Modelling and linearization

Seborg: Chapter 2 + 3.4 (lin.)

Skogestad: Ch. 11

Reference group process control:
Need 4 students (volunteers)

Mathematical Modeling of Chemical Processes

Mathematical Model (Eykhoff, 1974)
“a representation of the essential aspects of an existing system (or a system to be constructed) which represents knowledge of that system in a usable form”

“Everything should be made as simple as possible, but no simpler.” (A. Einstein)

“All models are wrong, but some are useful.”

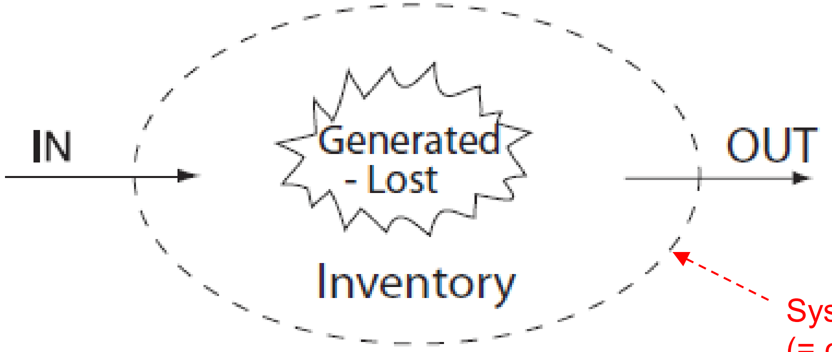
General Modeling Principles

- The model equations are at best an approximation to the real process.
- Modeling inherently involves compromise between
  - Model accuracy and complexity
  - and: Cost and effort required to develop model
- Process modeling is both an art and a science.
  - Creativity (art) is required to make simplifying assumptions that result in an appropriate model.
- Dynamic models of chemical processes consist of:
  - ordinary differential equations (ODE)
  - and/or partial differential equations (PDE)
  - plus related algebraic equations (AE).

11.2 Modeling: Dynamic balances

Balance principle ("Conservation laws"): Applies to mass, mols of molecules, energy and momentum

This gives what is known as "first principles model" or "physical model" or "nonlinear state space model"



System boundary
(= control volume)

Figure 11.1: The balance principle

$$\boxed{\underbrace{\text{Change Inventory}}_{\text{accumulated in the system}} = \underbrace{\text{In} - \text{Out}}_{\text{through the system's boundary}} + \underbrace{\text{Generated} - \text{Loss}}_{\text{internally in the system}}}$$

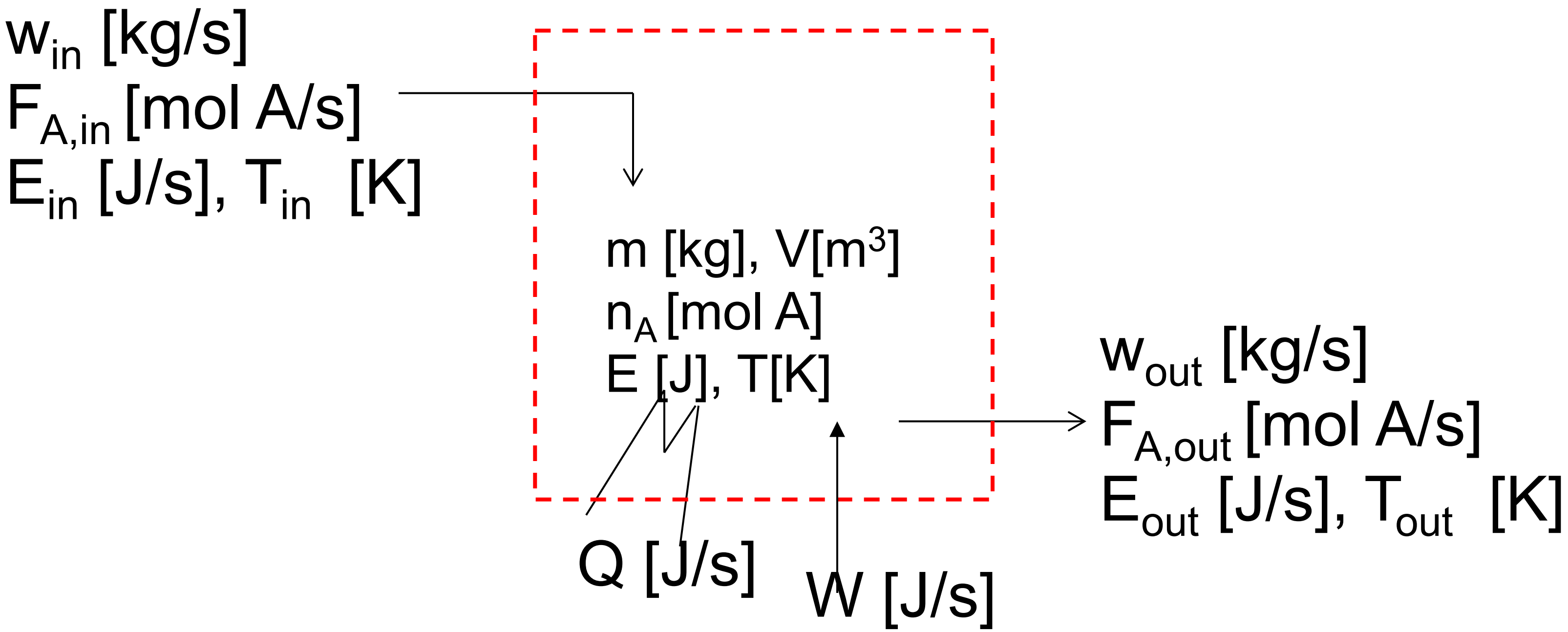
=0 for mass and energy

In this chapter, the terms "change," "in," "out," "generated" and "loss" are always per unit of time. Mathematically, the general balance equation *per unit of time* is (see (2.8) on page 42):

$$\boxed{\frac{dB}{dt} = B_{\text{in}} - B_{\text{out}} + \overbrace{B_{\text{generated}} - B_{\text{loss}}}^{\text{=0 for mass and energy}}} \quad [\frac{\text{kg}}{\text{s}}, \frac{\text{mol}}{\text{s}}, \frac{\text{J}}{\text{s}}, \ldots] \qquad (11.2)$$

For reactions [mol]

General process system



w_{in} [kg/s]
$F_{A,in}$ [mol A/s]
E_{in} [J/s], T_{in} [K]

m [kg], V[m^3]
n_A [mol A]
E [J], T[K]

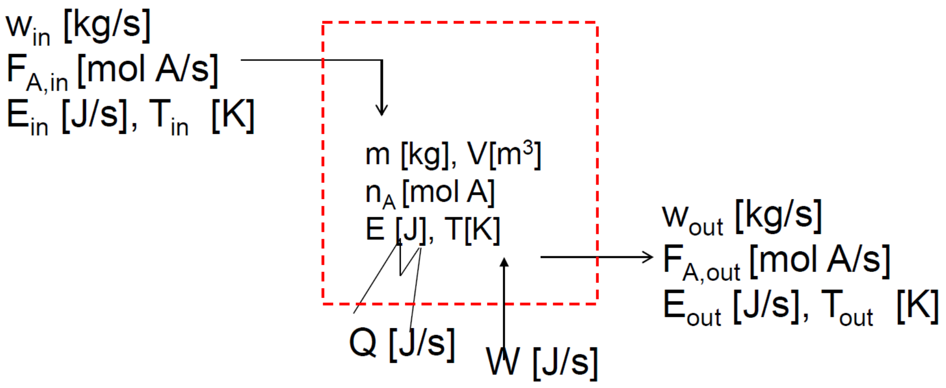
w_{out} [kg/s]
$F_{A,out}$ [mol A/s]
E_{out} [J/s], T_{out} [K]

Q [J/s]

W [J/s]

