_\mathrm{ref}\right)+P(t)\right] - w(t)c_\mathrm{p}\left(T(t)-T_\mathrm{ref}\right)$$

$$V\rho c_\mathrm{p}\frac{\mathrm{d}}{\mathrm{d}t}T(t) = w(t)c_\mathrm{p}\left[T_\mathrm{e}(t)-T(t)\right]+P(t)$$

# Stirred tank with variable volume

**Assumptions**

- V is **not** constant
- No heat loss to the outside
- Well-mixed tank $T_s = T(t)$




**Global mass balance**

$$w_s(t) \neq w_e(t)$$

$$\begin{pmatrix}\text{rate of mass}\\ \text{accumulation}\end{pmatrix} = \begin{pmatrix}\text{input mass}\\ \text{flow rate}\end{pmatrix} - \begin{pmatrix}\text{output mass}\\ \text{flow rate}\end{pmatrix}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\rho V(t)\right] = w_\mathrm{e}(t) - w_\mathrm{s}(t)$$

$$\rho \frac{\mathrm{d}}{\mathrm{d}t} V(t) = w_\mathrm{e}(t) - w_\mathrm{s}(t)$$

# Stirred tank with variable volume (cont'd)

**Global energy balance**

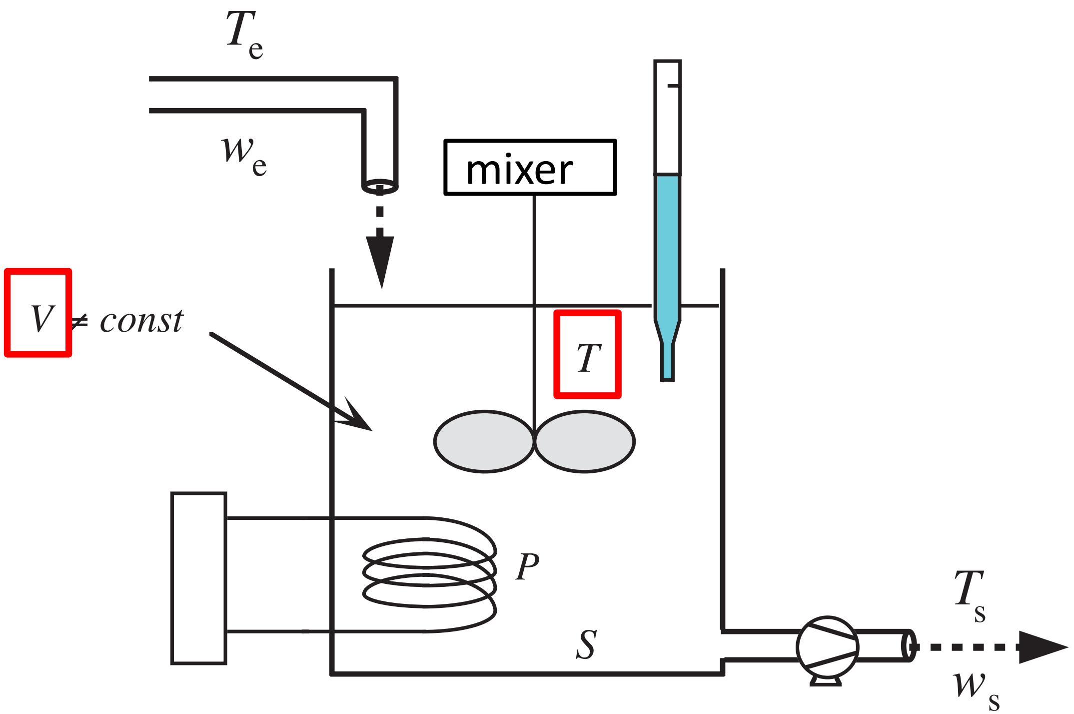
$$\begin{pmatrix}\text{rate of energy}\\ \text{accumulation}\end{pmatrix} = \begin{pmatrix}\text{rate of}\\ \text{input energy}\end{pmatrix} - \begin{pmatrix}\text{rate of}\\ \text{output energy}\end{pmatrix}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[V(t)\rho c_\mathrm{p}\left(T(t)-T_\mathrm{ref}\right)\right]=\left[w_\mathrm{e}(t)c_\mathrm{p}\left(T_\mathrm{e}(t)-T_\mathrm{ref}\right)+P(t)\right]-w_\mathrm{s}(t)c_\mathrm{p}\left(T(t)-T_\mathrm{ref}\right)$$

$$\rho\frac{\mathrm{d}}{\mathrm{d}t}V(t)=w_\mathrm{e}(t)-w_\mathrm{s}(t)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}T(t)=\frac{w_\mathrm{e}(t)}{V(t)\rho}\left[T_\mathrm{e}(t)-T(t)\right]+\frac{P(t)}{V(t)\rho c_\mathrm{p}}$$

# Stirred tank with variable volume (cont'd)




$$\rho \frac{\mathrm{d}}{\mathrm{d}t} V(t) = w_e(t) - w_s(t)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} T(t) = \frac{w_e(t)}{V(t)\rho}\left[T_e(t) - T(t)\right] + \frac{P(t)}{V(t)\rho c_p}$$

# Stirred tank with variable volume (cont'd)

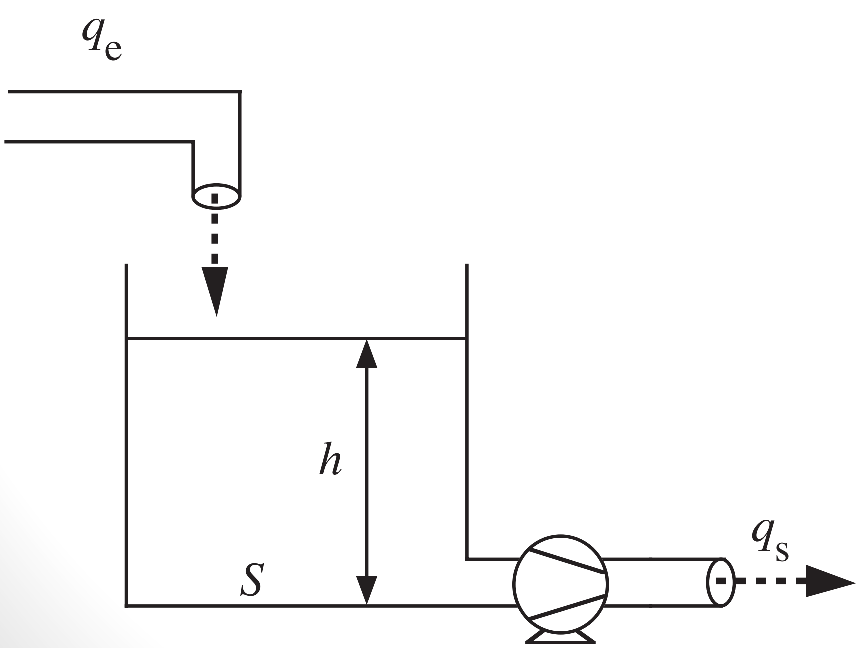
**Specific cases**

**a)** If $V$ is <u>constant</u>:

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t)=0$$

$$w(t):=w_{\mathrm{e}}(t)=w_{\mathrm{s}}(t)$$

$$V\rho c_{\mathrm{p}}\frac{\mathrm{d}}{\mathrm{d}t}T(t)=w(t)c_{\mathrm{p}}\left[T_{\mathrm{e}}(t)-T(t)\right]+P(t)$$




**b)** If $T$ is <u>constant</u>:

**Mass balance**

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\rho V(t)\right]=\rho q_{\mathrm{e}}(t)-\rho q_{\mathrm{s}}(t)$$

ou

$$S\frac{\mathrm{d}}{\mathrm{d}t}h(t)=q_{\mathrm{e}}(t)-q_{\mathrm{s}}(t)$$

**c)** If $V$ and $T$ are <u>constant</u> (steady state):

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t)=0 \quad \text{et} \quad \frac{\mathrm{d}}{\mathrm{d}t}T(t)=0$$

giving

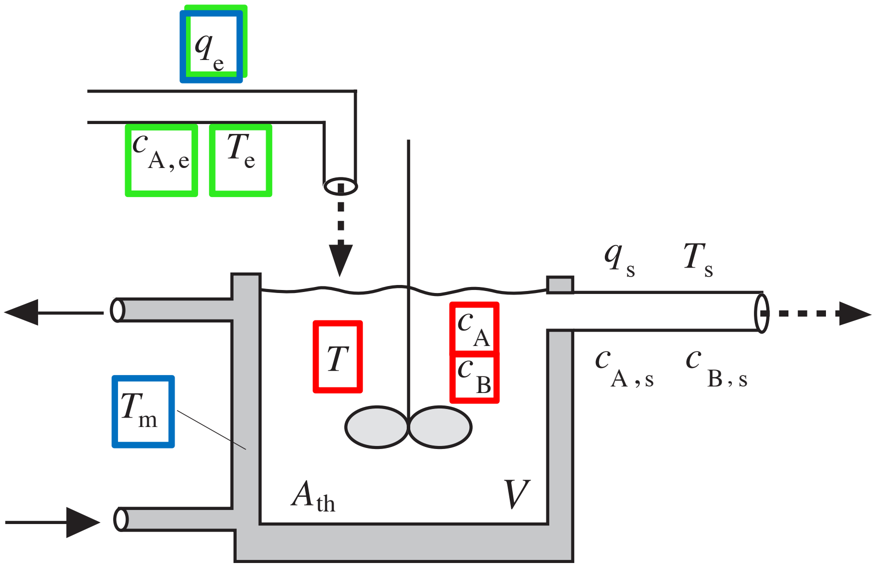
$$\bar{w}:=\bar{w}_{\mathrm{e}}=\bar{w}_{\mathrm{s}}$$

$$\bar{P}=\bar{w}c_{\mathrm{p}}\left(\bar{T}-\bar{T}_{\mathrm{e}}\right)$$

# Continuously stirred reactor

**Exothermic** chemical reaction

$$A \rightarrow B$$




**Global mass balance**

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho V) = \rho q_e(t) - \rho q_s(t) = 0$$

that is: $q(t) := q_e(t) = q_s(t)$

**Assumptions**

- First-order reaction

$$r(t) = k(t) c_A(t)$$

with

$$k(t) = k_0 \, exp\left(\frac{-E_a}{RT(t)}\right)$$

(Arrhénius law)

- Well-mixed reactor:

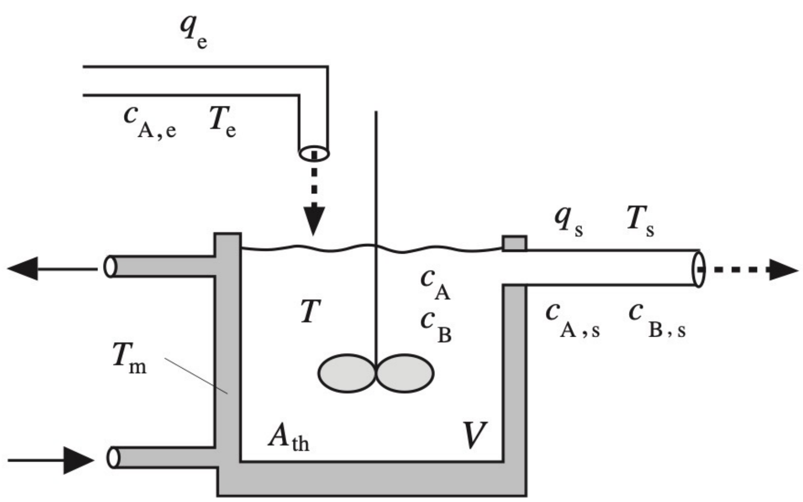
$$T_s(t) = T(t)$$
$$c_{A,s}(t) = c_A(t)$$
$$c_{B,s}(t) = c_B(t)$$

