Aalto University

Linearisation of nonlinear models: Example

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Example I

Linearisation of nonlinear models

Example I

Consider two chemical species A and B in a solvent feed entering a chemical reactor

- The two species react to form a third one, the product component P
- $A + 2B \longrightarrow P$

Liquid-phase chemical reactor

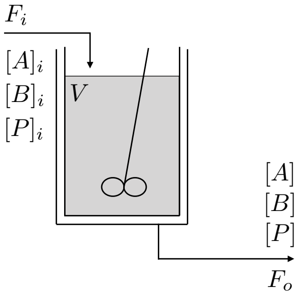
⇝ Volume $V(t)$

Temperature is constant

⇝ $T(t) = \text{constant}$

Volumetric flow-rates

⇝ $F_i(t)$ and $F_o(t)$



Assuming perfect mixing, our main interest is in the concentrations inside the reactor

⇝ The concentration of species as a function of time $[A](t)$, $[B](t)$, and $[P](t)$

- (Interest also in $V(t)$, because we do not want to flood/dry the tank)

Example I (cont.)

Total mass balance

$$\underbrace{\frac{\mathrm{d}M(t)}{\mathrm{d}t}}_{\text{(mass/time)}} = \underbrace{\frac{\mathrm{d}V(t)\rho_0(t)}{\mathrm{d}t}}_{\text{(volume × (mass / volume) / time)}}$$

$$= \underbrace{\rho_i(t)}_{\text{(mass / volume)}} \underbrace{F_i(t)}_{\text{(volume / time)}} - \underbrace{\rho_o(t)}_{\text{(mass / volume)}} \underbrace{F_o(t)}_{\text{(volume / time)}}$$

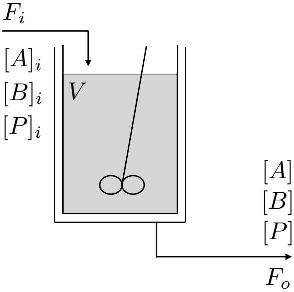
Assuming (!) that the density is does not depend on the concentration of A, B and P, we get

$$\rho_o(t) = \rho_i(t) = \rho \quad \rightsquigarrow \quad \rho \neq \rho(t)$$

$\rightsquigarrow$ Density does not depend on time

The resulting total mass balance,

$$\rightsquigarrow \quad \frac{\mathrm{d}V(t)}{\mathrm{d}t} = F_i(t) - F_o(t)$$



Example I (cont.)

Component mass balance

Let $[A]$, $[B]$ and $[P]$ be molar concentrations (moles/volume) of species A, B and P

- Based on some kinetic modelling, we are given the stoichiometric equation

$$A + 2B \xrightarrow{k} P$$

Assuming that there is no product P in the feed ($[P]_i(t) = 0$ for all $t \geq t(0)$), we have

$$\begin{aligned}
\frac{\mathrm{d}\,V(t)[A](t)}{\mathrm{d}t} &= F_i(t)[A]_i(t) - F_o(t)[A]_o(t) + V(t)r_A(t) \\
\frac{\mathrm{d}\,V(t)[B](t)}{\mathrm{d}t} &= F_i(t)[B]_i(t) - F_o(t)[B]_o(t) + V(t)r_B(t) \\
\frac{\mathrm{d}\,V(t)[P](t)}{\mathrm{d}t} &= F_i(t)\cancel{[P]_i(t)} - F_o(t)[P]_o(t) + V(t)r_P(t)
\end{aligned}$$

$r_A(t)$, $r_B(t)$ and $r_P(t)$ denote generation/consumption rates of species A, B and P

- Given per unit volume, and assume we know the reaction rate constant k

$\rightsquigarrow$ $\left(\dfrac{\text{moles}}{\text{time}}\right) \Big/ \text{volume}$

Example I (cont.)

$$A + 2B \xrightarrow{k} P$$

We can assume that the reaction rate per unit volume for component A is second order

- We can also assume that it depends on the composition of both $A(t)$ and $B(t)$

$$r_A(t) = -k[A](t)[B](t), \quad \text{(rate of generation of } A\text{, per unit volume)}$$

The stoichiometric equation tells us that one mole of A reacts with two moles of B

- ... to produce one mole of P

We can also write the generation rates (per unit volume) for the remaining species

$$r_B(t) = -2k[A](t)[B](t)$$
$$r_P(t) = k[A](t)[B](t)$$

At this point, we need to substitute their expressions in the mass balances

Example I (cont.)

