# Exercise to MATLAB Course lecture 3 

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## 1 Problem formulation

A chemical isothermal reactor (Van de Vusse) is studied in this example. The relationship from the feed flow rate $u$ into the reactor to the concentration of the product $y$ at the outlet of the reactor is modeled by the following non-linear state space model.

$$
\begin{align*}
\dot{x_{1}} & =-k_{1} x_{1}-k_{3} x_{1}^{2}+\left(v-x_{1}\right) u  \tag{1}\\
\dot{x_{2}} & =k_{1} x_{1}-k_{2} x_{2}-x_{2} u  \tag{2}\\
y & =x_{2} \tag{3}
\end{align*}
$$

where the reaction rate coefficients are given by $k_{1}=50, k_{2}=100, k_{3}=10$. The concentration of the by-product into the reactor, $v$, is treated as an unknown constant or slowly varying disturbance with nominal value $v^{s}=10$.

The following steady state nominal (equilibrium) values are given:

$$
\begin{align*}
v^{s} & =10,  \tag{4}\\
u^{s} & =25,  \tag{5}\\
x_{1}^{s} & =2.5,  \tag{6}\\
y^{s} & =x_{2}^{s}=1 . \tag{7}
\end{align*}
$$

The above model may be written as a vector Ordinary Differential Equation (ODE) model of the form

$$
\begin{align*}
\dot{x} & =f(x, u, v)  \tag{8}\\
y & =g(x) \tag{9}
\end{align*}
$$

where

$$
x=\left[\begin{array}{l}
x_{1}  \tag{10}\\
x_{2}
\end{array}\right], f(x, u, v)=\left[\begin{array}{l}
f_{1} \\
f_{2}
\end{array}\right],
$$

where

$$
\begin{align*}
& f_{1}=-k_{1} x_{1}-k_{3} x_{1}^{2}+\left(v-x_{1}\right) u,  \tag{11}\\
& f_{2}=k_{1} x_{1}-k_{2} x_{2}-x_{2} u . \tag{12}
\end{align*}
$$

Furthermore the output equation is linear in this example due to $y=x_{2}$ in the model.

## 2 Exercise Tasks

Use MATLAB in all tasks below. Write an m-file script for the solutions. Write with advantage separate m-file scripts for Tasks 3 and 4 below.

1. Show that the given steady state nominal values, $v^{s}, u^{s}, x_{1}^{s}, x_{2}^{s}$, actually is equilibrium values so that $\dot{x_{1}^{s}}=0$ and $\dot{x_{2}^{s}}=0$.
2. We want to define the time interval

$$
\begin{equation*}
0 \leq t \leq t_{f} \tag{13}
\end{equation*}
$$

and with a step length parameter, $h=0.001$, and final time instant $t_{f}=0.3$. Define a vector

$$
t=\left[\begin{array}{lllll}
0 & h & 2 h & \cdots & t_{f} \tag{14}
\end{array}\right]
$$

in MATLAB using the : (column) operator. Find the number of discrete time instants, $N$, in the discrete time vector, $t$.
3. Simulate (solve) the differential equation $\dot{x}=f(x, u), y=g(x)$ by using the explicit Euler method for integration. Implement the simulation in a for-loop. Store the solutions in data matrices $X$ for the states $x^{T}, Y$ for the output $y=y(t)$. Plot the results. Assume that the initial values for the states are $x_{1}(t=0)=x_{1}^{s}$ and $x_{2}(t=0)=x_{2}^{s}$. Specify a step in the input feed flow rate from $u=25$ to $u=30$ at time $t=\frac{t_{f}}{2}$.
4. Simulate (solve) the differential equation $\dot{x}=f(x, u), y=g(x)$ by using the built in ODE solver, ode15s for the integration. Plot the results and compare with the Euler simulation results from the previous task. Assume that the initial values for the states are $x_{1}(t=0)=0$ and $x_{2}(t=0)=0$. Specify a step in the input feed flow rate from $u=25$ to $u=30$ at time $t=\frac{t_{f}}{2}$.
5. In the response from the input $u$ to the output $y=x_{2}$ there is a so called "inverse response". Use the zoom MATLAB figure function to display this better. Plot the response from $u$ to $y=x_{2}$ in one figure.
6. Assume that the model, $\dot{x}=f(x, u, v)$ is linearized around the nominal values $x^{s}, u^{s}$ and $v^{s}$. Find the time constants of the system (around nominal values).
Find the Jacobian system matrix