- Homogeneous cooling jacket
- Heat loss negligible

# Continuously stirred reactor (cont'd)

**Partial molar balance for component A**

$A \rightarrow B$



# Continuously stirred reactor (cont'd)

**Partial molar balance for component A**

$$\begin{pmatrix}\text{variation in the number}\\ \text{of moles of A in the}\\ \text{reactor per unit of time}\end{pmatrix} = \begin{pmatrix}\text{input molar}\\ \text{flow rate of A}\end{pmatrix} - \begin{pmatrix}\text{output molar}\\ \text{flow rate of A}\end{pmatrix} - \begin{pmatrix}\text{consumed number}\\ \text{of moles of A}\\ \text{per unit of time}\end{pmatrix}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[Vc_{\mathrm{A}}(t)\right] = q(t)c_{\mathrm{A,e}}(t) - q(t)c_{\mathrm{A}}(t) - Vr(t)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}c_{\mathrm{A}}(t) = \frac{q(t)}{V}\left[c_{\mathrm{A,e}}(t) - c_{\mathrm{A}}(t)\right] - k_0\exp\left[\frac{-E_{\mathrm{a}}}{RT(t)}\right]c_{\mathrm{A}}(t)$$

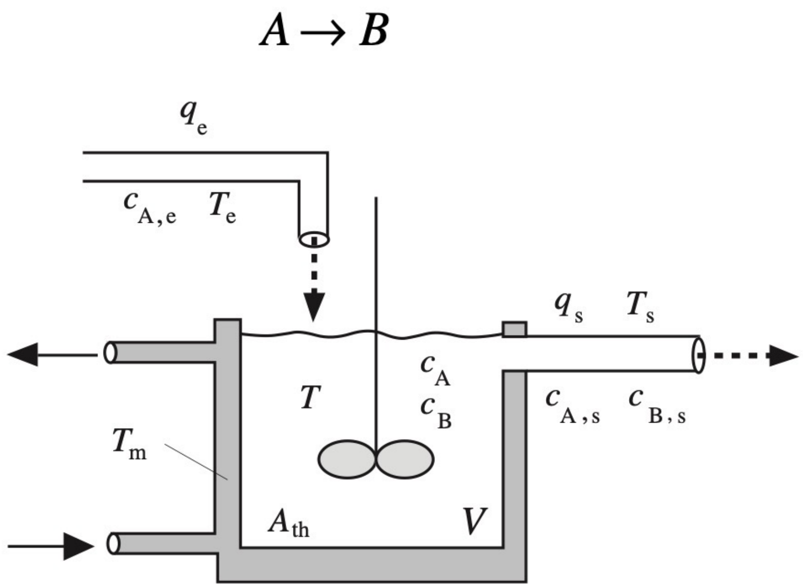
**Partial molar balance for component B**

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[Vc_{\mathrm{B}}(t)\right] = -q(t)c_{\mathrm{B}}(t) + Vr(t)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}c_{\mathrm{B}}(t) = -\frac{q(t)}{V}c_{\mathrm{B}}(t) + k_0\exp\left[\frac{-E_{\mathrm{a}}}{RT(t)}\right]c_{\mathrm{A}}(t)$$

# Continuously stirred reactor (cont'd)

**Global energy balance**



# Continuously stirred reactor (cont'd)

**Global energy balance**

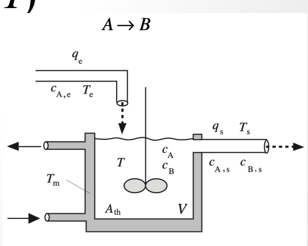
$$\begin{pmatrix}\text{Accumulated}\\ \text{power}\end{pmatrix} = \begin{pmatrix}\text{Power exchanged}\\ \text{with the jacket}\end{pmatrix} + \begin{pmatrix}\text{difference between}\\ \text{input and output}\\ \text{power}\end{pmatrix} + \begin{pmatrix}\text{Power generated}\\ \text{by chemical reaction}\end{pmatrix}$$

$$V\rho c_{\mathrm{p}} \frac{\mathrm{d}}{\mathrm{d}t} T(t) = UA_{\mathrm{th}}\left[T_{\mathrm{m}}(t) - T(t)\right] + \rho q(t) c_{\mathrm{p}}\left[T_{\mathrm{e}}(t) - T(t)\right] + (-\Delta H) V r(t)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} T(t) = \frac{UA_{\mathrm{th}}}{V\rho c_{\mathrm{p}}}\left[T_{\mathrm{m}}(t) - T(t)\right] + \frac{q(t)}{V}\left[T_{\mathrm{e}}(t) - T(t)\right] + \frac{(-\Delta H)}{\rho c_{\mathrm{p}}} k_0 \exp\left[\frac{-E_{\mathrm{a}}}{RT(t)}\right] c_{\mathrm{A}}(t)$$

**Characteristic variables**

- Constant parameters: $V, \rho, c_{\mathrm{p}}, U, A_{\mathrm{th}}, k_0, R, E_{\mathrm{a}}, (-\Delta H)$
- Independent variables: $q(t), c_{\mathrm{A,e}}(t), T_{\mathrm{e}}(t), T_{\mathrm{m}}(t)$
- Dependent variables (states): $c_{\mathrm{A}}(t), c_{\mathrm{B}}(t), T(t)$



# Bioreactions

- Involve micro-organisms and enzyme catalysts.
- The basis for production of a wide variety of pharmaceuticals and healthcare and food products.
- Important industrial processes that involve bioreactions include fermentation and wastewater treatment.

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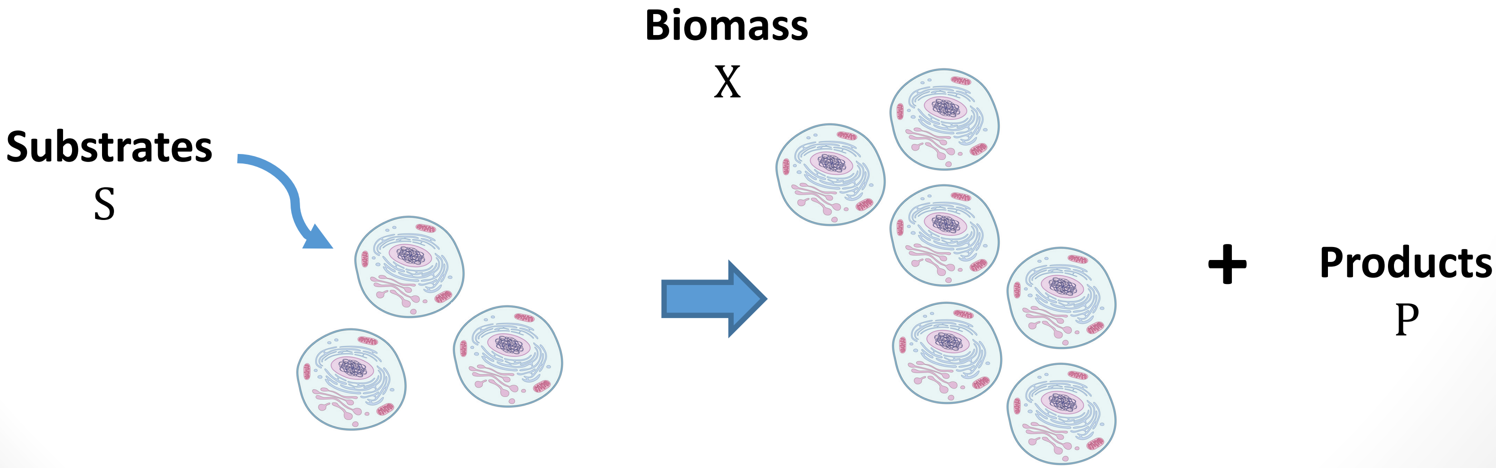
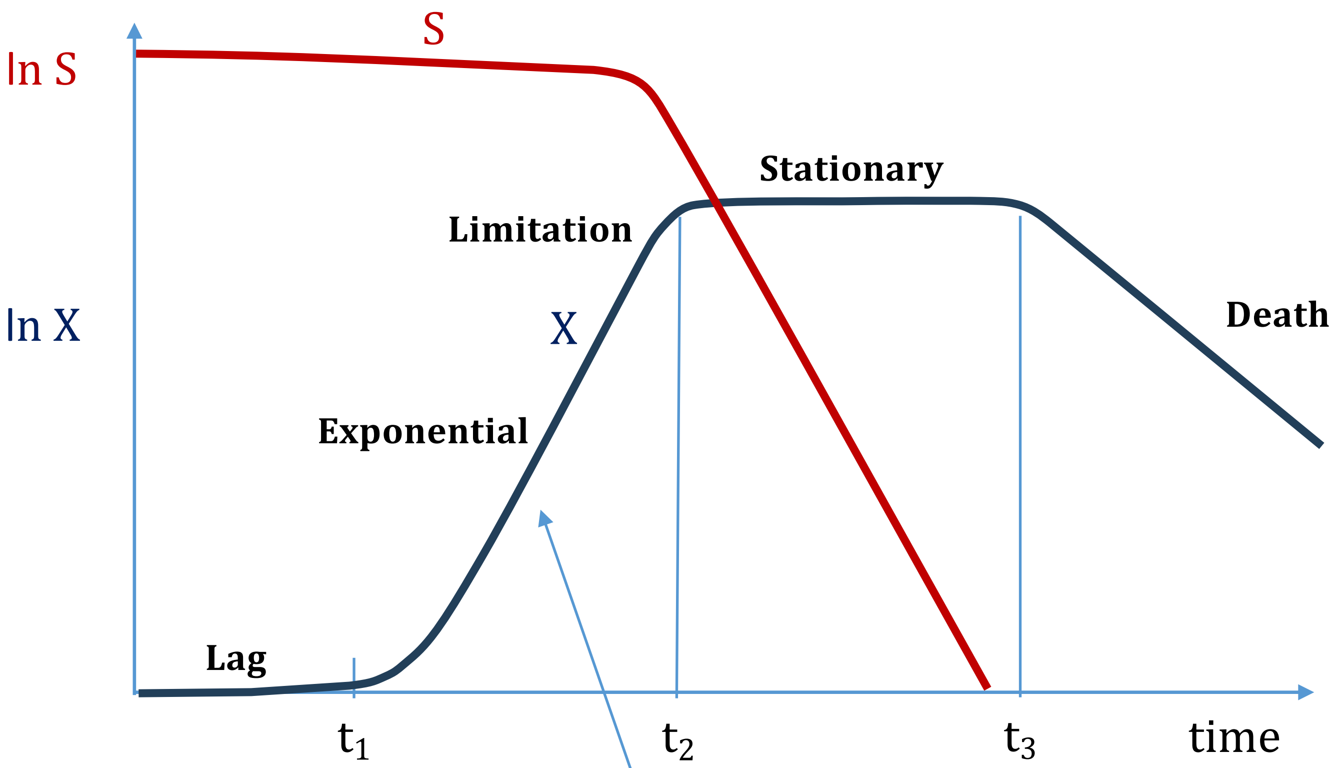


# Basic growth kinetics in a batch




$$r_g = \mu X$$

# Growth kinetics

## Monod Equation

$$r_g = \mu X$$

## Specific Growth Rate

$$\mu = \mu_{max} \frac{S}{S + K_s}$$

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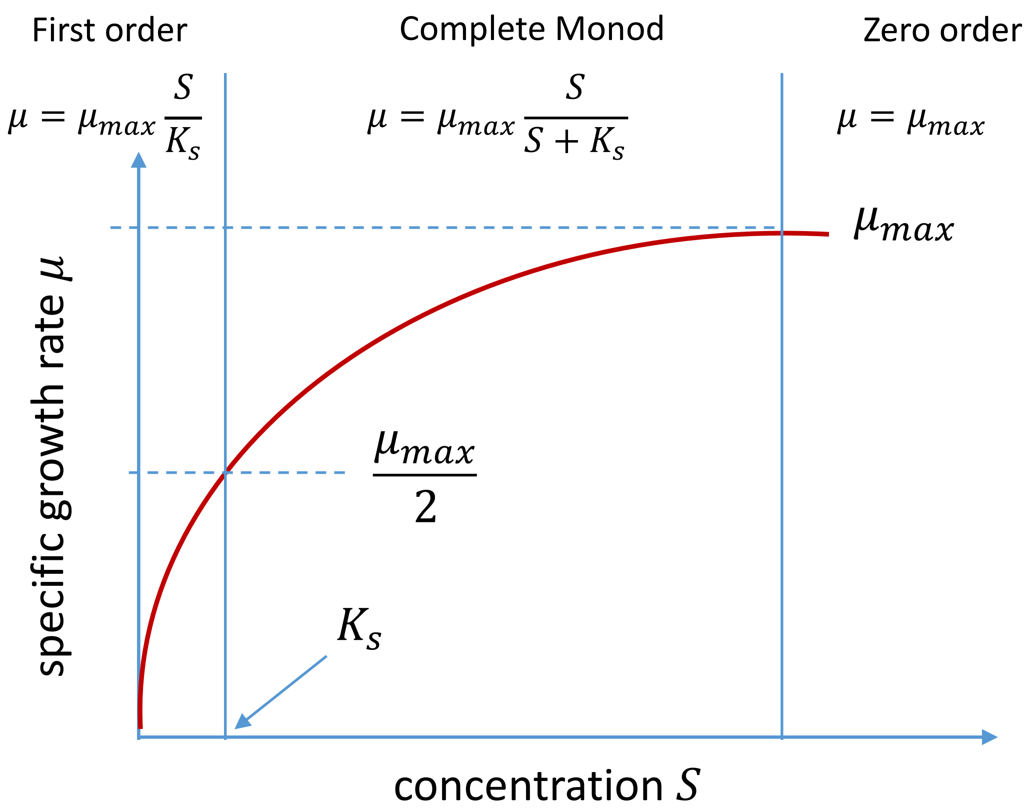