Consider the mass balance for component A and differentiate with respect to time

$$\begin{aligned}\frac{\mathrm{d}\,V(t)[A](t)}{\mathrm{d}t} &= V(t)\frac{\mathrm{d}[A](t)}{\mathrm{d}t} + [A](t)\frac{\mathrm{d}\,V(t)}{\mathrm{d}t}\\ &= F_i(t)[A]_i(t) - F_o(t)[A](t) - V(t)\underbrace{k[A](t)[B](t)}_{-r_A}\end{aligned}$$

Dividing by $V(t)$ and rearranging terms, we get

$$\frac{\mathrm{d}[A](t)}{\mathrm{d}t} = \frac{F_i(t)}{V(t)}[A]_i(t) - \frac{F_o(t)}{V(t)}[A](t) - \frac{V(t)}{V(t)}k[A](t)[B](t) - \frac{1}{V(t)}\frac{\mathrm{d}\,V(t)}{\mathrm{d}t}[A](t)$$

From the total mass balance, we know that $\dfrac{\mathrm{d}\,V(t)}{\mathrm{d}t} = F_i(t) - F_o(t)$

$$\begin{aligned}\frac{\mathrm{d}[A](t)}{\mathrm{d}t} &= \frac{F_i(t)}{V(t)}[A_i](t) - \cancel{\frac{F_o(t)}{V(t)}[A](t)} - k[A](t)[B](t) - \frac{F_i(t)}{V(t)}[A](t) + \cancel{\frac{F_o(t)}{V(t)}[A](t)}\\ &= \frac{F_i(t)}{V(t)}\Big([A]_i(t) - [A](t)\Big) - k[A](t)[B](t)\end{aligned}$$

Example I (cont.)

We can proceed similarly for component B and component P to get their dynamics

$$\rightsquigarrow \quad \frac{\mathrm{d}[B](t)}{\mathrm{d}t} = \frac{F_i(t)}{V(t)}\Big([B]_i(t) - [B](t)\Big) - 2k[A](t)[B](t)$$

$$\rightsquigarrow \quad \frac{\mathrm{d}[P](t)}{\mathrm{d}t} = \frac{F_i(t)}{V(t)}\Big(\underbrace{[P]_i(t)}_{=0} - [P](t)\Big) + k[A](t)[B](t)$$

Example I (cont.)

Altogether, we have model equations involving 4 state variables and 4 input variables

$$\frac{\mathrm{d}[A](t)}{\mathrm{d}t} = \frac{F_i(t)}{V(t)}([A]_i(t) - [A](t)) - k[A](t)[B](t)$$
$$\frac{\mathrm{d}[B](t)}{\mathrm{d}t} = \frac{F_i(t)}{V(t)}([B]_i(t) - [B](t)) - 2k[A](t)[B](t)$$
$$\frac{\mathrm{d}[P](t)}{\mathrm{d}t} = -\frac{F_i(t)}{V(t)}[P](t) + k[A](t)[B](t)$$
$$\frac{\mathrm{d}V(t)}{\mathrm{d}t} = F_i(t) - F_o(t)$$

The state equations of the model consists of four first-order differential equations

- $\rightsquigarrow$ Thus four state variables, they are associated with the derivatives
- $\rightsquigarrow$ Variables $V(t)$, $[A](t)$, $[B](t)$ and $[P](t)$ have dynamics

As for the four (five) input variables, some are controls others are disturbances

- $\rightsquigarrow$ $F_i(t)$, $F_o(t)$, $[A]_i(t)$, $[B]_i(t)$ (and $[P]_i(t)$)

Example I (cont.)

