Modelling and linearization

Seborg: Chapter 2 + 3.4 (lin.)

Skogestad: Ch. 11

Chapter 2

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)

Chapter 2

General Modeling Principles

- The model equations are at best an approximation to the real process.
- "All models are wrong, but some are useful."
- 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 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

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

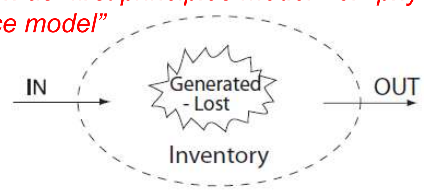


Figure 11.1: The balance principle

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

=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):

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

For reactions [mol]

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)

Chapter 2

- Conservation Laws

Theoretical models of chemical processes are based on conservation laws.

Conservation of Mass

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

The total mass balance per unit of time is

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

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 $w_{\text{in}} - w_{\text{out}}$ [kg/s] are the mass flow rates for for the entering and exiting streams (bulk flow). By introducing the density, we get

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

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

Chapter 2

- Conservation Laws

Conservation of Component i

$$\left\{\begin{matrix}\text{rate of component i}\\ \text{accumulation}\end{matrix}\right\} = \left\{\begin{matrix}\text{rate of component i}\\ \text{in}\end{matrix}\right\}$$

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

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

Chapter 2

Conservation of Energy

The general law of energy conservation is also called the First Law of Thermodynamics. It can be expressed as:

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

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

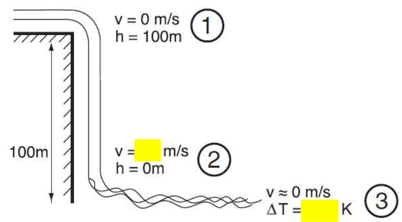
The total energy of a thermodynamic system, U=U_{tot}, is the sum of its internal energy, kinetic energy, and potential energy: $U_{tot} = U_{int} + U_{KE} + U_{PE}$ (2-9)

The general energy balance (4.10) over a time period Δt with $\Delta U = U_f - U_0$ gives, as $\Delta t \to 0$, the dynamic energy balance:

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

Here, U [J] is the internal energy for the system (inside the control volume), while $H_{\text{in}} - H_{\text{out}}$ is the sum of internal energy in the streams plus the flow work that the streams perform on the system as they are "pushed" in or out of the system. The term $-p_{\text{ex}}\frac{dV}{dt}$ is the work supplied to the system when its volume changes; it is negligible for most systems. Q [J/s] is supplied heat (through the system's wall), while W_s [J/s] is supplied useful mechanical work (usually shaft work, for example, from a compressor,

Can usually neglect kinetic and potential energy in energy balance



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

Thermal energy is included in internal energy (U).

Energy balance (for 1 kg water):

$gh_1 = ½ v_2^2 = c_P T_3$ [J/kg]

where

$g = 10$ m/s^2

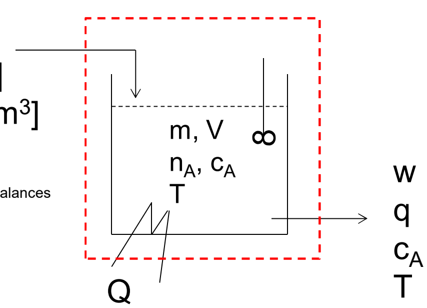
$c_P = 1$ kcal/kg,K = 4184 J/kg,K

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 on itslearning or here:
  http://www.nt.ntnu.no/users/skoge/prosessregulering/course-material/

Example 1. Mixing tank (CSTR)

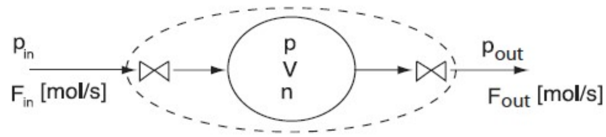
w_F [kg/s]
q_F [m^3/s]
c_{AF} [mol/m^3]
T_F [K]



Task:
Formulate mass, component and energy balances to find expressions for dV/dt, dc_A/dT, dT/dt
Assume:
- 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, τ_r
- Find time constant τ 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

Overall dynamic model

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

Linearization (Linear model)

- What is a linear system?
  - Satisfies the superposition principle, that is, the total response is the sum of individual responses. Let
    - $f(u_1)=y_1(t)$
    - $f(u_2)=y_2(t)$

    Then
    - $f(k_1\ u_1+k_2\ u_2) = k_1\ y_1(t) + k_2\ y_2(t)$
- Why linearize?
  - Much simpler mathematics (transfer functions)
  - All real systems behave linearly for small deviations from steady state (using control!)
- How?