# Mass yield coefficients

The biomass yield on substrate

$$Y_{X/S} = \frac{r_g}{r_s}$$

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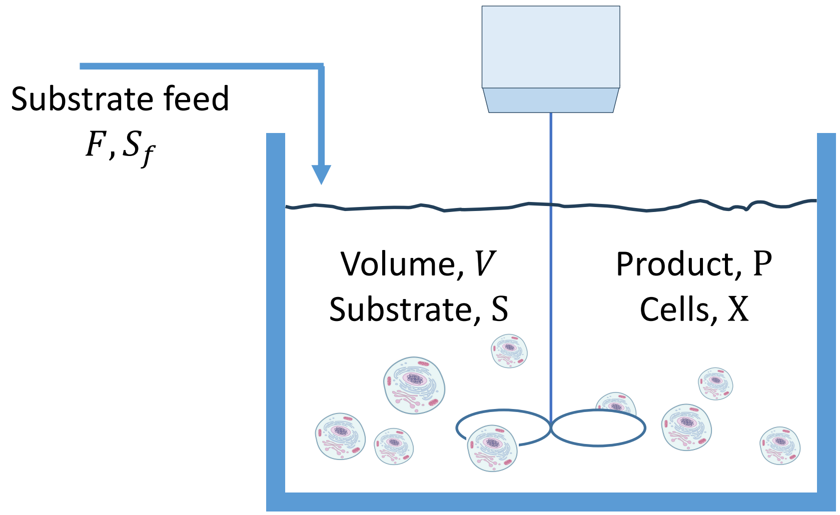
The yield product-biomass

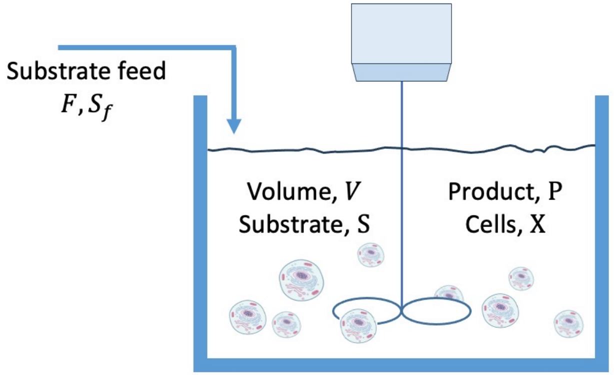
$$Y_{P/X} = \frac{r_p}{r_g} \qquad Y_{P/X} = \frac{mass\ of\ product\ formed}{mass\ of\ new\ cells\ formed}$$

# Fed-batch bioreactors

- Biological reactions typically performed in a batch or fed-batch reactor.
- Fed-batch reactors are widely used in the pharmaceutical and other process industries.



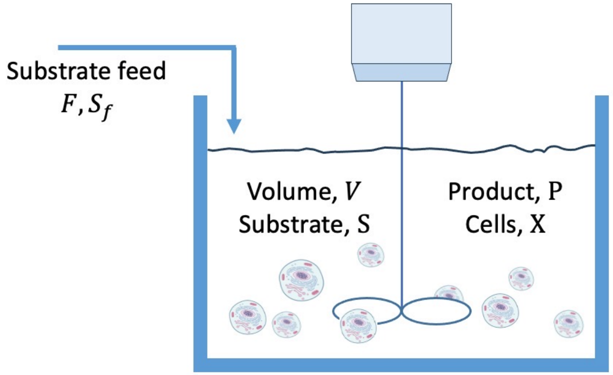
# Fed-batch bioreactors




## Modeling assumptions

1. The exponential cell growth stage
2. Perfectly mixed broth (cells + liquid), homogeneous
3. Isothermal reactor operation
4. The liquid density is constant
5. The cell growth rate $r_g$ given by the Monod equation

# Fed-batch bioreactors




## Modeling assumptions

1. The exponential cell growth stage
2. Perfectly mixed broth (cells + liquid), homogeneous
3. Isothermal reactor operation
4. The liquid density is constant
5. The cell growth rate $r_g$ given by the Monod equation
6. The rate of product formation per unit volume $r_p$ can be expressed as

$$r_p = Y_{P/X} r_g$$

$$Y_{P/X} = \frac{mass\ of\ product\ formed}{mass\ of\ new\ cells\ formed}$$

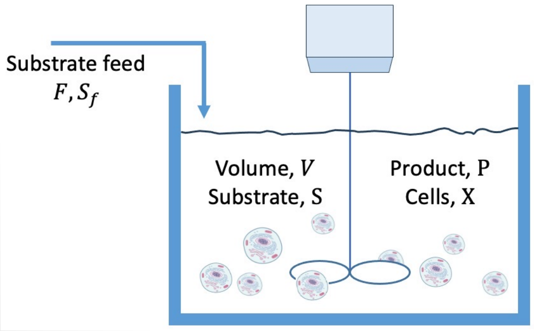
# Fed-batch bioreactors

## Individual Component Balances

$$r_g = \mu_{max} \frac{S}{S + K_s} X$$

Cells:

$$\frac{d(XV)}{dt} = V r_g$$



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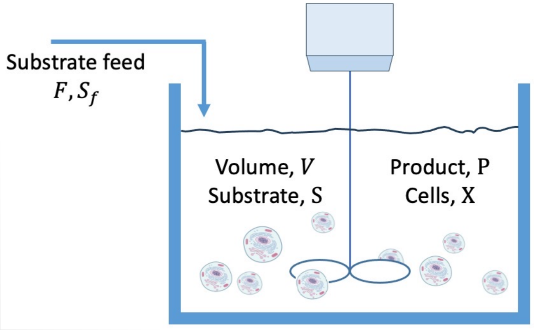
$$\frac{d(PV)}{dt} = V r_p$$



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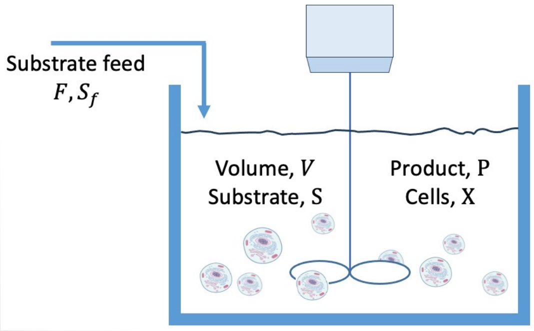
Product:

$$\frac{d(PV)}{dt} = V r_p$$

Substrate:

$$\frac{d(SV)}{dt} = F S_f - \frac{1}{Y_{X/S}} V r_g$$




**Note:** in some books Yield coefficients are defined as

$$Y^*_{X/S} = \frac{mass\ of\ new\ cells\ formed}{mass\ of\ substrate\ consumed\ to\ form\ cells}$$

$$Y^*_{P/S} = \frac{mass\ of\ product\ formed}{mass\ of\ substrate\ consumed\ to\ form\ product}$$

$$\frac{d(SV)}{dt} = F S_f - \frac{1}{Y^*_{X/S}} V r_g - \frac{1}{Y^*_{P/S}} V r_p$$

# Fed-batch bioreactors

Individual Component Balances

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Substrate:

$$\frac{d(SV)}{dt} = F S_f - \frac{1}{Y_{X/S}} V r_g$$

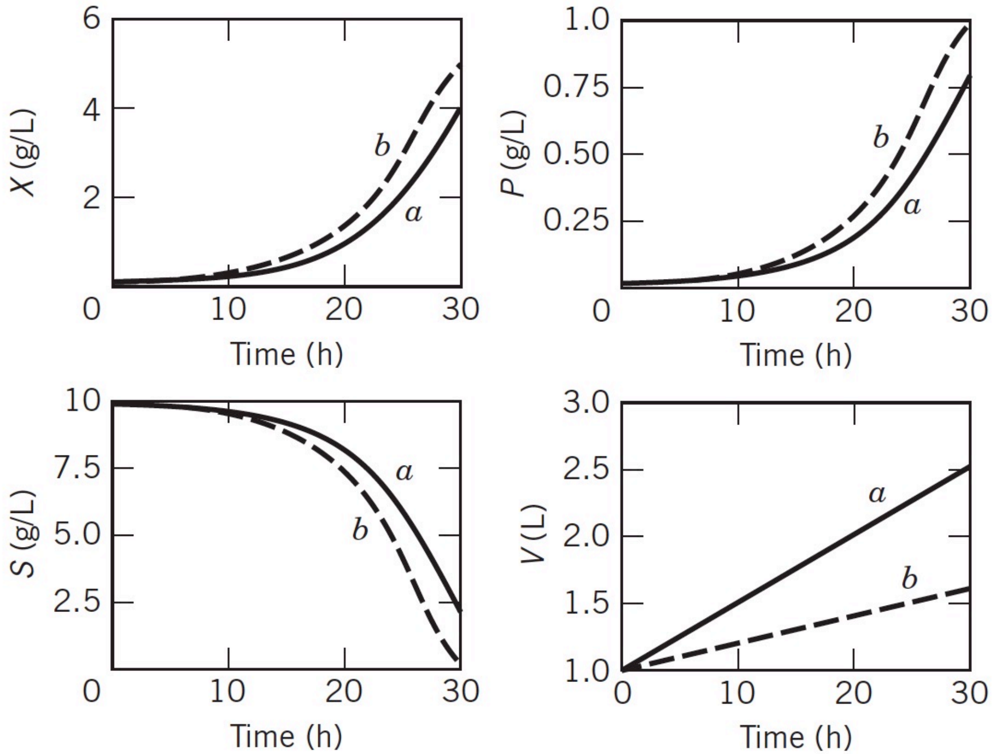
Overall Mass Balance

Mass:

$$\frac{dV}{dt} = F$$

# Fed-batch bioreactor simulation*

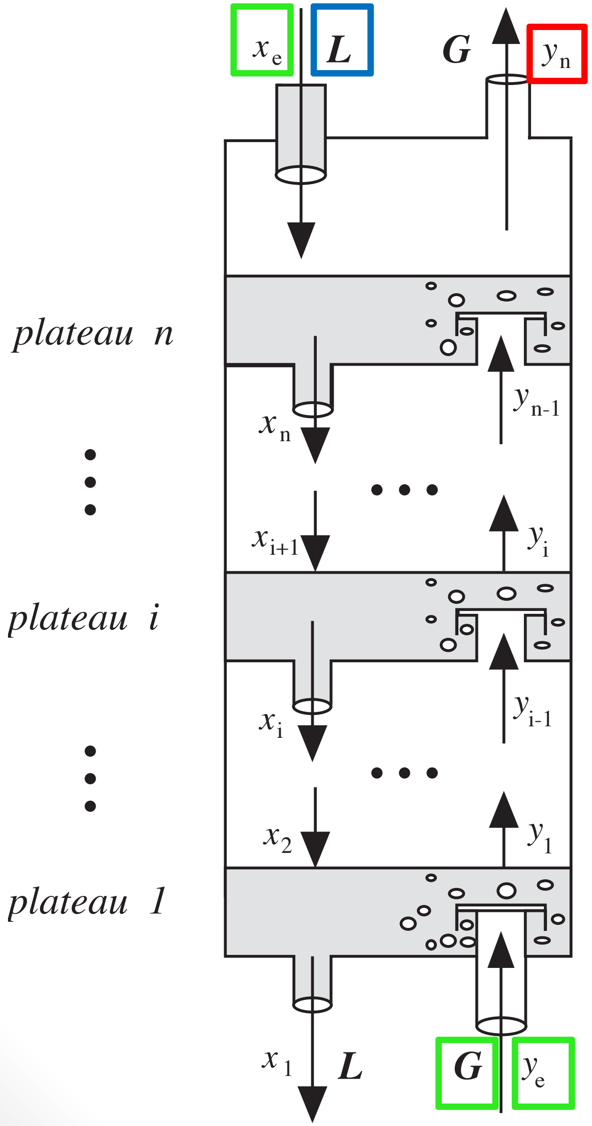
a (solid): F = 0.05 L/h; b (dashed): F = 0.02 L/h).