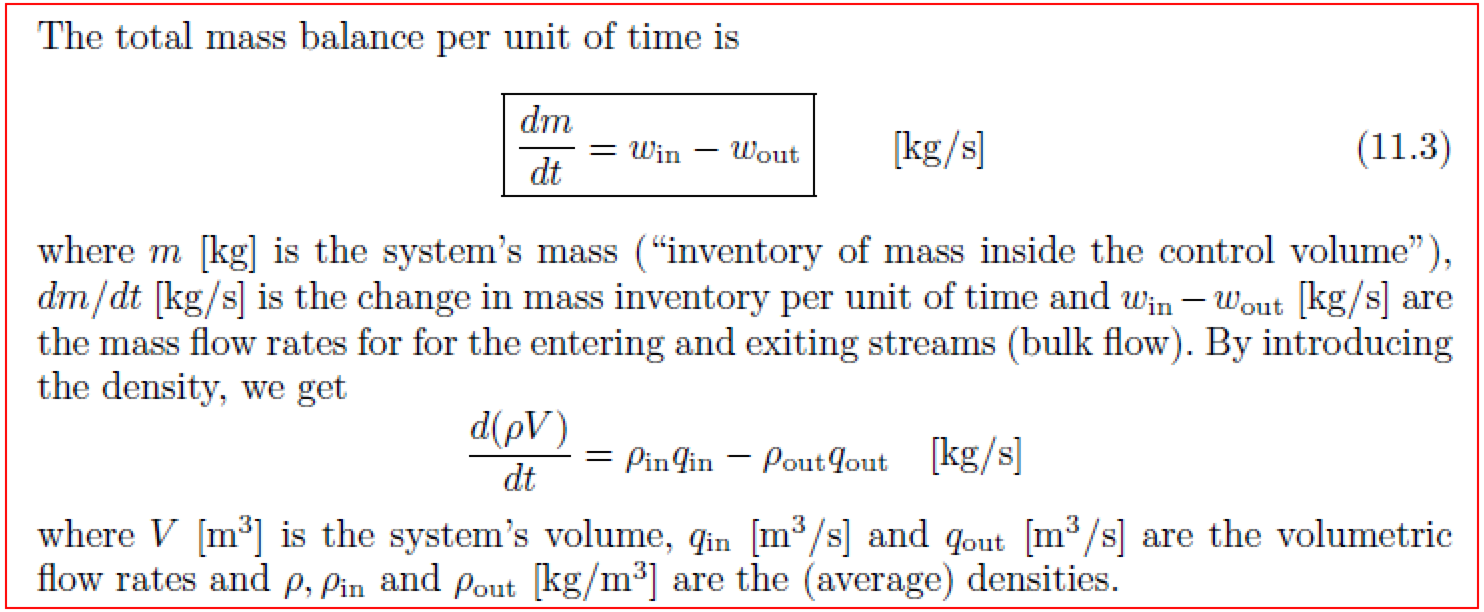
Formulate balances for mass (m), energy (E) and component mass (n_A)

- Mass (m) and energy (E) are conserved quantities (no generation or loss)
- Chemical components (A) may be generated by chemical reactions. G_A [mol A/s]



Mass balance:

$$\begin{Bmatrix}\text{rate of mass}\\ \text{accumulation}\end{Bmatrix}=\begin{Bmatrix}\text{rate of mass}\\ \text{in}\end{Bmatrix}-\begin{Bmatrix}\text{rate of mass}\\ \text{out}\end{Bmatrix}\qquad (2\text{-}6)$$



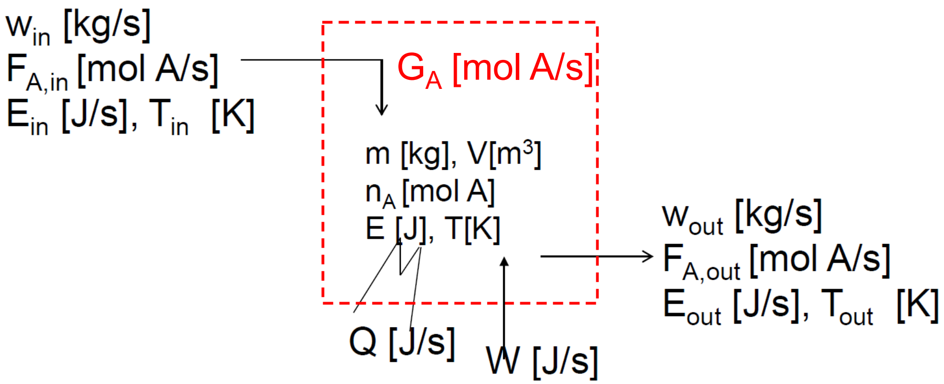
The total mass balance per unit of time is

$$\boxed{\frac{dm}{dt}=w_{\rm in}-w_{\rm out}}\qquad [\mathrm{kg/s}]\qquad (11.3)$$

where m [kg] is the system's mass ("inventory of mass inside the control volume"), dm/dt [kg/s] is the change in mass inventory per unit of time and $w_{\rm in}-w_{\rm out}$ [kg/s] are the mass flow rates for for the entering and exiting streams (bulk flow). By introducing the density, we get

$$\frac{d(\rho V)}{dt}=\rho_{\rm in}q_{\rm in}-\rho_{\rm out}q_{\rm out}\quad [\mathrm{kg/s}]$$

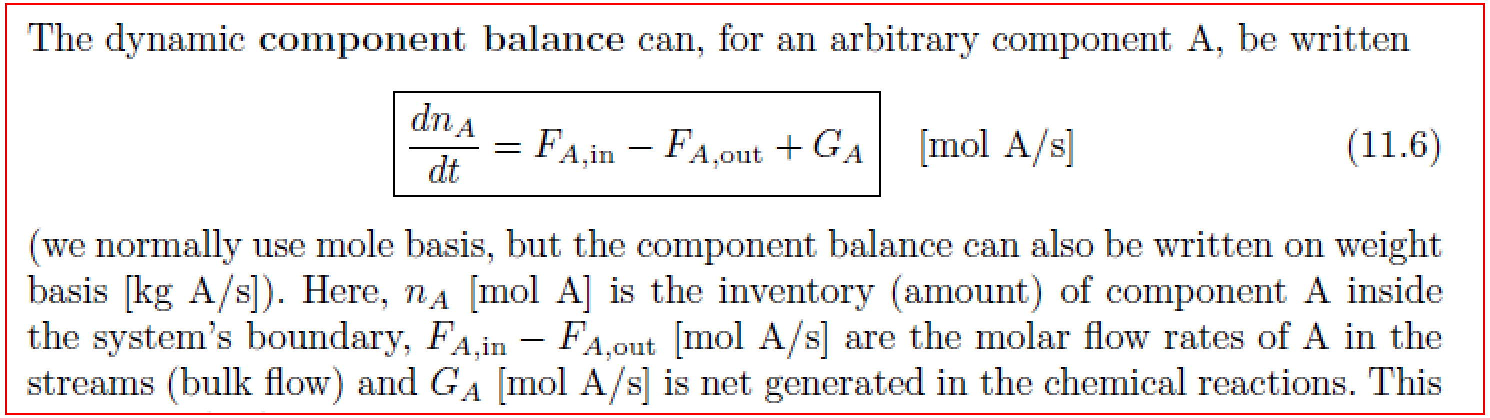
where V [m^3] is the system's volume, $q_{\rm in}$ [m^3/s] and $q_{\rm out}$ [m^3/s] are the volumetric flow rates and ρ, $\rho_{\rm in}$ and $\rho_{\rm out}$ [kg/m^3] are the (average) densities.



Molar component balance:

$$\begin{Bmatrix}\text{rate of component i}\\ \text{accumulation}\end{Bmatrix} = \begin{Bmatrix}\text{rate of component i}\\ \text{in}\end{Bmatrix}$$

$$-\begin{Bmatrix}\text{rate of component i}\\ \text{out}\end{Bmatrix} + \begin{Bmatrix}\text{rate of component i}\\ \text{produced}\end{Bmatrix} \qquad (2\text{-}7)$$

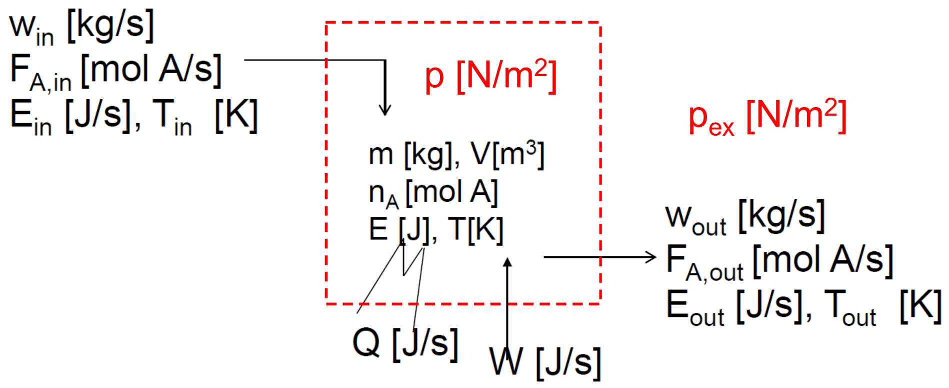


The dynamic **component balance** can, for an arbitrary component A, be written

$$\boxed{\frac{dn_A}{dt} = F_{A,\text{in}} - F_{A,\text{out}} + G_A} \quad [\text{mol A/s}] \qquad (11.6)$$

(we normally use mole basis, but the component balance can also be written on weight basis [kg A/s]). Here, n_A [mol A] is the inventory (amount) of component A inside the system's boundary, $F_{A,\text{in}} - F_{A,\text{out}}$ [mol A/s] are the molar flow rates of A in the streams (bulk flow) and G_A [mol A/s] is net generated in the chemical reactions. This

Energy balance (=First Law of Thermodynamics)



$$\left\{\begin{matrix}\textbf{rate of energy}\\ \textbf{accumulation}\end{matrix}\right\} = \left\{\begin{matrix}\textbf{rate of energy in}\\ \textbf{by convection}\end{matrix}\right\} - \left\{\begin{matrix}\textbf{rate of energy out}\\ \textbf{by convection}\end{matrix}\right\}$$

$$+\left\{\begin{matrix}\textbf{net rate of heat addition}\\ \textbf{to the system from}\\ \textbf{the surroundings}\end{matrix}\right\} + \left\{\begin{matrix}\textbf{net rate of work}\\ \textbf{performed on the system}\\ \textbf{by the surroundings}\end{matrix}\right\} \qquad \textbf{(2-8)}$$

$$\frac{dE}{dt} = E_{in} - E_{out} + Q + W \quad [\mathrm{J/s}]$$

Energy is a conserved quantity (no generation or loss).