Four initial conditions (at $t = 0$) are needed for determining the temporal evolution

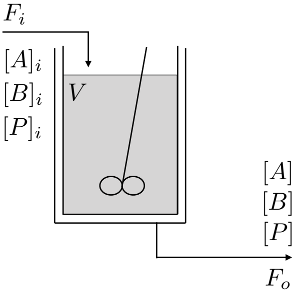
$\rightsquigarrow$ $V(0)$, $[A](0)$, $[B](0)$ and $[P](0)$

To determine the temporal evolution, we also need to set the inputs to be applied

$\rightsquigarrow$ $F_i(t)$, $F_o(t)$, $[A]_i(t)$, $[B]_i(t)$ (and $[P]_i(t)$)

- From the initial time $t = 0$ onwards

$$\begin{bmatrix} \dot{V} \\ [\dot{A}] \\ [\dot{B}] \\ [\dot{P}] \end{bmatrix} = \begin{bmatrix} F_i - F_o \\ \frac{F_i}{V}([A]_i - [A]) - k[A][B] \\ \frac{F_i}{V}([B]_i - [B]) - 2k[A][B] \\ -\frac{F_i}{V}[P] + k[A][B] \end{bmatrix}$$



Note how the state equations of the state-space model contains also a parameter, k

$\rightsquigarrow$ We assumed it to be time-invariant (that is, $k \neq k(t)$)

Example I (cont.)

$$\begin{bmatrix} \dot{V} \\ [\dot{A}] \\ [\dot{B}] \\ [\dot{P}] \end{bmatrix} = \begin{bmatrix} F_i - F_o \\ \dfrac{F_i}{V}([A]_i - [A]) - k[A][B] \\ \dfrac{F_i}{V}([B]_i - [B]) - 2k[A][B] \\ -\dfrac{F_i}{V}[P] + k[A][B] \end{bmatrix}$$

$$= \begin{bmatrix} f_1\left(V, [A], [B], [P], F_i, F_o, [A]_i[B]_i, [P]_i | k, B\right) \\ f_2\left(V, [A], [B], [P], F_i, F_o, [A]_i[B]_i, [P]_i | k, B\right) \\ f_3\left(V, [A], [B], [P], F_i, F_o, [A]_i[B]_i, [P]_i | k, B\right) \\ f_4\left(V, [A], [B], [P], F_i, F_o, [A]_i[B]_i, [P]_i | k, B\right) \end{bmatrix}$$

$\rightsquigarrow$ For the state variables, $x(t)$

$$x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \\ x_4(t) \end{bmatrix} = \begin{bmatrix} V(t) \\ [A](t) \\ [B](t) \\ [P](t) \end{bmatrix}$$

Example I (cont.)

$$\begin{bmatrix} \dot{V} \\ [\dot{A}] \\ [\dot{B}] \\ [\dot{P}] \end{bmatrix} = \begin{bmatrix} F_i - F_o \\ \frac{F_i}{V}([A]_i - [A]) - k[A][B] \\ \frac{F_i}{V}([B]_i - [B]) - 2k[A][B] \\ -\frac{F_i}{V}[P] + k[A][B] \end{bmatrix}$$

$$= \begin{bmatrix} f_1\left(V, [A], [B], [P], F_i, F_o, [A]_i, [B]_i, [P]_i | k, B\right) \\ f_2\left(V, [A], [B], [P], F_i, F_o, [A]_i, [B]_i, [P]_i | k, B\right) \\ f_3\left(V, [A], [B], [P], F_i, F_o, [A]_i, [B]_i, [P]_i | k, B\right) \\ f_4\left(V, [A], [B], [P], F_i, F_o, [A]_i, [B]_i, [P]_i | k, B\right) \end{bmatrix}$$

⇝ For the input variables, $u(t)$

$$u(t) = \begin{bmatrix} u_1(t) \\ u_2(t) \\ u_3(t) \\ u_4(t) \end{bmatrix} \begin{bmatrix} F_i(t) \\ F_o(t) \\ [A]_i(t) \\ [B]_i(t) \end{bmatrix},$$

Example I (cont.)