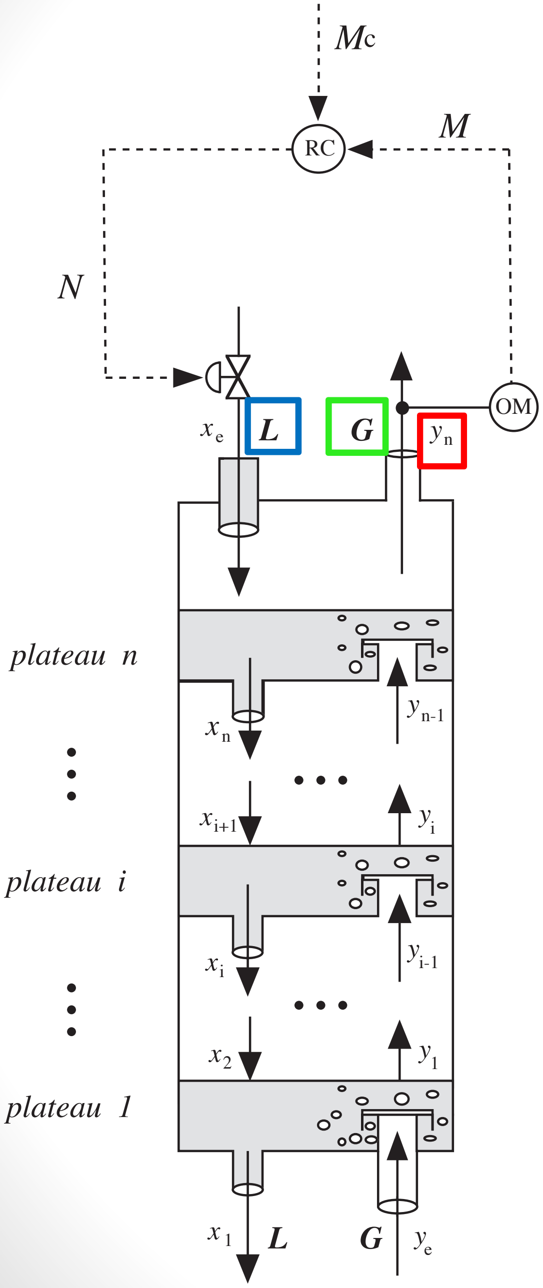

| Model Parameters | | | Simulation Conditions | | |
|---|---|---|---|---|---|
| $\mu_{max}$ | 0.20 | $h^{-1}$ | $S_f$ | 10.0 | g/L |
| $K_S$ | 1.0 | g/L | $X(0)$ | 0.05 | g/L |
| $Y_{X/S}$ | 0.5 | g/g | $S(0)$ | 10.0 | g/L |
| $Y_{P/X}$ | 0.2 | g/g | $P(0)$ | 0.0 | g/L |
| | | | $V(0)$ | 1.0 | L |

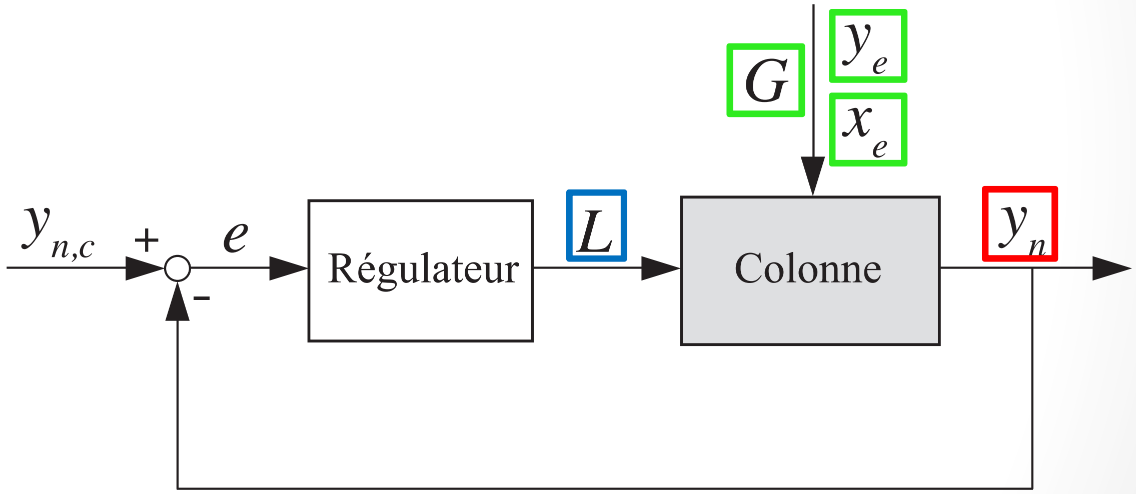
* from Process Dynamic and control by Seborg et al.

# Absorption column



# Control of the absorption column



# State-space representation of systems


$$\dot{y}(t) = -3y(t) + 2u(t)z(t) \quad y(0)$$
$$\dot{z}(t) = 2y(t) - z(t) \quad z(0)$$

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Behavior of $y(t)$ and $z(t)$ for $t \geq 0$ depends on $u(t \geq 0)$ but also on $y(0)$ and $z(0)$!

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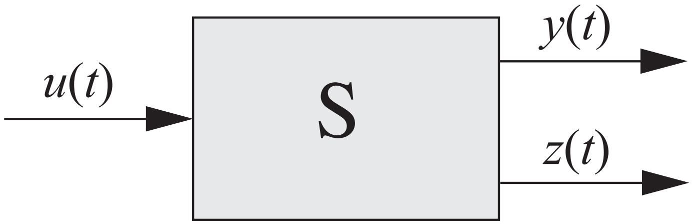



$$\dot{y}(t) = -3y(t) + 2u(t)z(t) \quad y(0)$$
$$\dot{z}(t) = 2y(t) - z(t) \quad z(0)$$

Behavior of $\mathrm{y}(t)$ and $\mathrm{z}(t)$ for $t \geq 0$ depends on $\mathrm{u}(t \geq 0)$ but also on $\mathrm{y}(0)$ and $\mathrm{z}(0)$!

The minimal required information to unambiguously determine future behavior of a dynamic deterministic system for $t \geq t_0$ is:

- the state of system at $t = t_0$
- the knowledge of the future inputs, i.e., $\mathrm{u}(t \geq t_0)$

# State-space models

$$
\left\{
\begin{aligned}
\dot{x}_1(t) &= f_1\left[x_1(t),\ \ldots,\ x_{\mathrm{n}}(t), u_1(t),\ \ldots,\ u_{\mathrm{p}}(t), t\right] && x_1(t_0) = x_{1,\,0} \\
\dot{x}_2(t) &= f_2\left[x_1(t),\ \ldots,\ x_{\mathrm{n}}(t), u_1(t),\ \ldots,\ u_{\mathrm{p}}(t), t\right] && x_2(t_0) = x_{2,\,0} \\
&\ \vdots \\
\dot{x}_{\mathrm{n}}(t) &= f_{\mathrm{n}}\left[x_1(t),\ \ldots,\ x_{\mathrm{n}}(t), u_1(t),\ \ldots,\ u_{\mathrm{p}}(t), t\right] && x_{\mathrm{n}}(t_0) = x_{\mathrm{n},\,0}
\end{aligned}
\right.
$$

$$
\left\{
\begin{aligned}
y_1(t) &= g_1\left[x_1(t),\ \ldots,\ x_{\mathrm{n}}(t), u_1(t),\ \ldots,\ u_{\mathrm{p}}(t), t\right] \\
y_2(t) &= g_2\left[x_1(t),\ \ldots,\ x_{\mathrm{n}}(t), u_1(t),\ \ldots,\ u_{\mathrm{p}}(t), t\right] \\
&\ \vdots \\
y_{\mathrm{q}}(t) &= g_{\mathrm{q}}\left[x_1(t),\ \ldots,\ x_{\mathrm{n}}(t), u_1(t),\ \ldots,\ u_{\mathrm{p}}(t), t\right]
\end{aligned}
\right.
$$

# State-space models

$$x(t)=\begin{bmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_n(t) \end{bmatrix} \qquad u(t)=\begin{bmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_p(t) \end{bmatrix} \qquad y(t)=\begin{bmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_q(t) \end{bmatrix}$$

**Vector of states** **Vector of inputs** **Vector of outputs**

**State equation**

$$\dot{x}(t)=f\left[x(t),\, u(t),\, t\right] \qquad x(t_0)=x_0$$

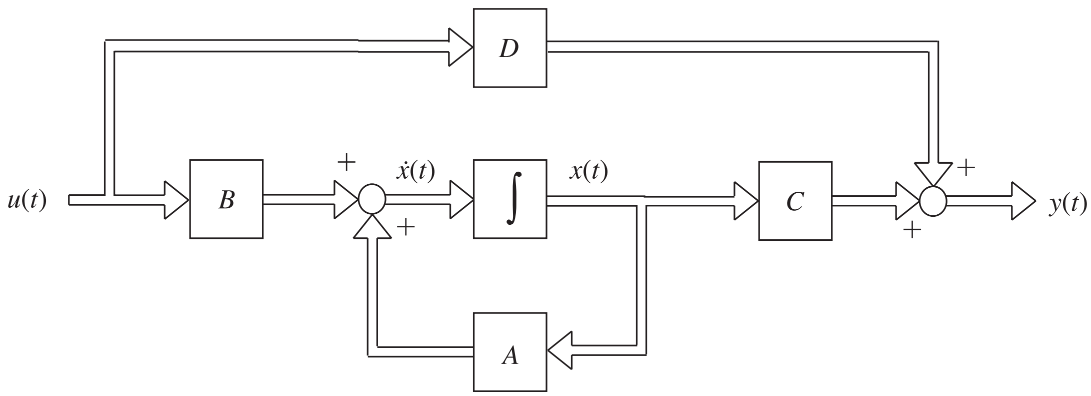
**Output equation**

$$y(t)=g\left[x(t),\, u(t),\, t\right]$$

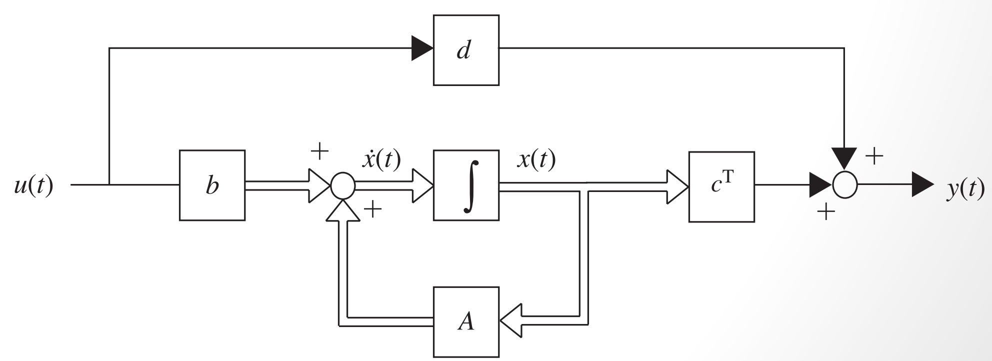
# Linear, stationary, state-space models