Heat of reaction is included in E with common reference state (usually elements)

The total energy of a thermodynamic system, E, is the sum of its internal energy, kinetic energy, and potential energy: E = U + KE + PE + other (surface energy, etc)

Also many forms of work: W = W_s + pV-work + other (electric, etc.)

where pV-work = $P_{in}q_{in} - p_{out}q_{out} - p_{ex}\, dV/dt$

1) Neglect KE and PE. 2) Neglect «other» work. 3) Introduce $H_{in}=U_{in} + p_{in}q_{in.}$ etc. Get:

$$\boxed{\frac{dU}{dt} = H_{\mathrm{in}} - H_{\mathrm{out}} + Q + W_s - p_{\mathrm{ex}}\frac{dV}{dt}} \quad [\mathrm{J/s}] \qquad (11.11)$$

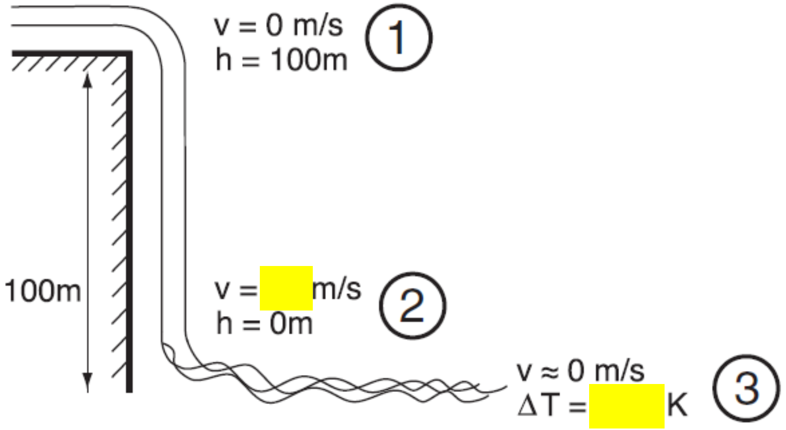
We usually prefer to work with enthalpy, and introducing $U = H - pV$ in (11.11), gives

$$\boxed{\frac{dH}{dt} = H_{\mathrm{in}} - H_{\mathrm{out}} + Q + W_s \underbrace{-(p_{\mathrm{ex}} - p)\frac{dV}{dt} + V\frac{dp}{dt}}_{\text{pressure−volume changes}}} \quad [\mathrm{J/s}] \qquad (11.12)$$

The term “pressure-volume changes” in (11.12) is often negligible.

- The term is exactly zero (also for gases) for cases with constant pressure and volume.
- The term is exactly zero (also for gases) for cases where the pressure is constant and equal to the surrounding’s pressure ($p = p_{\mathrm{ex}}$=constant).
- Even with varying pressure, the term is approximately zero for liquids and solids, because the volume V is relatively small for such systems.

Can usually neglect kinetic and potential energy in energy balance



Conclusion:
- Process plants: Typically
  - $v < 10$ m/s,
  - $H < 100$ m,
  - $\Delta T = 0.24$ K is negligible

⇒ Can neglect KE and PE compared to temperature changes (changes in U)

$$E = U + \cancel{KE} + \cancel{PE}$$

Waterfall: (1) potential energy -> (2) kinetic energy -> (3) thermal energy

Thermal energy is included in internal energy (U).

Proof: Energy balance (for m=1kg water): $PE_1 = KE_2 = U_3$

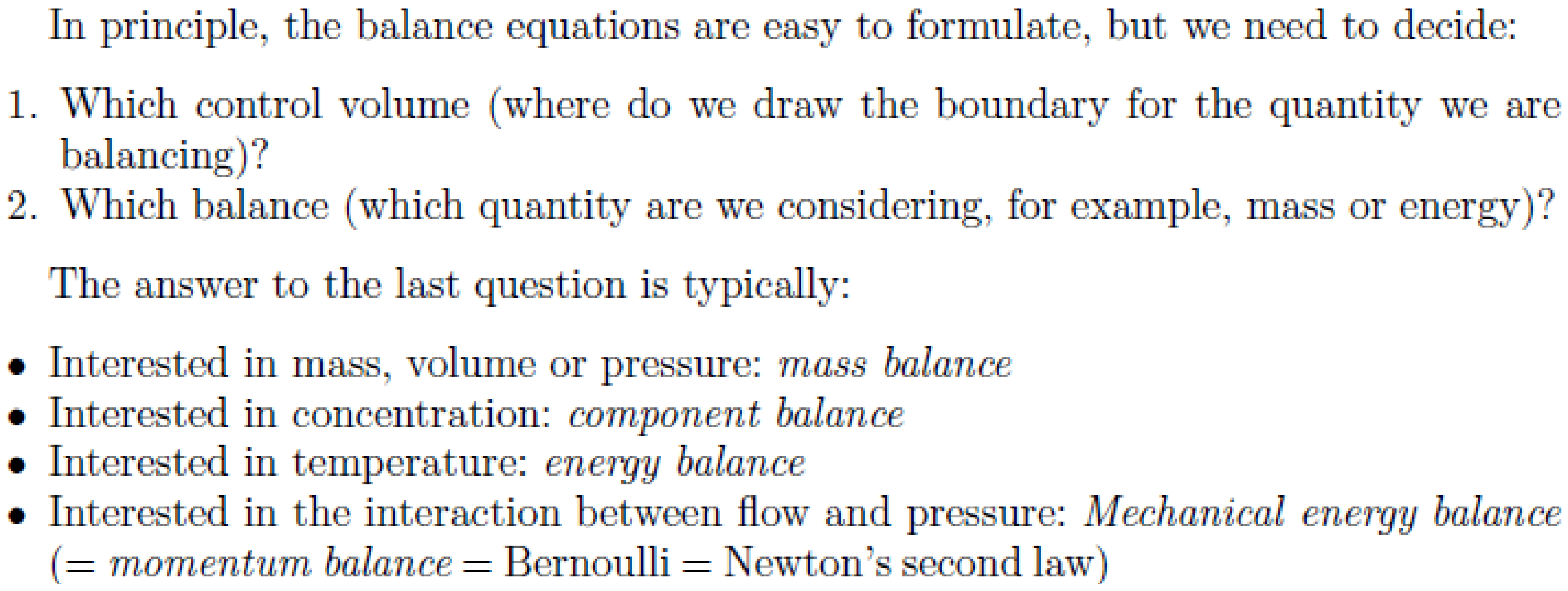
$mgh_1 = \frac{1}{2} mv_2^2 = mc_P T_3$ [J]

where

$g = 10$ m/s^2

$c_P = 1$ kcal/kg,K $= 4184$ J/kg,K

Which control volume and which balance?



In principle, the balance equations are easy to formulate, but we need to decide:

1. Which control volume (where do we draw the boundary for the quantity we are balancing)?
2. Which balance (which quantity are we considering, for example, mass or energy)?

The answer to the last question is typically:

- Interested in mass, volume or pressure: *mass balance*
- Interested in concentration: *component balance*
- Interested in temperature: *energy balance*
- Interested in the interaction between flow and pressure: *Mechanical energy balance* (= *momentum balance* = Bernoulli = Newton's second law)

Dot notation

- In the control field (EE), a dot means derivative (of quantity inside boundary)
- But in other fields (ME) it may mean a transfer rate (through boundary)
- For this reason I usually avoid dot-notation

$$\text{Control field: } \dot{V} = \frac{dV}{dt} = \text{derivative [m3/s]}$$
$$\text{Other fields: } \dot{V} = q = \text{flowrate [m3/s]}$$

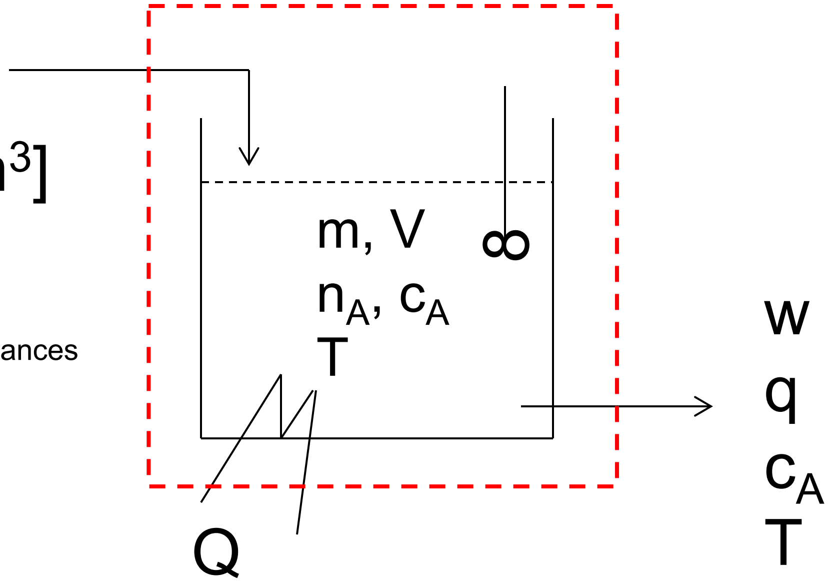
Dynamic modeling. Examples

- You should do many examples!
- See my book: CHEMICAL AND ENERGY PROCESS ENGINEERING, CRC Press (Taylor & Francis Group), 2009, Chapter 11..
- Chapter 11 on dynamics available here:

  http://folk.ntnu.no/users/skoge/prosessregulering/course-material/

Example 1. Mixing tank (CSTR)