$$
\begin{bmatrix} \dot{V} \\ \dot{[A]} \\ \dot{[B]} \\ \dot{[P]} \end{bmatrix} = \begin{bmatrix} F_i - F_o \\ \frac{F_i}{V}([A]_i - [A]) - k[A][B] \\ \frac{F_i}{V}([B]_i - [B]) - 2k[A][B] \\ -\frac{F_i}{V}[P] + k[A][B] \end{bmatrix}
$$

$$
= \begin{bmatrix} f_1\left(V, [A], [B], [P], F_i, F_o, [A]_i, [B]_i, [P]_i | k, B\right) \\ f_2\left(V, [A], [B], [P], F_i, F_o, [A]_i, [B]_i, [P]_i | k, B\right) \\ f_3\left(V, [A], [B], [P], F_i, F_o, [A]_i, [B]_i, [P]_i | k, B\right) \\ f_4\left(V, [A], [B], [P], F_i, F_o, [A]_i, [B]_i, [P]_i | k, B\right) \end{bmatrix}
$$

⇝ For the parameter(s), θ_x

$$
\theta_x = \begin{bmatrix} \theta_1^x \\ \theta_2^x \end{bmatrix} = \begin{bmatrix} k \\ B \end{bmatrix}
$$

Strictly speaking, B is embedded in the state variable V and hence not a parameter

- We still need to know it's value to be able to computations

Example I (cont.)

$$\begin{bmatrix} \dot{V} \\ [\dot{A}] \\ [\dot{B}] \\ [\dot{P}] \end{bmatrix} = \begin{bmatrix} F_i - F_o \\ \frac{F_i}{V}([A]_i - [A]) - k[A][B] \\ \frac{F_i}{V}([B]_i - [B]) - 2k[A][B] \\ -\frac{F_i}{V}[P] + k[A][B] \end{bmatrix}$$

For compactness, we can now write the state-space equations using the control notation

$$\underbrace{\begin{bmatrix} \dot{x_1} \\ \dot{x_2} \\ \dot{x_3} \\ \dot{x_4} \end{bmatrix}}_{\dot{x}} = \underbrace{\begin{bmatrix} f_1(x, u|\theta_x) \\ f_2(x, u|\theta_x) \\ f_3(x, u|\theta_x) \\ f_4(x, u|\theta_x) \end{bmatrix}}_{f(x, u|\theta_x)} = \begin{bmatrix} u_1 - u_2 \\ \frac{u_1}{x_1}(u_3 - x_2) - kx_2x_3 \\ \frac{u_1}{x_1}(u_4 - x_3) - 2kx_2x_3 \\ -\frac{u_1x_4}{x_1} + kx_2x_3 \end{bmatrix}$$

Example I (cont.)

Let $x'(t) = [x(t) - x_{SS}(t)]$, $u'(t) = [u(t) - u_{SS}(t)]$, for some steady-state (x_{SS}, u_{SS})

We write a linearised model, $\dot{x}'(t) = Ax'(t) + Bu'(t)$ by computing matrix A and B

$$A = \begin{bmatrix} \frac{\partial f_1(x,u)}{\partial x_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial x_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial x_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial x_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_2(x,u)}{\partial x_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial x_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial x_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial x_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_3(x,u)}{\partial x_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial x_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial x_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial x_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_4(x,u)}{\partial x_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial x_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial x_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial x_4}\Big|_{x_{SS},u_{SS}} \end{bmatrix}$$

$$B = \begin{bmatrix} \frac{\partial f_1(x,u)}{\partial u_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial u_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial u_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_1(x,u)}{\partial u_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_2(x,u)}{\partial u_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial u_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial u_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_2(x,u)}{\partial u_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_3(x,u)}{\partial u_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial u_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial u_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_3(x,u)}{\partial u_4}\Big|_{x_{SS},u_{SS}} \\ \frac{\partial f_4(x,u)}{\partial u_1}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial u_2}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial u_3}\Big|_{x_{SS},u_{SS}} & \frac{\partial f_4(x,u)}{\partial u_4}\Big|_{x_{SS},u_{SS}} \end{bmatrix}$$