$$\dot{x}(t) = Ax(t) + Bu(t) \quad x(0) = x_0$$

$$y(t) = Cx(t) + Du(t)$$

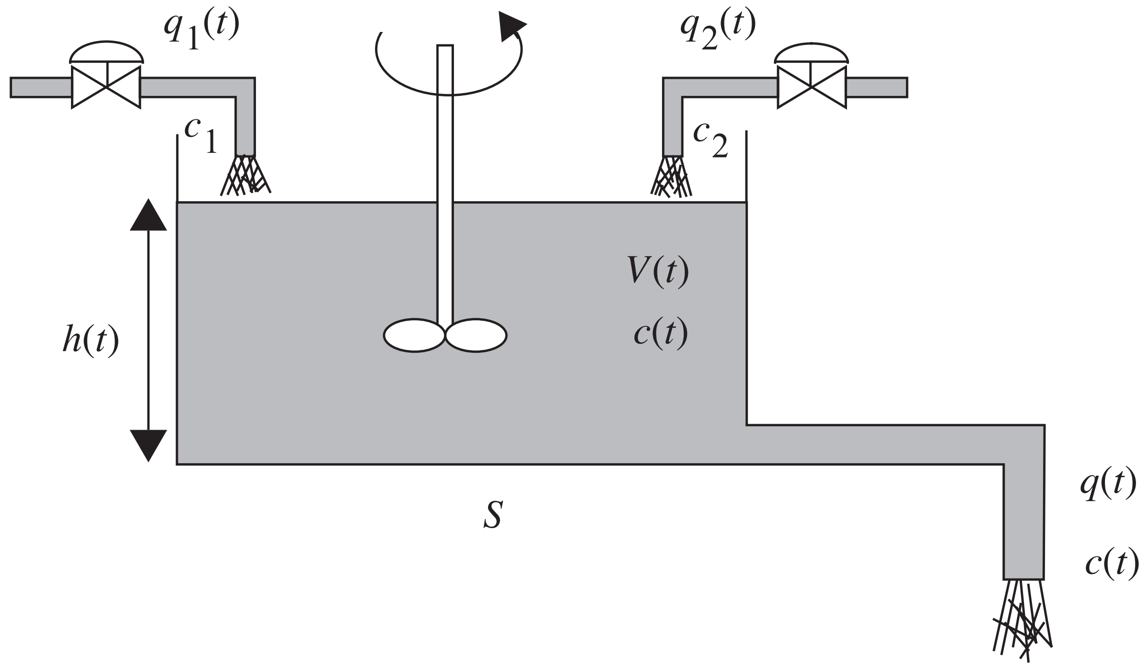



Multivariable




Monovariable

# Mixing tank example




$$q(t) = k\sqrt{h(t)}$$

$$\rho S \frac{\mathrm{d}}{\mathrm{d}t} h(t) = \rho q_1(t) + \rho q_2(t) - \rho q(t) \qquad \left[\frac{\text{kg}}{\text{s}}\right]$$

$$\rho S \frac{\mathrm{d}}{\mathrm{d}t} \left[c(t) h(t)\right] = \rho c_1 q_1(t) + \rho c_2 q_2(t) - \rho c(t) q(t) \qquad \left[\frac{\text{kgP}}{\text{s}}\right]$$

# Mixing tank state-space model

$$x_1(t) = h(t)$$
$$x_2(t) = c(t)$$

**states**

$$u_1(t) = q_1(t)$$
$$u_2(t) = q_2(t)$$

**inputs**

$$y_1(t) = h(t)$$
$$y_2(t) = \frac{c(t)}{c_1}$$

**outputs**

$$\dot{x}_1(t) = \frac{1}{S}\left[u_1(t) + u_2(t) - k\sqrt{x_1(t)}\right] \qquad x_1(0) = h(0)$$

$\rightarrow$

$$\dot{x}_2(t) = \frac{1}{Sx_1(t)}\left\{\left[c_1 - x_2(t)\right]u_1(t) + \left[c_2 - x_2(t)\right]u_2(t)\right\} \qquad x_2(0) = c(0)$$

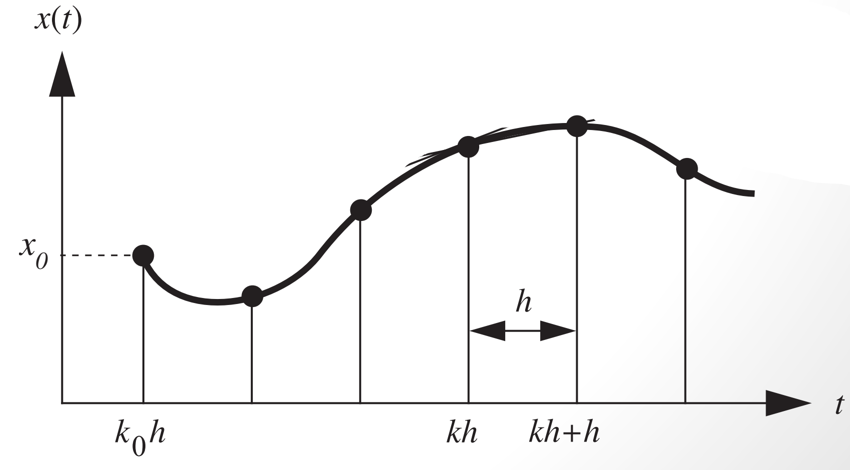
# Once having a nonlinear model – what to do?

**Simulation:** Determine the state $x(t)$ and the output $y(t)$ for $t \geq t_0$ starting from $x(t_0)$ and using the knowledge of $u(t)$ for $t \geq t_0$.

**For** $t = kh$

$$\dot{x}(kh) = f\left[x(kh),\, u(kh)\right] \qquad x(k_0 h) = x_0$$

$$y(kh) = g\left[x(kh),\, u(kh)\right]$$



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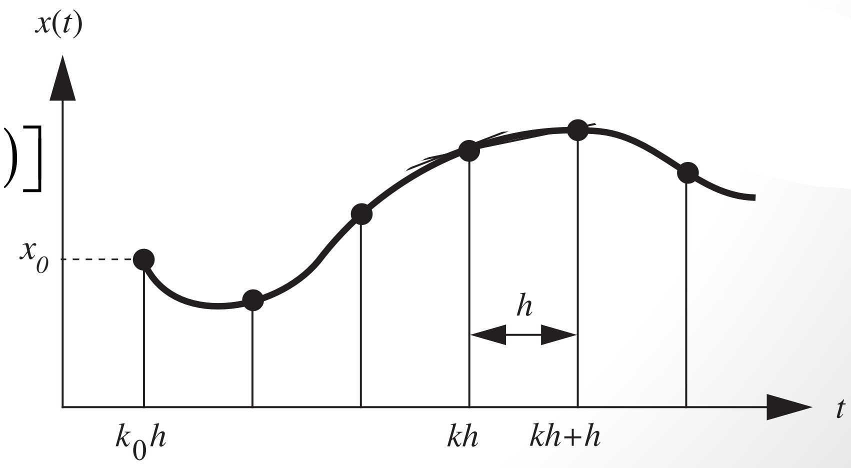
$$\dot{x}(kh) = f[x(kh), u(kh)] \qquad x(k_0 h) = x_0$$

$$y(kh) = g[x(kh), u(kh)]$$

**Euler**

$$\dot{x}(kh) \simeq \frac{x(kh+h) - x(kh)}{h}$$

$$x(kh+h) = x(kh) + hf[x(kh), u(kh)]$$



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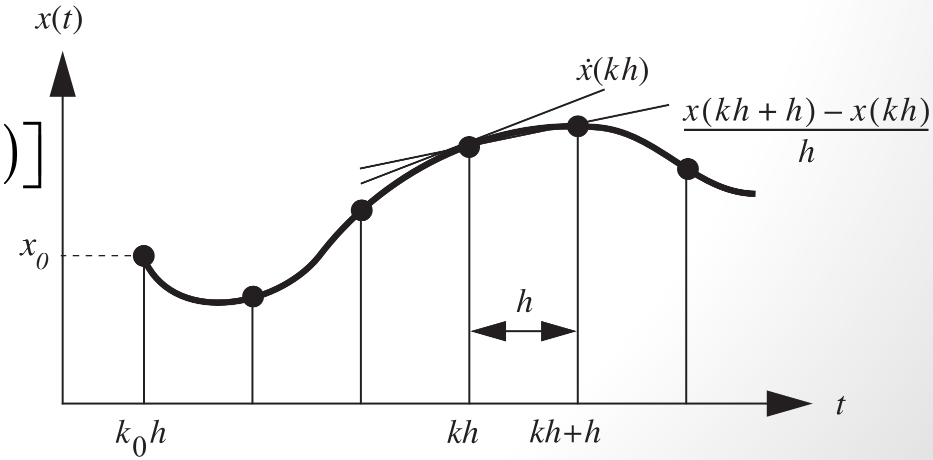


# Exact (feedback) linearization

Nonlinear model

$$\dot{x}_1(t) = \frac{1}{S}\left[u_1(t) + u_2(t) - k\sqrt{x_1(t)}\right]$$

$$A\dot{h}(t) = u(t) - k\sqrt{h(t)}$$

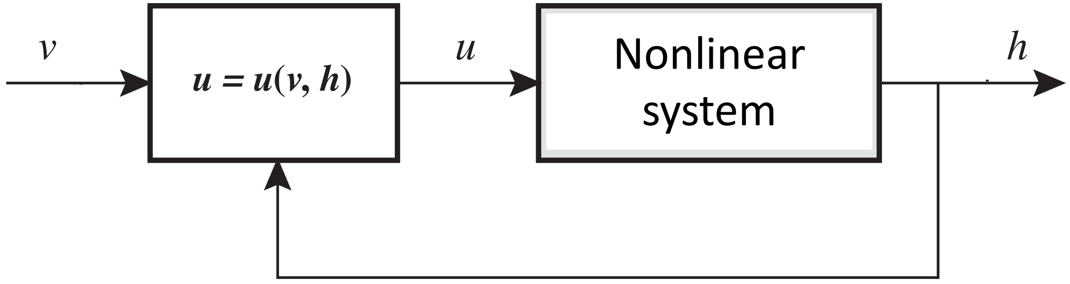
# Exact (feedback) linearization

Nonlinear model

$$A\dot{h}(t) = u(t) - k\sqrt{h(t)}$$

If we could measure $h(t)$, then we could define a new input that satisfies

$$u(t) - k\sqrt{h(t)} = Av(t)$$



# Exact (feedback) linearization

Nonlinear model

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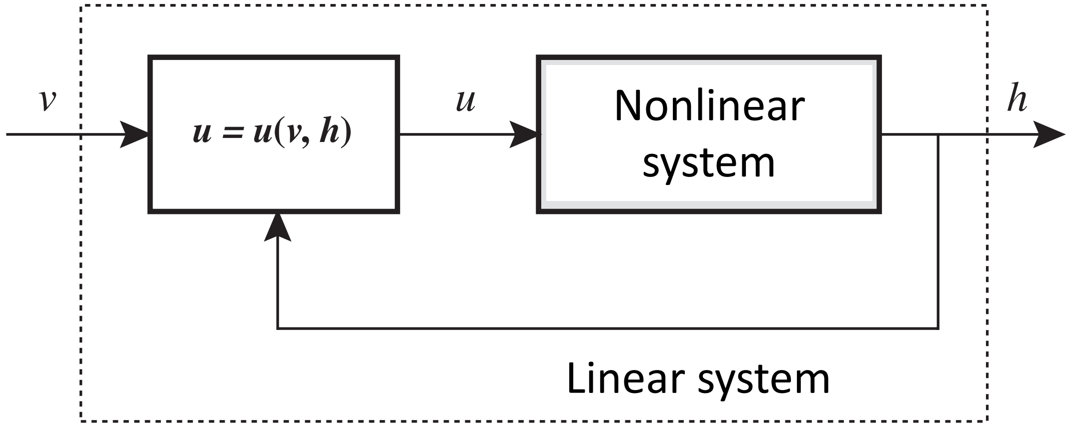
If we could measure $h(t)$, then we could define a new input that satisfies