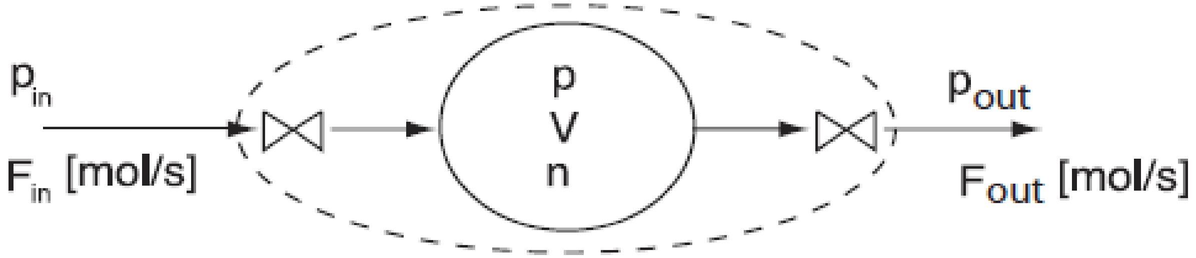
w_F [kg/s]
q_F [m^3/s]
c_{AF} [mol/m^3]
T_F [K]



Task:
Formulate mass, component and energy balances to find expressions for dV/dt, dc_A/dT, dT/dt
Assume:
- Perfect mixing
- No reaction
- Constant density
- Constant heat capacity
- Single phase (liquid)
- Do NOT assume constant volume V

Example 2. Buffer tank on gas pipeline

(Example 11.10)



Task:

- Find residence time, $¿_r$
- Find time constant ¿ for dynamic response
- Hint: Find expression for dp/dt and rearrange to standard form to find time constant (gives dynamics for effect of changes in p_{in} on p, F_{in}, etc.)

Note: Only one mass (mole) balance, so this is a first-order system

Assume:

- T constant; Ideal gas, pV = nRT
- Linear valves: $F_{in} = c\,(p_{in}-p)$, $F_{out}= c(p-p_{out})$

Gas dynamics are very fast!

Data at steady state:
p_{in}=10.1 bar, p=10 bar, p_{out}=9.9 bar, V = 10m^3, F_{in}=F_{out} = 100 mol/s, T=300K

Summary: Dynamic modeling

- Use of the "balance principles" (resulting in differential equations) combined with other equations for equilibrium, heat transfer etc. (resulting in algebraic equations), gives in a "nonlinear state space model" on the general form:

Balance equations: $\frac{dx_1}{dt} = f_1(x_1, x_2, u)$

Additional algebraic equations: $0 = f_2(x_1, x_2, u)$

where

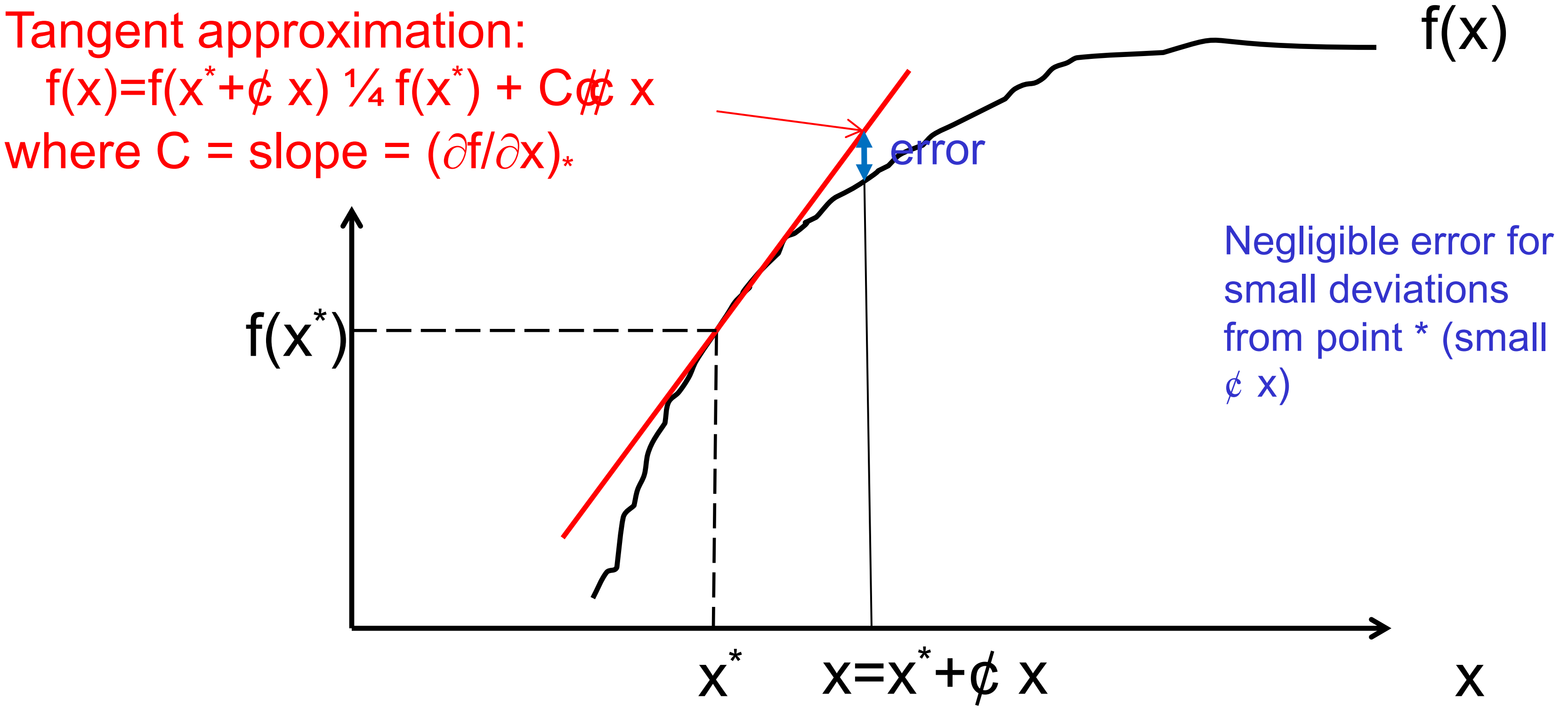
u - independent variables (inputs, disturbances)

x - states (internal model variables) - dependent variables

$y = g(x_1, x_2, u)$ - output variables (measurements)

- The states x_1, x_2… are usually the balanced quantities (mass, energy, molar holdup). It is possible to redefine the states, for example, to replace x_1=H (energy) by x_1=T (temperature), but this requires work (see example), so we often don't do it.

Linearization = Tangent approximation = Taylor series expansion



Tangent approximation:
$f(x)=f(x^*+¢\ x)$ ¼ $f(x^*) + C¢\ x$
where C = slope = $(\partial f/\partial x)_*$

Negligible error for small deviations from point * (small ¢ x)

Example: $f(x) = \sqrt{x}$. Linearize around point x*=1.

$\Delta x = x - x^* = x - 1$, $f(x^*) = 1$, $C = (\partial f/\partial x)_* = 1/(2\sqrt{x^*}) = 0.5$

x	$f(x) = \sqrt{x}$	$\approx f(x^*) + C\,\Delta x$
0		
0.5		
1	1	$1 + 0.5 \cdot 0 = 1$
2		

Linearization (Linear model)

- What is a linear system?

1. Gain k = $\Delta y/\Delta u$ is constant, independent of magnitude of Δu.

2. **Satisfies the superposition principle:** that is, the total response is the sum of individual responses. Let

  - $f(u_1)=y_1(t)$ y_1 = change in temperature when change u_1 (put on heater)
  - $f(u_2)=y_2(t)$ y_2 = change in temperature when change u_2 (open window)

  Then

  - $f(u_1+u_2) = y_1(t) + y_2(t) = y(t)$ (y=change in y with both at same time)

- Why linearize?
  - Much simpler mathematics (transfer functions)
  - All real systems behave linearly for small deviations from steady state (using control!)
- How linearize?

1. Linearize nonlinear dynamic model (e.g., obtained from balance equations):

$$dx/dt = f(x,u)$$

to get a linear «state space» model in deviation variables ($\Delta x(t) = x(t) - x^*$, etc.):

$$d\Delta x/dt = A\ \Delta x + B\ \Delta u$$

where $A = (\partial f/\partial x)_*$ and $B = (\partial f/\partial u)_*$ are constants (matrices in the general case).

Linearization of dynamic model. Proof of «How»

Dynamic model (e.g., from balance equations)

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

where x are the (internal, model) states and u are the independent variables.