Example I (cont.)

$$\begin{bmatrix} \dot{x_1} \\ \dot{x_2} \\ \dot{x_3} \\ \dot{x_4} \end{bmatrix} = \begin{bmatrix} u_1 - u_2 \\ \frac{u_1}{x_1}(u_3 - x_2) - kx_2x_3 \\ \frac{u_1}{x_1}(u_4 - x_3) - 2kx_2x_3 \\ -\frac{u_1x_4}{x_1} + kx_2x_3 \end{bmatrix}$$

By taking the partial derivatives of f with respect to the state variables x, we obtain

$$A =$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ -\frac{u_1(u_3 - x_2)}{x_1^2}\Big|_{x_{SS},u_{SS}} & (-\frac{u_1}{x_1} - kx_3)\Big|_{x_{SS},u_{SS}} & -kx_2\Big|_{x_{SS},u_{SS}} & 0 \\ -\frac{u_1(u_4 - x_3)}{x_1^2}\Big|_{x_{SS},u_{SS}} & -2kx_3\Big|_{x_{SS},u_{SS}} & (-\frac{u_1}{x_1} - 2kx_2)\Big|_{x_{SS},u_{SS}} & 0 \\ \frac{u_1x_4}{x_1^2}\Big|_{x_{SS},u_{SS}} & k & kx_2\Big|_{x_{SS},u_{SS}} & -\frac{u_1}{x_1}\Big|_{x_{SS},u_{SS}} \end{bmatrix}$$

For some fixed point (x_{SS}, u_{SS})

Example I (cont.)

$$\begin{bmatrix} \dot{x_1} \\ \dot{x_2} \\ \dot{x_3} \\ \dot{x_4} \end{bmatrix} = \begin{bmatrix} u_1 - u_2 \\ \dfrac{u_1}{x_1}(u_3 - x_2) - kx_2x_3 \\ \dfrac{u_1}{x_1}(u_4 - x_3) - 2kx_2x_3 \\ -\dfrac{u_1x_4}{x_1} + kx_2x_3 \end{bmatrix}$$

By taking the partial derivatives of f with respect to the input variables u, we obtain

$$B = \begin{bmatrix} 1 & -1 & 0 & 0 \\ \left.\dfrac{u_3 - x_2}{x_1}\right|_{x_{SS},u_{SS}} & 0 & \left.\dfrac{u_1}{x_1}\right|_{x_{SS},u_{SS}} & 0 \\ \left.\dfrac{u_4 - x_3}{x_1}\right|_{x_{SS},u_{SS}} & 0 & 0 & \left.\dfrac{u_1}{x_1}\right|_{x_{SS},u_{SS}} \\ -\left.\dfrac{x_4}{x_1}\right|_{x_{SS},u_{SS}} & 0 & 0 & 0 \end{bmatrix}$$

Again, for some fixed point (x_{SS}, u_{SS})

The nonlinear model linearised around (x_{SS}, u_{SS})

$$\dot{x}'(t) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ -\dfrac{u_1(u_3-x_2)}{x_1^2} & -\dfrac{u_1}{x_1} - kx_3 & -kx_2 & 0 \\ -\dfrac{u_1(u_4-x_3)}{x_1^2} & -2kx_3 & -\dfrac{u_1}{x_1} - 2kx_2 & 0 \\ \dfrac{u_1 x_4}{x_1^2} & k & kx_2 & -\dfrac{u_1}{x_1} \end{bmatrix}_{SS} x'(t)$$

$$+ \begin{bmatrix} 1 & -1 & 0 & 0 \\ \dfrac{u_3-x_2}{x_1} & 0 & \dfrac{u_1}{x_1} & 0 \\ \dfrac{u_4-x_3}{x_1} & 0 & 0 & \dfrac{u_1}{x_1} \\ -\dfrac{x_4}{x_1} & 0 & 0 & 0 \end{bmatrix}_{SS} u'(t)$$

Assuming that we can measure all the state variables, for $y'(t) = y(t) - y_{SS}$ we have

$$y'(t) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} x'(t) + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} u'(t)$$

What is y_{SS}?