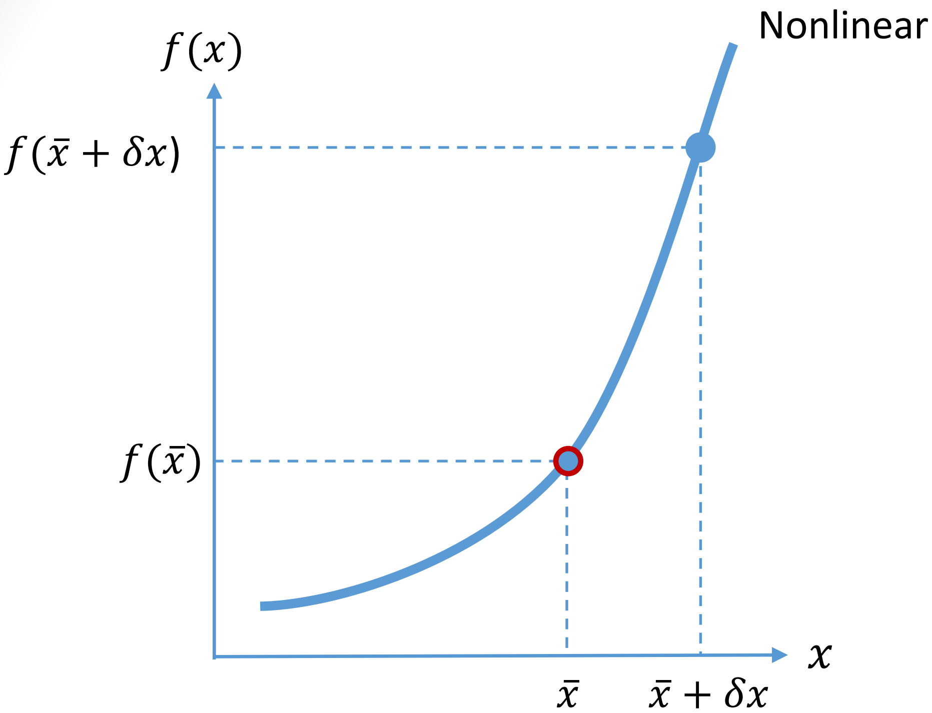
$$u(t) - k\sqrt{h(t)} = Av(t)$$

And our system becomes linear:

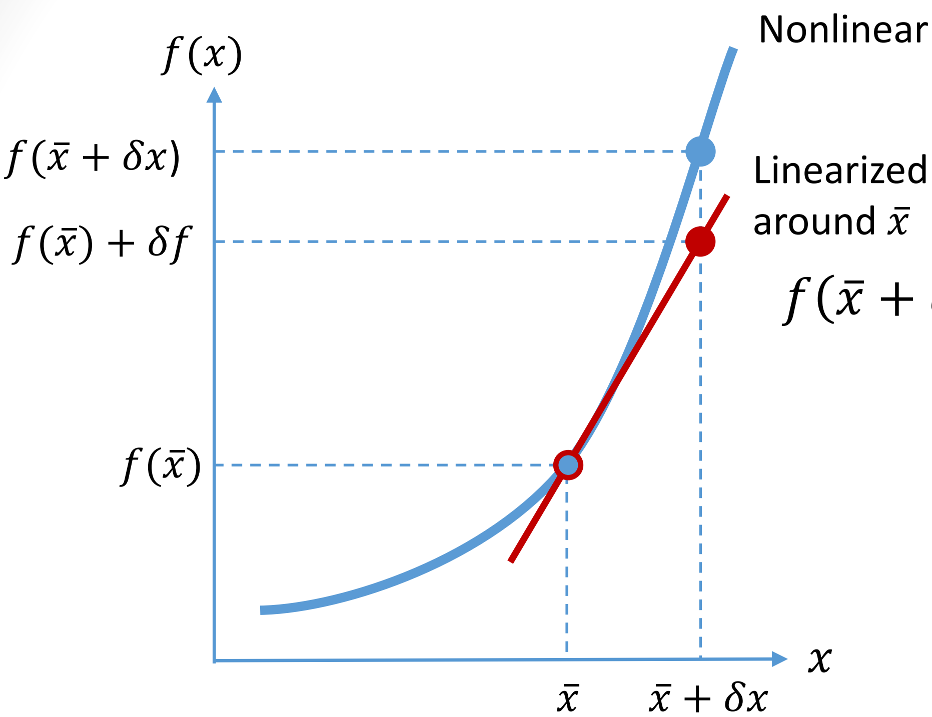
$$\dot{h}(t) = v(t)$$



# Approximate linearization

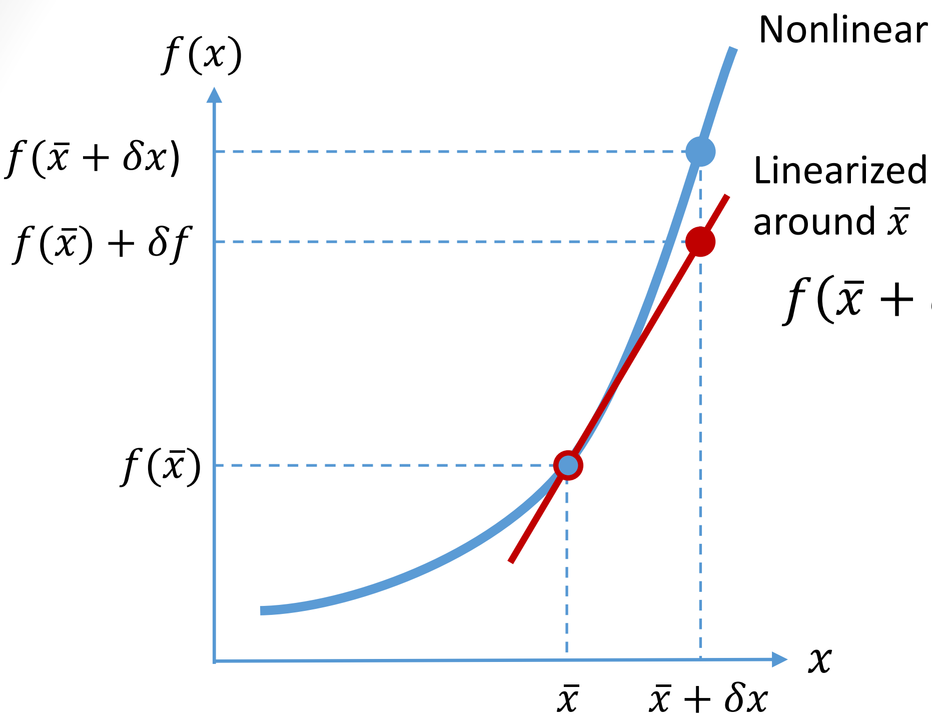


# Approximate linearization




$$f(\bar{x}+\delta x) \cong f(\bar{x}) + \frac{df}{dx}(\bar{x})\,\delta x = f(\bar{x}) + \delta f$$

# Approximate linearization




$$f(\bar{x}+\delta x) \cong f(\bar{x}) + \frac{df}{dx}(\bar{x})\,\delta x = f(\bar{x}) + \delta f$$

Depending on the control problem (tracking or regulation), we can perform linearization around:

**Nominal trajectories**

$$\dot{\bar{x}} = f\left[\bar{x}(t), \bar{u}(t), t\right] \qquad \bar{x}(0) = x_0$$

$$\bar{y}(t) = g\left[\bar{x}(t), \bar{u}(t), t\right]$$

**Stationary point**

$$0 = f\left[\bar{x}, \bar{u}\right]$$

$$\bar{y} = g\left[\bar{x}, \bar{u}\right]$$

# Linearization procedure
(around a stationary point)

$$\dot{x}(t) = f\left[x(t), u(t)\right] \qquad x(0) = x_0$$

$$y(t) = g\left[x(t), u(t)\right]$$

**Equilibrium point**

$$0 = f\left[\bar{x}, \bar{u}\right]$$

$$\bar{y} = g\left[\bar{x}, \bar{u}\right]$$

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(around a stationary point)

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$$y(t) = g\left[x(t), u(t)\right]$$

**Equilibrium point**

$$0 = f\left[\bar{x}, \bar{u}\right]$$
$$\bar{y} = g\left[\bar{x}, \bar{u}\right]$$

**Taylor series**

$$\dot{x} = f\left[\bar{x}, \bar{u}\right] + \left.\frac{\partial f}{\partial x}\right|_{\bar{u}, \bar{x}} (x - \bar{x}) + \left.\frac{\partial f}{\partial u}\right|_{\bar{u}, \bar{x}} (u - \bar{u}) + \text{Higher-order terms (h.o.t.)}$$
$$y = g\left[\bar{x}, \bar{u}\right] + \left.\frac{\partial g}{\partial x}\right|_{\bar{u}, \bar{x}} (x - \bar{x}) + \left.\frac{\partial g}{\partial u}\right|_{\bar{u}, \bar{x}} (u - \bar{u}) + \text{Higher-order terms (h.o.t.)}$$

# Linearization procedure (cont'd)

$$\dot{x} = f[\bar{x}, \bar{u}] + \left.\frac{\partial f}{\partial x}\right|_{\bar{u},\, \bar{x}} (x - \bar{x}) + \left.\frac{\partial f}{\partial u}\right|_{\bar{u},\, \bar{x}} (u - \bar{u})$$

$$y = g[\bar{x}, \bar{u}] + \underbrace{\left.\frac{\partial g}{\partial x}\right|_{\bar{u},\, \bar{x}} \underbrace{(x - \bar{x})}_{\delta x}}_{\delta y_x} + \underbrace{\left.\frac{\partial g}{\partial u}\right|_{\bar{u},\, \bar{x}} \underbrace{(u - \bar{u})}_{\delta u}}_{\delta y_u}$$

# Linearization procedure (cont'd)

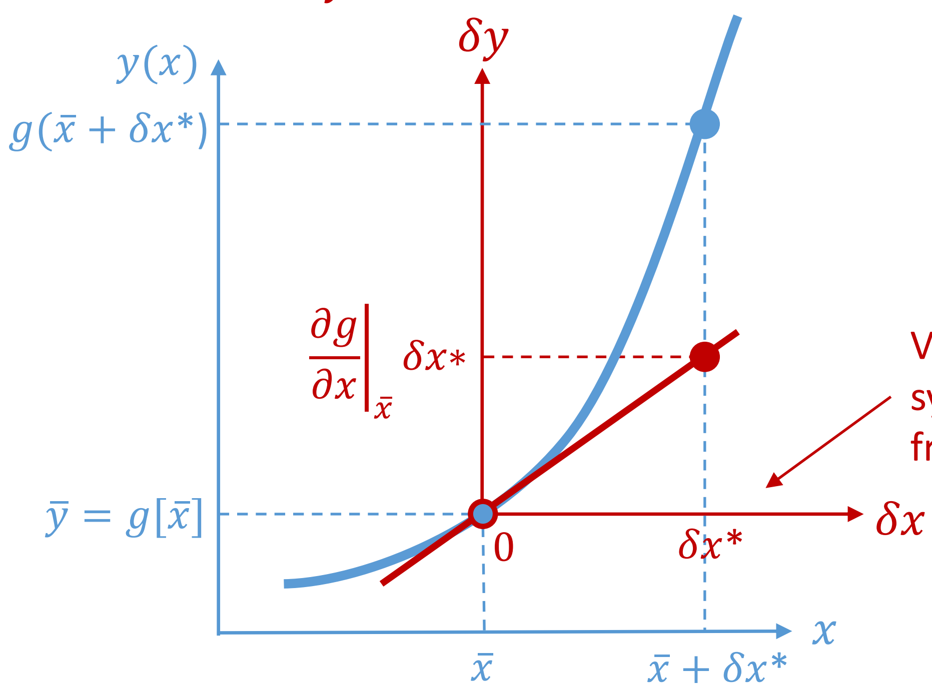
$$\dot{x} = f[\bar{x}, \bar{u}] + \left.\frac{\partial f}{\partial x}\right|_{\bar{u},\,\bar{x}} (x - \bar{x}) + \left.\frac{\partial f}{\partial u}\right|_{\bar{u},\,\bar{x}} (u - \bar{u})$$

$$y = g[\bar{x}, \bar{u}] + \left.\frac{\partial g}{\partial x}\right|_{\bar{u},\,\bar{x}} (x - \bar{x}) + \left.\frac{\partial g}{\partial u}\right|_{\bar{u},\,\bar{x}} (u - \bar{u})$$

$\delta x$

$\delta y$

For illustration purposes, consider only one argument $x$, i.e., neglect $u$




Variables in the linearized system are **deviations** from $\bar{x}$ and $\bar{y}$

# Linearization procedure (cont'd)

$$\dot{x} = f[\bar{x}, \bar{u}] + \left.\frac{\partial f}{\partial x}\right|_{\bar{u},\,\bar{x}} (x - \bar{x}) + \left.\frac{\partial f}{\partial u}\right|_{\bar{u},\,\bar{x}} (u - \bar{u})$$