RHS: First-order Taylor series expansion of non-linear term gives linear approximation

$$f(x,u) \approx \underbrace{f(x^*,u^*)}_{f^*} + \underbrace{\left(\frac{\delta f}{\delta u}\right)^* \Delta u + \left(\frac{\delta f}{\delta x}\right)^* \Delta x}_{\Delta f}$$

where $\Delta u = u - u^*$ and $\Delta x = x - x^*$ are deviations from the nominal trajectory,

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

LHS:

$$\frac{dx}{dt} = \frac{d(\Delta x + x^*)}{dt} = \frac{d\Delta x}{dt} + f^*$$

Note: f^* on LHS cancels against f^* on RHS

Conclusion: Set LHS=RHS (f* drops out!):

$$\boxed{\frac{d\Delta x}{dt} = \Delta f = \underbrace{\left(\frac{\delta f}{\delta x}\right)^*}_{A} \Delta x + \underbrace{\left(\frac{\delta f}{\delta u}\right)^*}_{B} \Delta u}$$

Note: We do <u>not</u> need to assume $\frac{dx^*}{dt} = f^* = 0$ (steady state)

But some things become simpler for normal case when we linearize around steady state:

Special case (slight extension) when we linearize around a steady state (f*=0):

Nonlinear model: V(t) dx/dt = f(x,u) (Here V(t) can be any function or variable)

Linear model becomes: V* dΔx/dt = Δf

Proof (assume that * is a steady state so f*=0).

Rewrite nonlinear model as: dx/dt = f/V

Linearize using brown box: dΔx/dt = (1/V*) Δf – (f*/V*^{2}) ΔV = (1/V*) Δf

QED

This is how I do it

1. Nonlinear model, $\frac{dx(t)}{dt} = f(x, u)$
2. Steady state (*), $f(x^*, u^*) = 0$
   - Use to find missing parameters
3. Introduce deviation variables
   - $\Delta x(t) = x(t) - x^*$, etc
4. Linearize model
   - Simplest is to do one term at a time:

     $\frac{dx}{dt} = f_1 + f_2 + f_3 \Rightarrow \frac{d\Delta x}{dt} = \Delta \mathrm{f}_1 + \Delta f_2 + \Delta f_3$, where $\Delta f_1 = \left.\frac{\partial f_1}{\partial x}\right|_* \Delta x + \left.\frac{\partial f_1}{\partial \mathrm{u}}\right|_* \Delta \mathrm{u}$
5. Analyze, simulate, plot

Example 1: Outflow from tank (bath-tub with no plug)

Nonlinear static model

$$q_{\text{out}} = k\sqrt{h} \quad \text{(turbulent outflow)}$$

$$\Rightarrow \Delta q_{\text{out}} = \left(\frac{\delta(k\sqrt{h})}{\delta h}\right)^* \Delta h = \frac{k}{\underbrace{2\sqrt{h^*}}_{}}\Delta h$$

- Note: Time constant for flow response (liquids)
  - Twice residence time for turbulent outflow
  - Equal to residence time for laminar outflow

  - Gas dynamics are much faster!

Start here part 3 - lecture 4 (10 sep 2024)

Example 2: CSTR

Notes

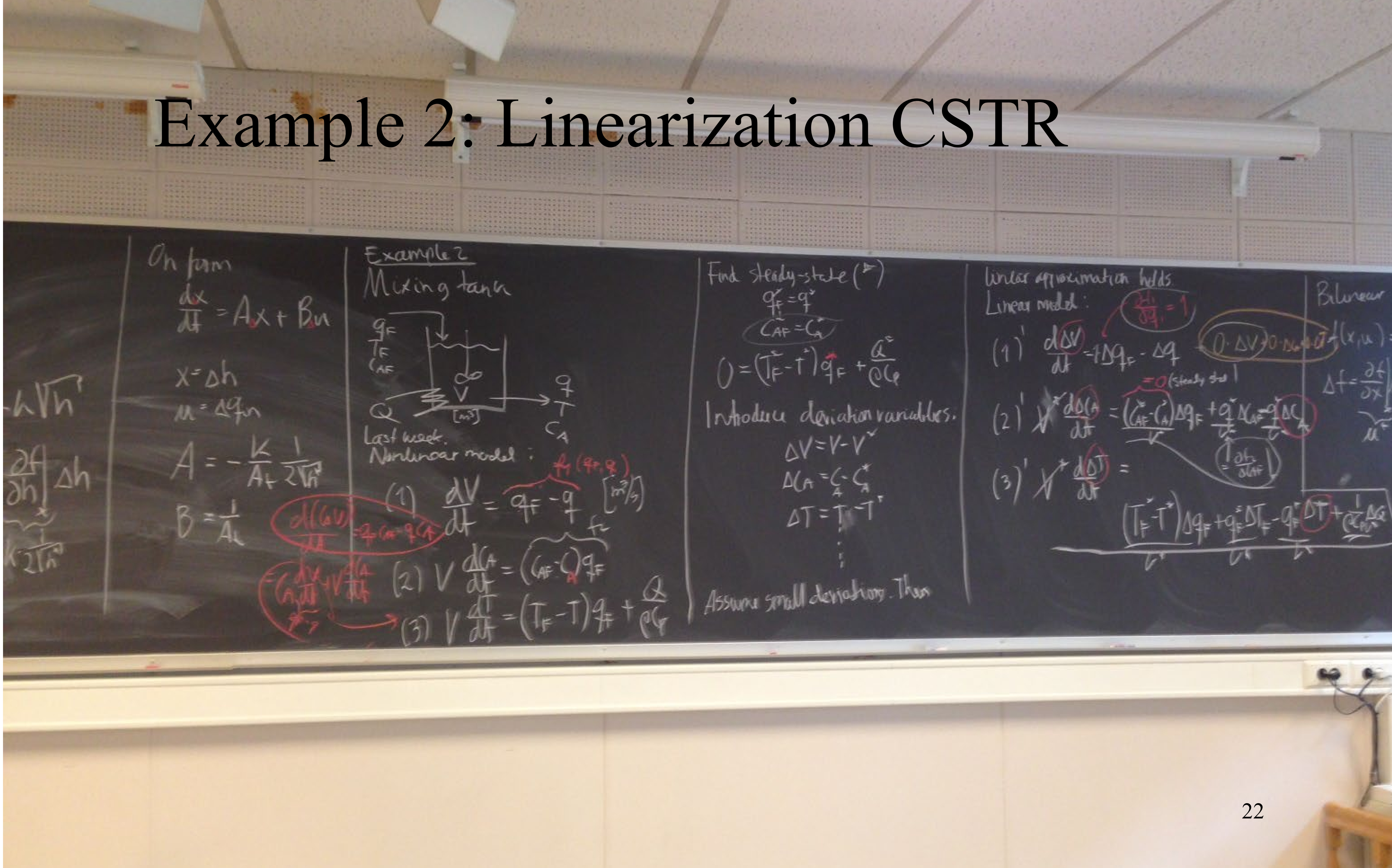
1. Bilinear term on RHS: $\Delta(xu) = x^* \Delta u + y^* \Delta u$

2. Linearize LHS:

Note: When you have a nonlinear model on the form $V(t)dT/dt = f$,
And you linearize a steady state, the linear version simply becomes $V^* d\Delta T/dt = \Delta f$, that is, you can use V^* on the left hand side.

Proof : See bottom of proof slide (in red)

Example 2: Linearization CSTR



$-k\sqrt{h}$

$\frac{\partial f}{\partial h}\Big|^{*}\Delta h$

$k\frac{1}{2\sqrt{h^*}}$

On form

$$\frac{dx}{dt} = Ax + Bu$$

$x = \Delta h$

$u = \Delta q_{in}$

$$A = -\frac{K}{A_t}\frac{1}{2\sqrt{h^*}}$$

$$B = \frac{1}{A_t}$$

$$\frac{d(c_A V)}{dt} = q_F c_{AF} - q c_A$$

$$= c_A\frac{dV}{dt} + V\frac{dc_A}{dt}$$

Example 2

Mixing tank

Last week.

Nonlinear model:

$$(1)\quad \frac{dV}{dt} = \overbrace{q_F - q}^{f_1(q_F,\, q)} \quad [m^3/s]$$

$$(2)\quad V\frac{dc_A}{dt} = \overbrace{(c_{AF} - c_A)\, q_F}^{f_2}$$

$$(3)\quad V\frac{dT}{dt} = (T_F - T)\, q_F + \frac{Q}{\rho c_p}$$

Find steady-state (*)

$q_F^* = q^*$

$c_{AF}^* = c_A^*$

$$0 = (T_F^* - T^*)\, q_F^* + \frac{Q^*}{\rho c_p}$$

Introduce deviation variables.

$\Delta V = V - V^*$

$\Delta c_A = c_A - c_A^*$

$\Delta T = T - T^*$

$\vdots$

Assume small deviations. Then linear approximation holds.