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

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

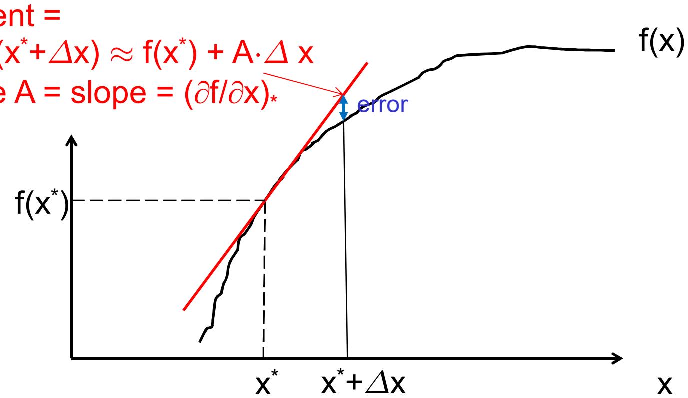
  to get a linear state space model in deviation variables:

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

  where A and B are constants (matrices).

Linearization = Tangent approximation = Taylor series expansion

Tangent =
$f(x)=f(x^*+\Delta x) \approx f(x^*) + A\cdot\Delta\ x$
where A = slope = $(\partial f/\partial x)_*$



Negligible error for small deviations from point * (small Δx)

Linearization. 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

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

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

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

If nominal is steady-state, then $\frac{dx^*}{dt} = f^* = 0$.

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: Get linear "state-space" model

deviation variables:

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

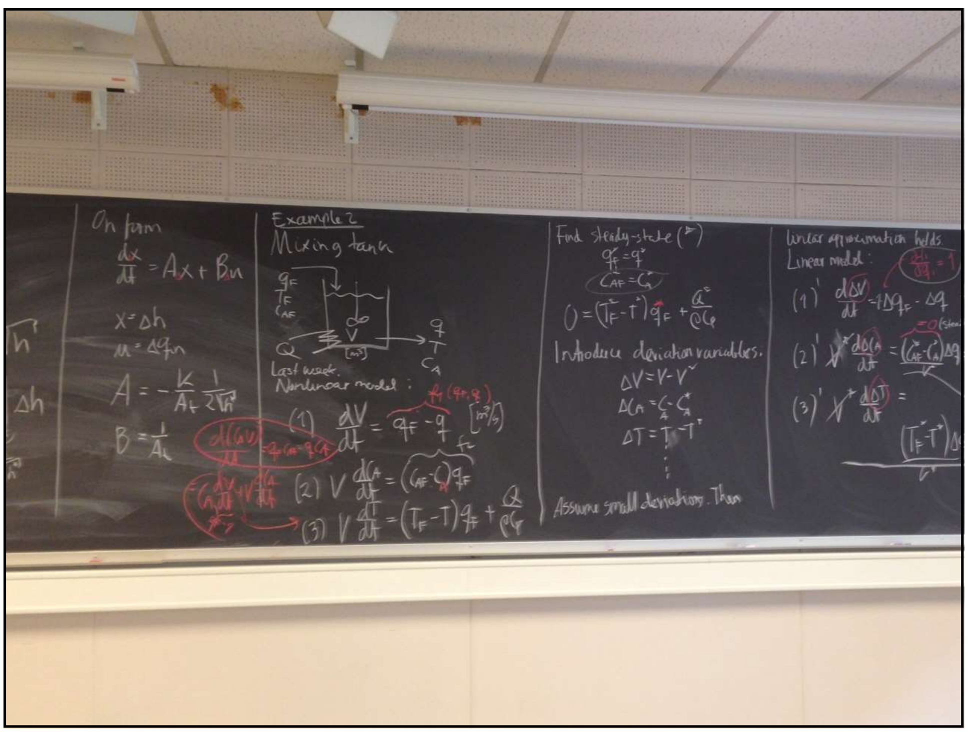
Summary linearization

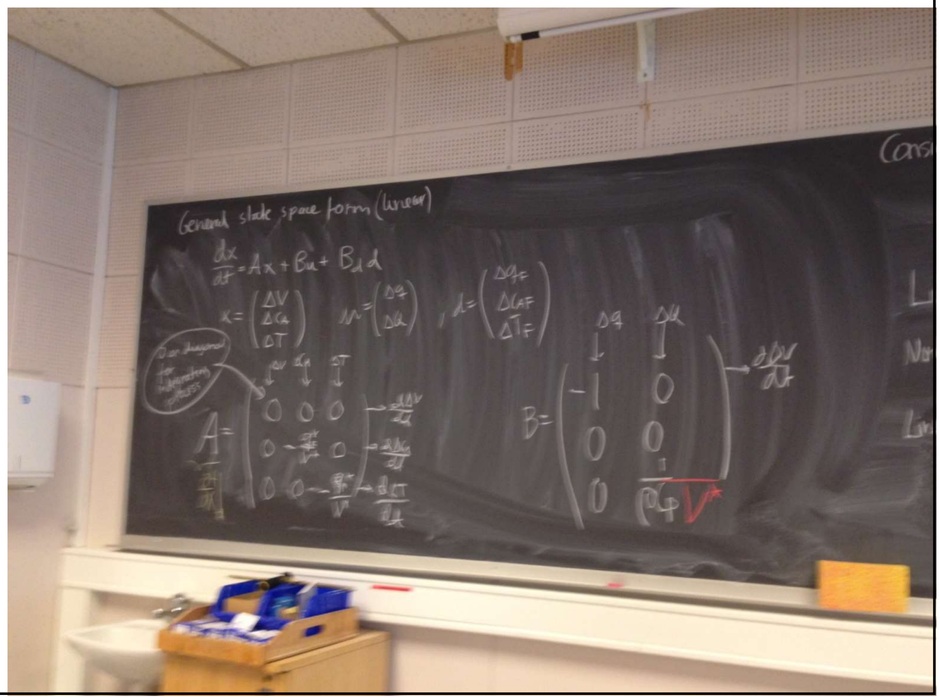
1. Nonlinear model: $\frac{dx}{dt} = f(x,u)$
2. Steady-state (find missing parameterx etc.): $\frac{dx^*}{dt} = f(x^*,u^*) = 0$
3. Introduce deviation variables: $\Delta x(t) = x(t) - x^*, \ \Delta u(t) = u(t) - u^*$
4. Linear model: $\frac{d\Delta x}{dt} = \Delta f = \underbrace{(\frac{\delta f}{\delta x})^*}_{A} \Delta x + \underbrace{(\frac{\delta f}{\delta u})^*}_{B} \Delta u$

Example 1: Bath tub with no plug

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

Example 2: Linearization CSTR



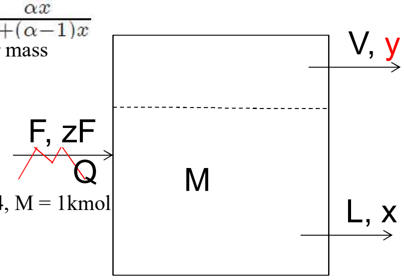


Example linearization: Flash

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

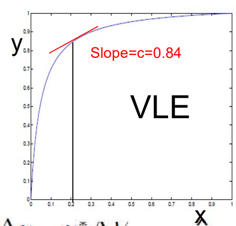
Solution

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

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

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:

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

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

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

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

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

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

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

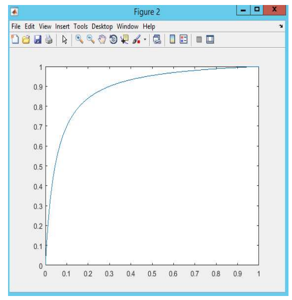
$$B_d = \begin{pmatrix} \frac{z_F^* - x^*}{M^*} & \frac{F^*}{M^*} \end{pmatrix} = \begin{pmatrix} 0.3 & 1 \end{pmatrix}$$

$$C = c = 0.84$$

```
% 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

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

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

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 $\boldsymbol{0}$ 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.

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