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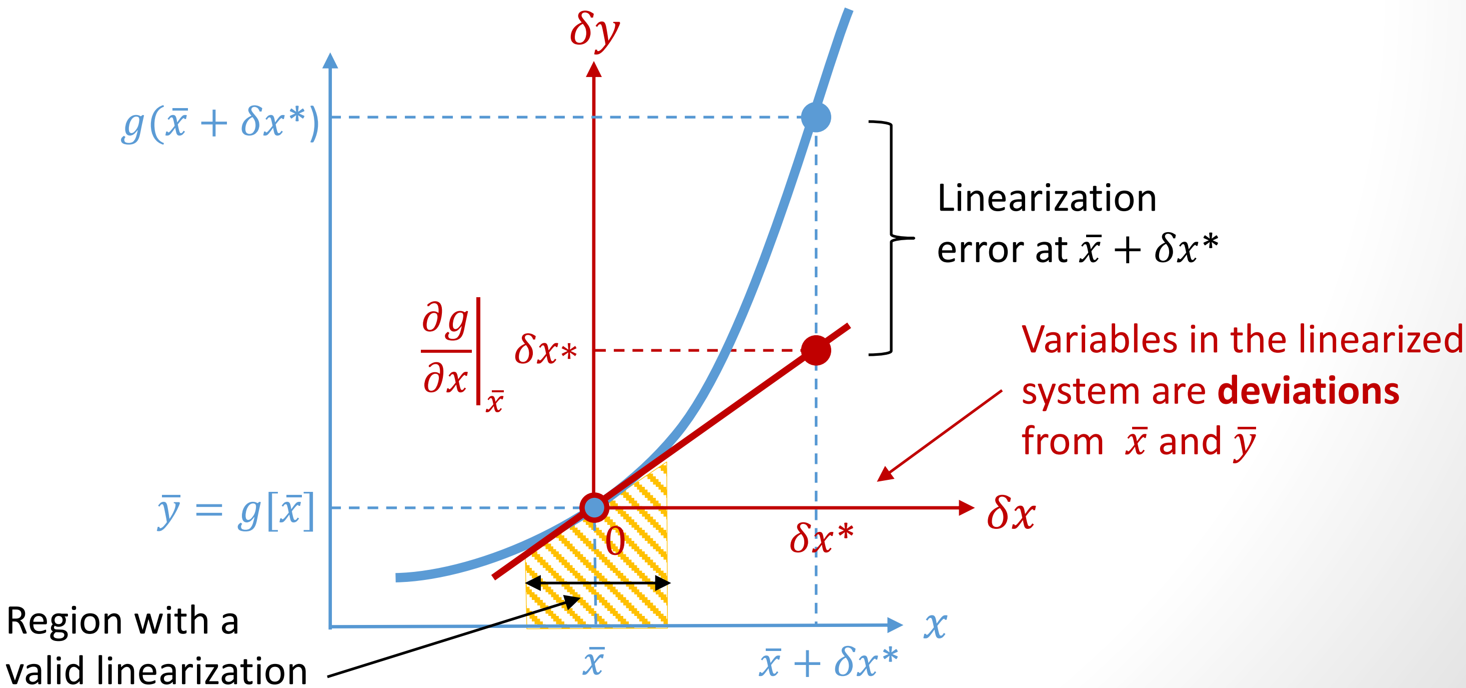

# Linearization procedure (cont'd)

**Deviations**

$$\delta x(t) := x(t) - \bar{x}$$
$$\delta u(t) := u(t) - \bar{u}$$
$$\delta y(t) := y(t) - \bar{y}$$

$$\dot{x} = f[\bar{x}, \bar{u}] + \left.\frac{\partial f}{\partial x}\right|_{\bar{u}, \bar{x}} (x - \bar{x}) + \left.\frac{\partial f}{\partial u}\right|_{\bar{u}, \bar{x}} (u - \bar{u}) + \text{h.o.t.}$$

$$y = g[\bar{x}, \bar{u}] + \left.\frac{\partial g}{\partial x}\right|_{\bar{u}, \bar{x}} (x - \bar{x}) + \left.\frac{\partial g}{\partial u}\right|_{\bar{u}, \bar{x}} (u - \bar{u}) + \text{h.o.t.}$$

# Linearization procedure (cont'd)

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**Linear approximation**

$$\delta \dot{x} = \left.\frac{\partial f}{\partial x}\right|_{\bar{u},\, \bar{x}} \delta x + \left.\frac{\partial f}{\partial u}\right|_{\bar{u},\, \bar{x}} \delta u \qquad \delta x(0) = x_0 - \bar{x}$$

$$\delta y = \left.\frac{\partial g}{\partial x}\right|_{\bar{u},\, \bar{x}} \delta x + \left.\frac{\partial g}{\partial u}\right|_{\bar{u},\, \bar{x}} \delta u$$

$$\delta \dot{x} = A\delta x + B\delta u \qquad \delta x(0) = x_0 - \bar{x}$$

$$\delta y = C\delta x + D\delta u$$

# Toy example: method 1

$$\dot{x} = -2x + 0,5(x+1)u \qquad x(0) = 1$$

**Equlibrium point**

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For $\bar{u} = 2$ , we obtain $\bar{x} = 1$

**Linear approximation of the nonlinearity**

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**Linear approximation of the nonlinearity**

$$xu \simeq \bar{x}\bar{u} + \bar{u}(x-\bar{x}) + \bar{x}(u-\bar{u})$$

**Deviations**

$$\delta x := x - \bar{x} \qquad \delta u := u - \bar{u}$$

$$xu \cong \bar{x}\bar{u} + \bar{u}\delta x + \bar{x}\delta u$$

**Linear approximation of the overall system**

$$\dot{x} = \left[-2x + 0,5(\bar{x}\bar{u} + \bar{u}\delta x + \bar{x}\delta u) + 0,5u\right]$$

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**Linear approximation of the overall system**

$$\dot{x} = \left[-2x + 0,5(\bar{x}\bar{u} + \bar{u}\delta x + \bar{x}\delta u) + 0,5u\right] - \left[-2\bar{x} + 0,5\bar{x}\bar{u} + 0,5\bar{u}\right]$$

$$= -2\delta x + 0,5(\bar{u}\delta x + \bar{x}\delta u) + 0,5\delta u$$

$$\delta\dot{x} = \dot{x}$$

$$\delta\dot{x} = -\delta x + \delta u \qquad \delta x(0) = 0$$

# Reminder: state-space matrices

**Linear approximation**

$$\delta\dot{x} = \left.\frac{\partial f}{\partial x}\right|_{\bar{u},\,\bar{x}} \delta x + \left.\frac{\partial f}{\partial u}\right|_{\bar{u},\,\bar{x}} \delta u \qquad \delta x(0) = x_0 - \bar{x}$$

$$\delta y = \left.\frac{\partial g}{\partial x}\right|_{\bar{u},\,\bar{x}} \delta x + \left.\frac{\partial g}{\partial u}\right|_{\bar{u},\,\bar{x}} \delta u$$

$$\delta\dot{x} = A\delta x + B\delta u \quad \delta x(0) = x_0 - \bar{x}$$

$$\delta y = C\delta x + D\delta u$$

**State-space representation of linear system**

$$\dot{x}(t) = Ax(t) + Bu(t) \quad x(0) = x_0$$

$$y(t) = Cx(t) + Du(t)$$

# State-space matrices

$$A:=\left.\frac{\partial f}{\partial x}\right|_{\bar{u},\bar{x}}=\left.\begin{bmatrix}\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n}\\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n}\\ \vdots & \vdots & \vdots & \vdots\\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n}\end{bmatrix}\right|_{\bar{u},\bar{x}}\qquad (n\times n)$$

$$B:=\left.\frac{\partial f}{\partial u}\right|_{\bar{u},\bar{x}}=\left.\begin{bmatrix}\frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} & \cdots & \frac{\partial f_1}{\partial u_p}\\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} & \cdots & \frac{\partial f_2}{\partial u_p}\\ \vdots & \vdots & \vdots & \vdots\\ \frac{\partial f_n}{\partial u_1} & \frac{\partial f_n}{\partial u_2} & \cdots & \frac{\partial f_n}{\partial u_p}\end{bmatrix}\right|_{\bar{u},\bar{x}}\qquad (n\times p)$$

$$C:=\left.\frac{\partial g}{\partial x}\right|_{\bar{u},\bar{x}}=\left.\begin{bmatrix}\frac{\partial g_1}{\partial x_1} & \frac{\partial g_1}{\partial x_2} & \cdots & \frac{\partial g_1}{\partial x_n}\\ \frac{\partial g_2}{\partial x_1} & \frac{\partial g_2}{\partial x_2} & \cdots & \frac{\partial g_2}{\partial x_n}\\ \vdots & \vdots & \vdots & \vdots\\ \frac{\partial g_q}{\partial x_1} & \frac{\partial g_q}{\partial x_2} & \cdots & \frac{\partial g_q}{\partial x_n}\end{bmatrix}\right|_{\bar{u},\bar{x}}\qquad (q\times n)$$

$$D:=\left.\frac{\partial g}{\partial u}\right|_{\bar{u},\bar{x}}=\left.\begin{bmatrix}\frac{\partial g_1}{\partial u_1} & \frac{\partial g_1}{\partial u_2} & \cdots & \frac{\partial g_1}{\partial u_p}\\ \frac{\partial g_2}{\partial u_1} & \frac{\partial g_2}{\partial u_2} & \cdots & \frac{\partial g_2}{\partial u_p}\\ \vdots & \vdots & \vdots & \vdots\\ \frac{\partial g_q}{\partial u_1} & \frac{\partial g_q}{\partial u_2} & \cdots & \frac{\partial g_q}{\partial u_p}\end{bmatrix}\right|_{\bar{u},\bar{x}}\qquad (q\times p)$$

# Toy example: method 2

$$\dot{x} = -2x + 0{,}5\left(x+1\right)u \qquad x\left(0\right) = 1$$

Monovariable system: $n = p = 1$

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$$\dot{x} = -2x + 0{,}5(x+1)u \qquad x(0) = 1$$

Monovariable system: $n = p = 1$

$$\dot{x} = f(x,u) \;\rightarrow f(x,u) = -2x + 0.5xu + 0.5u$$

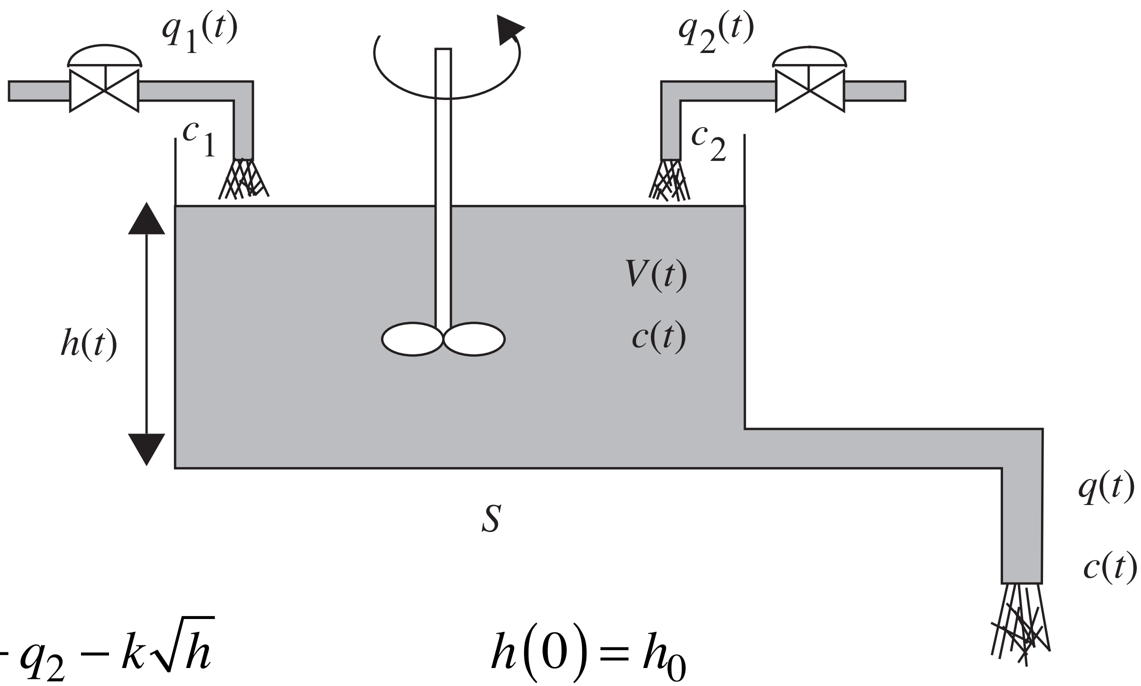
$$A = \left.\frac{\partial f(x,u)}{\partial x}\right|_{\bar{x},\bar{u}} = \left.\frac{\partial(-2x + 0.5xu + 0.5u)}{\partial x}\right|_{\bar{x},\bar{u}} = -2 + 0.5\bar{u} = -1$$