Linear model:

$$\frac{\partial f_1}{\partial q_F} = 1$$

$$(1)'\quad \frac{d\Delta V}{dt} = 1\cdot\Delta q_F - \Delta q + 0\cdot\Delta V + 0\cdot\Delta c_A + 0\cdot\Delta T$$

$$(2)'\quad \cancel{V^*}\frac{d\Delta c_A}{dt} = \frac{\overbrace{(c_{AF}^* - c_A^*)}^{=0\ (\text{steady state})}}{V^*}\Delta q_F + \frac{q^*}{V^*}\Delta c_{AF} - \frac{q^*}{V^*}\Delta c_A$$

$$= \frac{\partial f_2}{\partial c_{AF}}$$

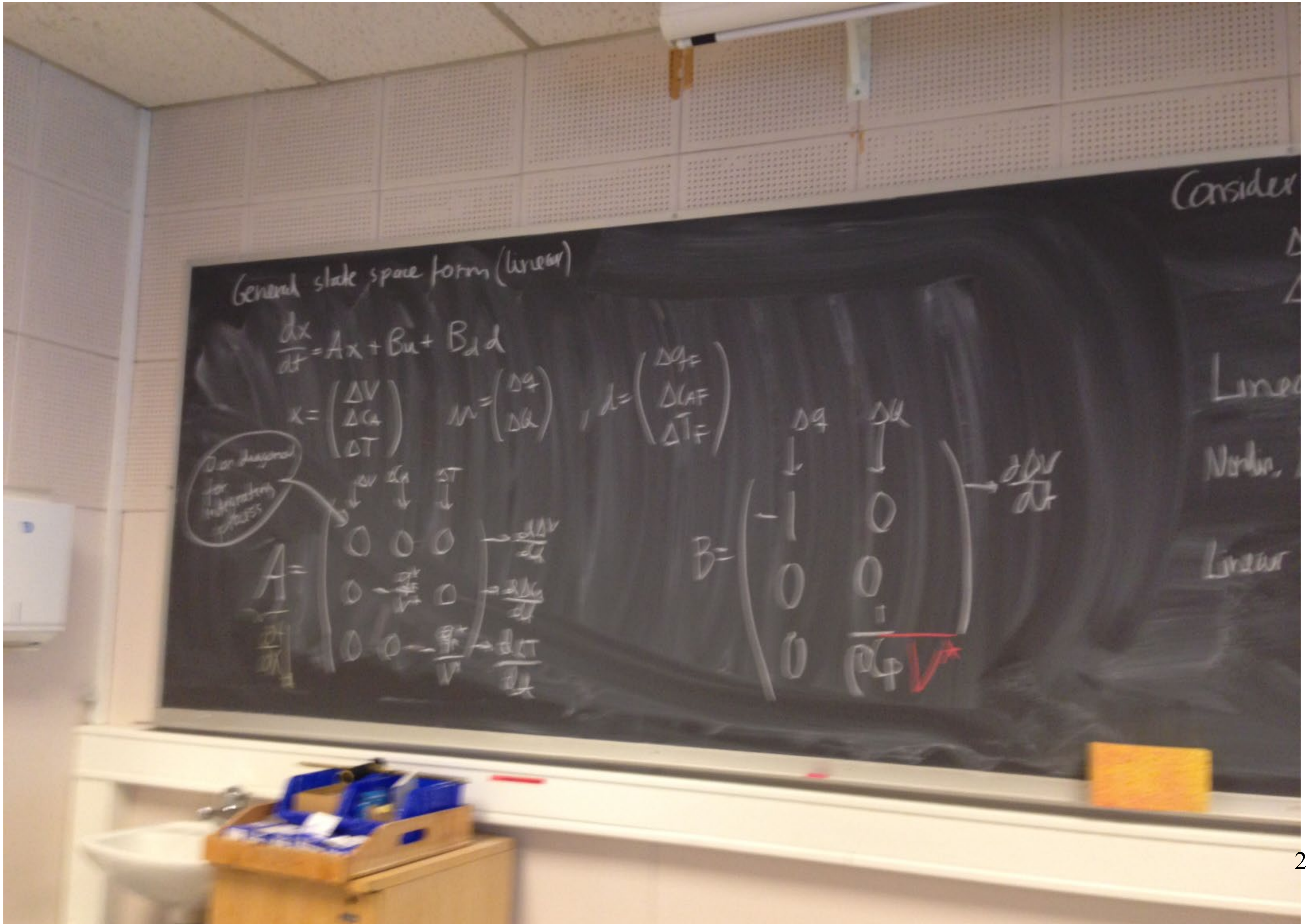
$$(3)'\quad \cancel{V^*}\frac{d\Delta T}{dt} = \frac{(T_F^* - T^*)\,\Delta q_F + q_F^*\,\Delta T_F - q_F^*\,\Delta T + \frac{1}{\rho c_p}\Delta Q}{V^*}$$

Bilinear

$f(x,u) =$

$\Delta f = \frac{\partial f}{\partial x}$

u^*



General state space form (linear)

$$\frac{dx}{dt} = Ax + Bu + B_d d$$

$$x = \begin{pmatrix} \Delta V \\ \Delta c_A \\ \Delta T \end{pmatrix}, \quad u = \begin{pmatrix} \Delta q \\ \Delta Q \end{pmatrix}, \quad d = \begin{pmatrix} \Delta q_F \\ \Delta c_{AF} \\ \Delta T_F \end{pmatrix}$$

0 on diagonal for integrating process

$$A = \begin{array}{c} \begin{array}{ccc} \Delta V & \Delta c_A & \Delta T \end{array} \\ \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\frac{q^*}{V^*} & 0 \\ 0 & 0 & -\frac{q^*}{V^*} \end{pmatrix} \end{array} \begin{array}{l} \to \frac{d\Delta V}{dt} \\ \to \frac{d\Delta c_A}{dt} \\ \to \frac{d\Delta T}{dt} \end{array}$$

$$B = \begin{array}{c} \begin{array}{cc} \Delta q & \Delta Q \end{array} \\ \begin{pmatrix} -1 & 0 \\ 0 & 0 \\ 0 & \frac{1}{\rho c_p V^*} \end{pmatrix} \end{array} \to \frac{d\Delta V}{dt}$$

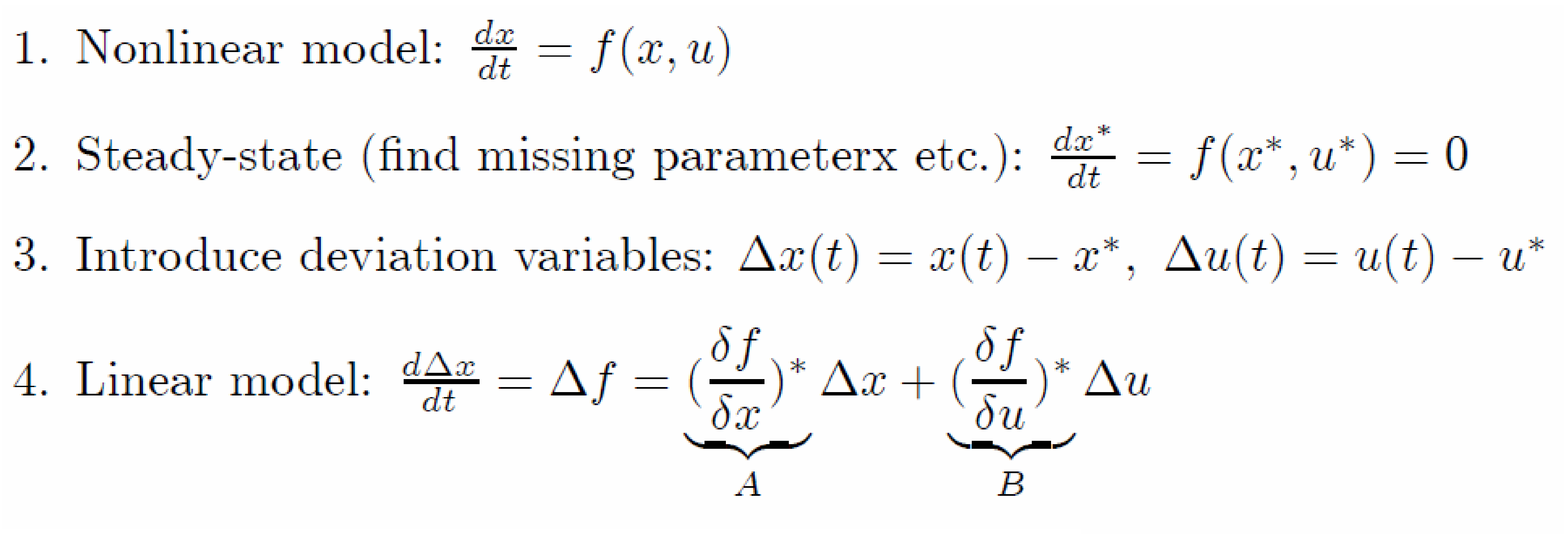
Consider

Linea

Nonlin.

Linear

Summary linearization

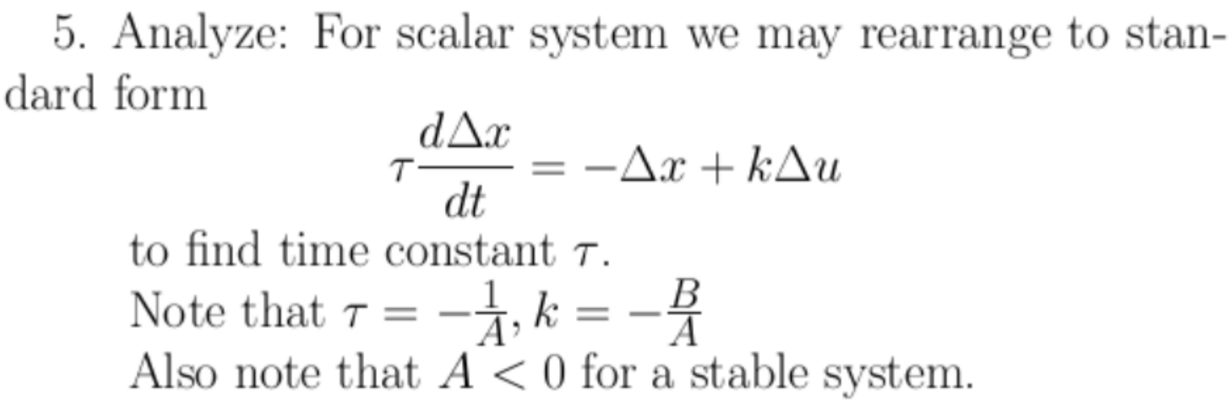


1. Nonlinear model: $\frac{dx}{dt} = f(x, u)$

2. Steady-state (find missing parameterx etc.): $\frac{dx^*}{dt} = f(x^*, u^*) = 0$

3. Introduce deviation variables: $\Delta x(t) = x(t) - x^*,\ \Delta u(t) = u(t) - u^*$

4. Linear model: $\frac{d\Delta x}{dt} = \Delta f = \underbrace{(\frac{\delta f}{\delta x})^*}_{A} \Delta x + \underbrace{(\frac{\delta f}{\delta u})^*}_{B} \Delta u$



5. Analyze: For scalar system we may rearrange to standard form

$$\tau \frac{d\Delta x}{dt} = -\Delta x + k\Delta u$$

to find time constant τ.
Note that $\tau = -\frac{1}{A}, k = -\frac{B}{A}$
Also note that $A < 0$ for a stable system.

Note: If you also have static model equations then I recommend to start by linearizing these

Linearize static model (for algebaic equations)

Static model

$y=f(x,u)$

Consider small deviations in u from nominal point where $y^*=f(x^*,u^*)$

Linear model in deviation variables ($\Delta x(t) = x(t) - x^*$, etc.):

$$\Delta y = C\,\Delta x + D\,\Delta u$$

where

$C = (\partial f/\partial x)_*$

$D = (\partial f/\partial u)_*$

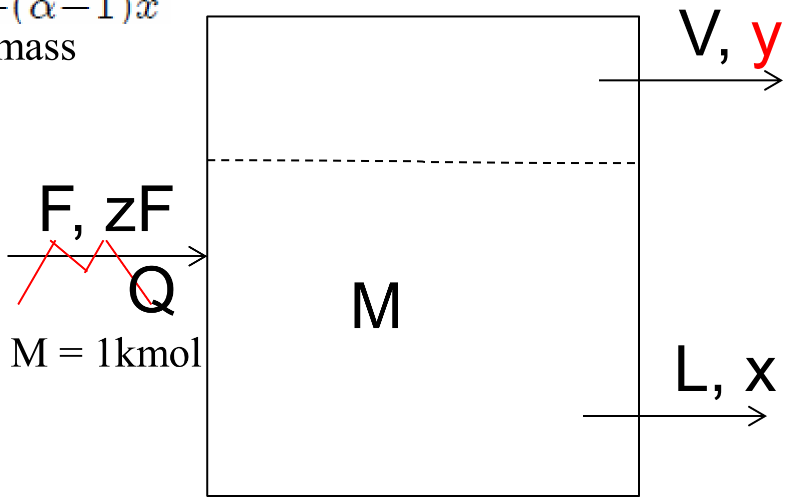
are constants (matrices in the general case)

Example 3 linearization: Flash

- Flash tank with two components (z_F,y,x: mole fraction light component)
- VLE: Assume constant relative volatility ®=21:

$$\alpha = \frac{y/x}{(1-y)/(1-x)} \Rightarrow y = \frac{\alpha x}{1+(\alpha-1)x}$$

- Model assumptions: Well mixed, neglect vapor mass
- p and M constant (using Q and L)
- u = V
- d = F, zF
- y = y (output)
- Nominal data: F^*=1 kmol/min, z^*_F=0.5, y^*=0.84, M = 1kmol



- Task: 1. Derive dynamic model + 2. Find nominal steady-state + 3. Linearize to find model (in deviation variables)

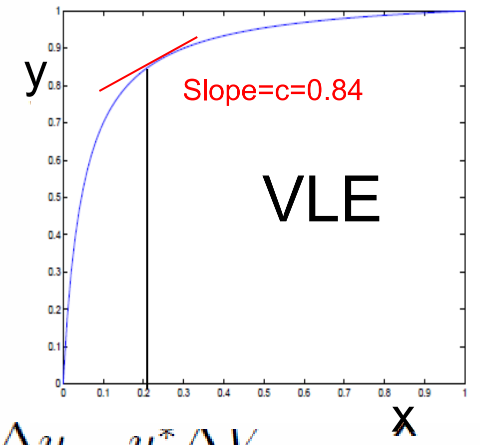
Solution

1. Overall and component balances [kmol/h]:

$$0 = \frac{dM}{dt} = F - L - V; \quad \frac{d(Mx)}{dt} = Fz_F - Lx - Vy$$

2. Find steady-state: $0 = F^* - L^* - V^*; \quad 0 = F^* z_F^* - L^* x^* - V^* y$
Combined with VLE ($\alpha = 21$) and given data ($F^* = 1, y^* = 0.84$):

$$x^* = 0.2, V^* = 0.469; L^* = 0.531$$



3. Linearize model.

Linearize balance equations:

$$0 = \Delta F - \Delta L - \Delta V$$

(I usually start by linearizing the static equations)

$$M\frac{d(\Delta x)}{dt} = F^*\Delta z_F + z_F^*\Delta F - L^*\Delta x - x^* \underbrace{\Delta L}_{\Delta F - \Delta V} - V^* \underbrace{\Delta y}_{c\Delta x} - y^*\Delta V$$

$$M\frac{d(\Delta x)}{dt} = -(L^* + cV^*)\Delta x - (y^* - x^*)\Delta V + F^*\Delta z_F + (z_F^* - x^*)\Delta F$$

Linearize VLE: $c = \left(\frac{dy}{dx}\right)^* = \frac{21}{1+20x^*} - \frac{21x^* \cdot 20}{(1+20x^*)^2} = 0.84$

$\Delta y = c\,\Delta x$

Conclusion.

Get:

$$\frac{dx}{dt} = Ax + Bu + B_d d; \quad y = Cx$$

where

$$x = \Delta x; y = \Delta y$$

$$u = \Delta V; d = \begin{pmatrix} \Delta F \\ \Delta z_F \end{pmatrix}$$

and

$$A = -\frac{L^* + cV^*}{M*} = -0.925 \ [\mathrm{min}^{-1}]$$

$$B = -\frac{y^* - x^*}{M*} = -0.64 \ [\mathrm{mol}^{-1}]$$

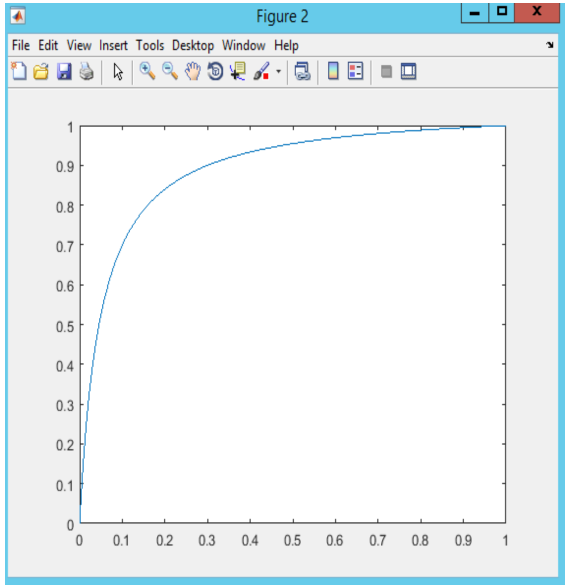
$$B_d = \begin{pmatrix} \frac{z_F^* - x^*}{M*} & \frac{F^*}{M*} \end{pmatrix} = \begin{pmatrix} 0.3 & 1 \end{pmatrix}$$

$$C = c = 0.84$$

```
% Using symbolic toolbox in Matlab
syms y x
f=21 - (y/x) / ((1-y)/(1-x)) % definition relative volatility=21
y=solve(f,y)
fplot(y,[0 1])
dydx(x)=diff(y,x)
dydx(0.2)
eval(ans)
```

Result:

```
f =21 - (y*(x - 1))/(x*(y - 1))
y =(21*x)/(20*x + 1)
dydx(x) =21/(20*x + 1) - (420*x)/(20*x + 1)^2
ans =21/25
ans =0.8400
```