$$B = \left.\frac{\partial f(x,u)}{\partial u}\right|_{\bar{x},\bar{u}} = 0.5\bar{x} + 0.5 = 1$$

$$\delta\dot{x} = A\delta x + B\delta u = -\delta x + \delta u$$

$$\delta x(0) = x(0) - \bar{x} = 0$$

# Mixing tank




$$S\dot{h} = q_1 + q_2 - k\sqrt{h} \qquad h(0) = h_0$$

$$\dot{c} = \frac{q_1}{Sh}(c_1 - c) + \frac{q_2}{Sh}(c_2 - c) \qquad c(0) = c_0$$

$$y_1 = h$$

$$y_2 = \frac{c}{c_1}$$

**Multivariable system** $n = p = q = 2$

# Mixing tank (cont'd)

**Operating point**

$$\left(\bar{q}_1, \bar{q}_2, \bar{h}, \bar{c}\right)$$

$$\overline{q_1}, \overline{q_2} \rightarrow \overline{u_1}, \overline{u_2}$$

$$\bar{h}, \bar{c} \rightarrow \overline{x_1}, \overline{x_2}$$

**Multivariable system** $n = p = q = 2$

$$A = \left.\frac{\partial f(x,u)}{\partial x}\right|_{\bar{x},\bar{u}} = \left.\begin{bmatrix} \frac{\partial f_1(x,u)}{\partial x_1} & \frac{\partial f_1(x,u)}{\partial x_2} \\ \frac{\partial f_2(x,u)}{\partial x_1} & \frac{\partial f_2(x,u)}{\partial x_2} \end{bmatrix}\right|_{\bar{x},\bar{u}}$$

$$\dot{h} = (q_1 + q_2 - k\sqrt{h})/S \rightarrow f_1$$

$$\dot{c} = \frac{q_1}{Sh}(c_1 - c) + \frac{q_2}{Sh}(c_2 - c) \rightarrow f_2$$

# Mixing tank (cont'd)

**Operating point**

$$\left(\bar{q}_1, \bar{q}_2, \bar{h}, \bar{c}\right)$$

$$\overline{q_1}, \overline{q_2} \rightarrow \overline{u_1}, \overline{u_2}$$

$$\bar{h}, \bar{c} \quad \rightarrow \overline{x_1}, \overline{x_2}$$

**Multivariable system** $n = p = q = 2$

$$A = \left.\frac{\partial f(x,u)}{\partial x}\right|_{\bar{x},\bar{u}} = \left.\begin{bmatrix} \frac{\partial f_1(x,u)}{\partial x_1} & \frac{\partial f_1(x,u)}{\partial x_2} \\ \frac{\partial f_2(x,u)}{\partial x_1} & \frac{\partial f_2(x,u)}{\partial x_2} \end{bmatrix}\right|_{\bar{x},\bar{u}}$$

$$\dot{h} = (q_1 + q_2 - k\sqrt{h})/S \quad \rightarrow f_1$$

$$\dot{c} = \frac{q_1}{Sh}(c_1 - c) + \frac{q_2}{Sh}(c_2 - c) \rightarrow f_2$$

$$a_{11} = \left.\frac{\partial f_1}{\partial h}\right|_{eq.p.} = -\frac{k}{2S\sqrt{\bar{h}}} \qquad a_{12} = \left.\frac{\partial f_1}{\partial c}\right|_{eq.p.} = 0$$

$$a_{21} = \left.\frac{\partial f_2}{\partial h}\right|_{eq.p.} = -\frac{\overline{q_1}}{S\bar{h}^2}(c_1 - \bar{c}) - \frac{\overline{q_2}}{S\bar{h}^2}(c_2 - \bar{c}) = \frac{1}{S\bar{h}^2}\left[\bar{c}(\overline{q_1} + \overline{q_2}) - c_1\overline{q_1} - c_2\overline{q_2}\right]$$

$$a_{22} = \left.\frac{\partial f_2}{\partial c}\right|_{eq.p.} = -\frac{\overline{q_1}}{S\bar{h}} - \frac{\overline{q_2}}{S\bar{h}}$$

# Mixing tank (cont'd)

$$B = \left.\frac{\partial f(x,u)}{\partial u}\right|_{\bar{x},\bar{u}} = \left.\begin{bmatrix} \frac{\partial f_1(x,u)}{\partial u_1} & \frac{\partial f_1(x,u)}{\partial u_2} \\ \frac{\partial f_2(x,u)}{\partial u_1} & \frac{\partial f_2(x,u)}{\partial u_2} \end{bmatrix}\right|_{\bar{x},\bar{u}}$$

$$\dot{h} = (q_1 + q_2 - k\sqrt{h})/S \quad \rightarrow f_1$$

$$\dot{c} = \frac{q_1}{Sh}(c_1 - c) + \frac{q_2}{Sh}(c_2 - c) \rightarrow f_2$$

$$b_{11} = \left.\frac{\partial f_1}{\partial q_1}\right|_{eq.p.} = \frac{1}{S} \qquad b_{12} = \left.\frac{\partial f_1}{\partial q_2}\right|_{eq.p.} = \frac{1}{S}$$

$$b_{21} = \left.\frac{\partial f_2}{\partial q_1}\right|_{eq.p.} = \frac{c_1 - \bar{c}}{S\bar{h}} \qquad b_{22} = \left.\frac{\partial f_2}{\partial q_2}\right|_{eq.p.} = \frac{c_2 - \bar{c}}{S\bar{h}}$$

# Mixing tank (cont'd)

$$B = \left.\frac{\partial f(x,u)}{\partial u}\right|_{\bar{x},\bar{u}} = \left.\begin{bmatrix} \frac{\partial f_1(x,u)}{\partial u_1} & \frac{\partial f_1(x,u)}{\partial u_2} \\ \frac{\partial f_2(x,u)}{\partial u_1} & \frac{\partial f_2(x,u)}{\partial u_2} \end{bmatrix}\right|_{\bar{x},\bar{u}}$$

$$\dot{h} = (q_1 + q_2 - k\sqrt{h})/S \quad \rightarrow f_1$$

$$\dot{c} = \frac{q_1}{Sh}(c_1 - c) + \frac{q_2}{Sh}(c_2 - c) \rightarrow f_2$$

$$b_{11} = \left.\frac{\partial f_1}{\partial q_1}\right|_{eq.p.} = \frac{1}{S} \qquad b_{12} = \left.\frac{\partial f_1}{\partial q_2}\right|_{eq.p.} = \frac{1}{S}$$

$$b_{21} = \left.\frac{\partial f_2}{\partial q_1}\right|_{eq.p.} = \frac{c_1 - \bar{c}}{S\bar{h}} \qquad b_{22} = \left.\frac{\partial f_2}{\partial q_2}\right|_{eq.p.} = \frac{c_2 - \bar{c}}{S\bar{h}}$$

$$c_{11} = 1 \qquad c_{12} = 0$$

$$c_{21} = 0 \qquad c_{22} = \frac{1}{c_1}$$

# Mixing tank (cont'd)



**Residence time**

At the operating point: $\dot{h} = (q_1 + q_2 - k\sqrt{h})/S = 0$

$$\theta := \frac{S\bar{h}}{\bar{q}_1 + \bar{q}_2} = \frac{S\sqrt{\bar{h}}}{k} \quad [\mathrm{s}]$$

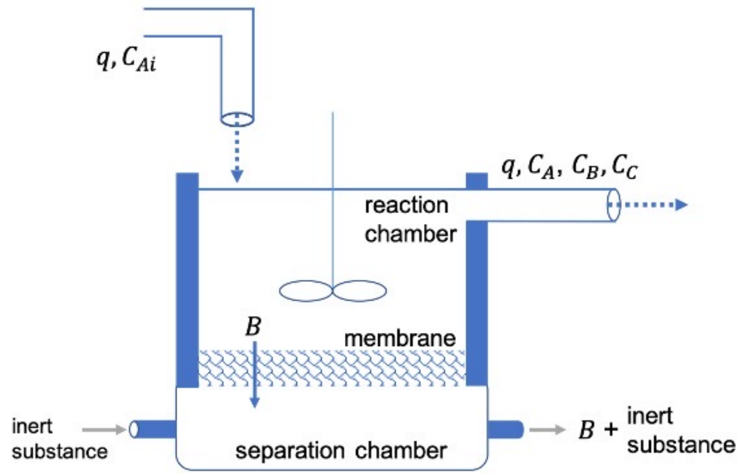
## Linear(ized) model

$$\begin{bmatrix} \delta\dot{h} \\ \delta\dot{c} \end{bmatrix} = \begin{bmatrix} -\dfrac{1}{2\theta} & 0 \\ 0 & -\dfrac{1}{\theta} \end{bmatrix} \begin{bmatrix} \delta h \\ \delta c \end{bmatrix} + \begin{bmatrix} \dfrac{1}{S} & \dfrac{1}{S} \\ \dfrac{c_1 - \bar{c}}{S\bar{h}} & \dfrac{c_2 - \bar{c}}{S\bar{h}} \end{bmatrix} \begin{bmatrix} \delta q_1 \\ \delta q_2 \end{bmatrix} \qquad \begin{bmatrix} \delta h(0) \\ \delta c(0) \end{bmatrix} = \begin{bmatrix} h_0 - \bar{h} \\ c_0 - \bar{c} \end{bmatrix}$$

$$\begin{bmatrix} \delta y_1 \\ \delta y_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & \dfrac{1}{c_1} \end{bmatrix} \begin{bmatrix} \delta h \\ \delta c \end{bmatrix}$$

# Exam problem example

1. **(30 points)** A reversible reaction $2A \leftrightarrow B + C$ takes place in a membrane reactor shown below. The reactor consists of a well-mixed reaction chamber and a separation chamber separated by a membrane. The membrane is permeable to compound $B$, whereas compounds $A$ and $C$ cannot pass through. Compound $B$ diffuses out of the reaction chamber through the membrane and is removed from the separation chamber by a stream of inert substance. The diffusion rate of $B$ through the membrane is $k_m A_m C_B \ [\frac{kmol}{min}]$, where $A_m$ is the effective area of the membrane. Compound $A$ is pumped into the reactor with the flow rate $q$ and the concentration $C_{Ai}$. $C_A$, $C_B$, and $C_C$ denote the concentrations of $A$, $B$, and $C$ in the reactor. Despite the diffusion of B through the membrane, the exit and feed flow rates are assumed equal because B is a small molecule, i.e., it is assumed that the reactor volume is constant. The temperature in the reactor is also constant. The reaction follows the mass action kinetics with the rate constants $k_1 = 0.5 \ \frac{m^3}{kmol \cdot min}$ (in the forward direction) and $k_2 = 2.5 \ \frac{m^3}{kmol \cdot min}$ (in the reverse direction).




For the parameter values: reactor volume $V = 3\ m^3$, feed flow rate $q = 0.25\ m^3/min$, mass transfer coefficient $k_m = 1.5\ m/min$, and input feed concentration $C_{Ai} = 10\ kmol/m^3$:

a) Write the mass balances for compounds $A$ and $B$.

b) Knowing that the effective membrane area at the steady-state is $A_m^{ss} = 4\ m^2$, and that the steady-state concentration of compound $A$ is five times the one of $B$, i.e., $C_A^{ss} = 5C_B^{ss}$, determine the steady-state concentrations of $A, B$, and $C$ in the reaction chamber.

c) The membrane degrades gradually and its effective area, $A_m$, changes in time. Derive the dynamic equations for deviations of concentrations $C_A$ and $C_B$ by linearizing the system of equations from a) around the steady-state derived in b).

d) Having the matrices in the states-space form, discuss how would you express in the Laplace domain the dependency of $C_A$ and $C_B$ on $A_m$. No explicit calculation is needed.