8.1 General

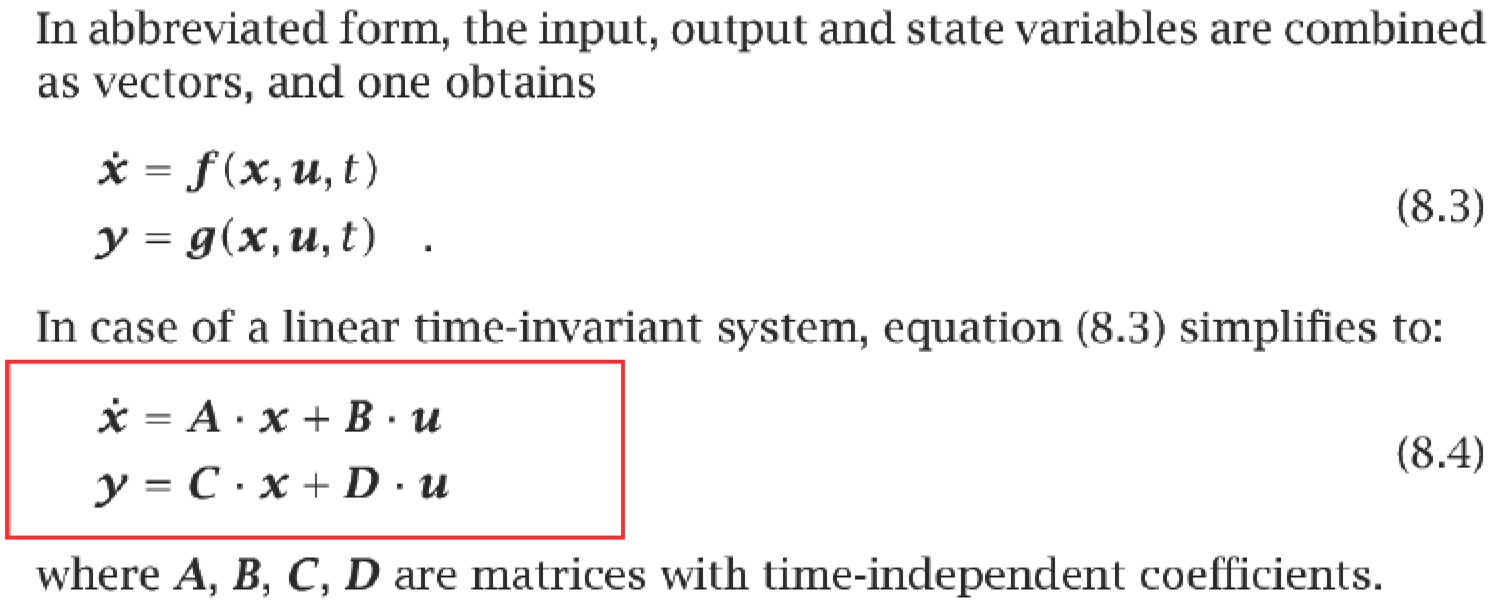
The relationship between the input and output variables of dynamic transfer systems may be described not just in terms of various differential equations, generally of a higher order, but also in terms of systems of first order differential equations. The variables that appear in addition to the input and output variables in such differential equation systems must conform to certain definite conditions, and are then generally characterised by the letter x as state variables.

The system of differential equations is then constructed in such a way that the n derivatives $\dot{x}_i$ of the state variables x_i are expressed as functions of these state variables and the p input variables u_i

$$\begin{aligned} \dot{x}_1 &= f_1(x_1, \ldots, x_n, u_1, \ldots, u_p, t) \\ &\vdots \\ \dot{x}_n &= f_n(x_1, \ldots, x_n, u_1, \ldots, u_p, t) \quad . \end{aligned} \tag{8.1}$$

The q output variables y_i are represented as functions of the state variables and input variables:

$$\begin{aligned} y_1 &= g_1(x_1, \ldots, x_n, u_1, \ldots, u_p, t) \\ &\vdots \\ y_q &= g_q(x_1, \ldots, x_n, u_1, \ldots, u_p, t) \quad . \end{aligned} \tag{8.2}$$



In abbreviated form, the input, output and state variables are combined as vectors, and one obtains

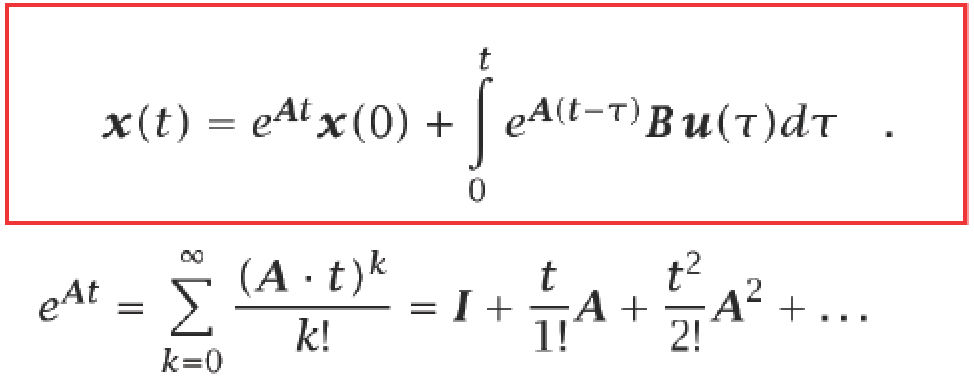
$$\begin{aligned}\dot{\boldsymbol{x}} &= \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},t)\\ \boldsymbol{y} &= \boldsymbol{g}(\boldsymbol{x},\boldsymbol{u},t)\quad .\end{aligned} \tag{8.3}$$

In case of a linear time-invariant system, equation (8.3) simplifies to:

$$\boxed{\begin{aligned}\dot{\boldsymbol{x}} &= \boldsymbol{A}\cdot\boldsymbol{x}+\boldsymbol{B}\cdot\boldsymbol{u}\\ \boldsymbol{y} &= \boldsymbol{C}\cdot\boldsymbol{x}+\boldsymbol{D}\cdot\boldsymbol{u}\end{aligned}} \tag{8.4}$$

where $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$, $\boldsymbol{D}$ are matrices with time-independent coefficients.

Solution



$$\boxed{\boldsymbol{x}(t) = e^{\boldsymbol{A}t}\boldsymbol{x}(0) + \int_0^t e^{\boldsymbol{A}(t-\tau)}\boldsymbol{B}\boldsymbol{u}(\tau)d\tau \quad .}$$

$$e^{\boldsymbol{A}t} = \sum_{k=0}^{\infty}\frac{(\boldsymbol{A}\cdot t)^k}{k!} = \boldsymbol{I} + \frac{t}{1!}\boldsymbol{A} + \frac{t^2}{2!}\boldsymbol{A}^2 + \dots$$

8.4 Controllability and observability

From the general solutions of the state space equations (8.49) and (8.54), some important statements about the described system can be derived. Among these characteristics are the controllability and the observability of the system - terms that were introduced by Kalman in 1960.

A system

$$\begin{aligned} \dot{\boldsymbol{x}} &= \boldsymbol{A} \cdot \boldsymbol{x} + \boldsymbol{B} \cdot \boldsymbol{u} \\ \boldsymbol{y} &= \boldsymbol{C} \cdot \boldsymbol{x} + \boldsymbol{D} \cdot \boldsymbol{u} \end{aligned} \tag{8.61}$$

is said to be controllable if its state $\boldsymbol{x}$ can be transferred from any arbitrary initial state $\boldsymbol{x}(t_0)$ to the final state $\mathbf{0}$ in finite time by means of an appropriate input value, the control vector $\boldsymbol{u}(t)$.

Correspondingly, the system (8.61) is said to be observable if from the known input vector $\boldsymbol{u}(t)$ and from the measurement of $\boldsymbol{y}(t)$ over a finite time interval, the initial state $\boldsymbol{x}(t_0)$ can be determined uniquely. For observable systems, one can design so-called state observers which generate estimates of the state variables from the input and output variables.

One can demonstrate, that a system with a single input variable u and a single output variable y is controllable , if the vectors

$$\boldsymbol{b},\ \boldsymbol{A}\cdot\boldsymbol{b},\ \boldsymbol{A}^2\cdot\boldsymbol{b},\ \ldots,\ \boldsymbol{A}^{n-1}\cdot\boldsymbol{b} \tag{8.62}$$

are linearly independent . Thus, the (n,n)-controllability matrix

$$\boxed{\boldsymbol{Q}_S = \left[\boldsymbol{b},\ \boldsymbol{A}\cdot\boldsymbol{b},\ \boldsymbol{A}^2\cdot\boldsymbol{b},\ \ldots,\ \boldsymbol{A}^{n-1}\cdot\boldsymbol{b}\right]} \tag{8.63}$$

is nonsingular if and only if the system is controllable. In other words, controllability is given when

$$\det \boldsymbol{Q}_S \neq 0 \quad . \tag{8.64}$$

A system with a single input variable u, n state variables and a single output variable y is said to be observable, if the vectors

$$\boldsymbol{c}^T,\ \boldsymbol{c}^T\cdot\boldsymbol{A},\ \ldots,\ \boldsymbol{c}^T\cdot\boldsymbol{A}^{n-1} \tag{8.65}$$

are linearly independent . In other words, observability is given if the (n,n)-observability matrix

$$\boxed{\boldsymbol{Q}_B = \begin{bmatrix} \boldsymbol{c}^T \\ \boldsymbol{c}^T\cdot\boldsymbol{A} \\ \vdots \\ \boldsymbol{c}^T\cdot\boldsymbol{A}^{n-1} \end{bmatrix}} \tag{8.66}$$

is nonsingular.

Minimum realization

- Unobservable states x are unintersting for us as they have no effect on the outputs (y)
- Uncontrollable states x cannot be effected by our inputs (u)
- Model from u to y: Eliminate unobsevable and uncontrollable* states to get model with fewest number of states («minimal realization»). Saves computation time.
- Corresponds to cancelling identical poles and zeros, (s+a)/(s+a), in transfer function
  - Note how much simpler it becomes with transfer functions (Laplace)

*But initial value of uncontrollable states will affect outputs, at least temporarily