$$
\begin{equation*}
A_{c}=\left.\frac{\partial f(x, u, v)}{\partial x^{T}}\right|_{0} \tag{15}
\end{equation*}
$$

where $\left.\right|_{0}$ means nominal values used in the arguments.

- Find $A_{c}$ and the time constants analytically. remember that the relationship between the eigenvalues, $\lambda_{1}$ and $\lambda_{2}$, and the time constants is, $T_{1}=-\frac{1}{\lambda_{1}}$ and $T_{2}=-\frac{1}{\lambda_{2}}$
- Find matrix $A_{c}$ numerically by using the function jacobi.m.


## Solutions

Some background and solution of topics regarding this exercise is presented in the following.

A linearized model around steady state is given by

$$
\begin{equation*}
\Delta \dot{x}=A_{c} \Delta x+B_{c} \Delta u \tag{16}
\end{equation*}
$$

where $\Delta x=x-x^{s}$ and $\Delta u=u-u^{s}$ and

$$
\begin{gather*}
A_{c}=\left[\begin{array}{ll}
\frac{\partial f_{1}}{\partial x_{1}} & \frac{\partial f_{1}}{\partial x_{2}} \\
\frac{\partial f_{2}}{\partial x_{1}} & \frac{\partial f_{2}}{\partial x_{2}}
\end{array}\right]_{x^{s}, u^{s}}=\left[\begin{array}{cc}
-k_{1}-2 k_{3} x_{1}^{s}-u^{s} & 0 \\
k_{1} & -k_{2}-u
\end{array}\right]=\left[\begin{array}{rr}
-125 & 0 \\
50 & -125
\end{array}\right], \\
B_{c}=\left[\begin{array}{c}
\frac{\partial f_{1}}{\partial u} \\
\frac{\partial f_{2}}{\partial u}
\end{array}\right]_{x^{s}, u^{s}}=\left[\begin{array}{r}
v^{s}-x_{1}^{s} \\
-x_{2}^{s}
\end{array}\right]=\left[\begin{array}{c}
7.5 \\
-1
\end{array}\right] . \tag{18}
\end{gather*}
$$

A discrete time model is obtained by using a zero order hold on the input and a sampling interval $h=0.002$, i.e.,

$$
\begin{align*}
x_{k+1} & =A x_{k}+B u_{k}+v,  \tag{19}\\
y_{k} & =D x_{k}, \tag{20}
\end{align*}
$$

where

$$
\begin{gather*}
A=e^{A c h}=\left[\begin{array}{lr}
0.7788 & 0 \\
0.0779 & 0.7788
\end{array}\right],  \tag{21}\\
B=A_{c}^{-1}\left(e^{A_{c} h}-I\right) B_{c}=\left[\begin{array}{r}
0.0133 \\
-0.0011
\end{array}\right], \tag{22}
\end{gather*}
$$

$$
D=\left[\begin{array}{ll}
0 & 1 \tag{23}
\end{array}\right], v=x^{s}-A x^{s}-B u^{s}+C\left(v-v^{s}\right)
$$

Choosing an LQ criterion

$$
\begin{equation*}
J_{i}=\frac{1}{2} \sum_{k=i}^{\infty}\left(Q\left(y_{k}-r\right)^{2}+P \Delta u_{k}^{2}\right) \tag{24}
\end{equation*}
$$

with

$$
\begin{equation*}
P=1, Q=500 \tag{25}
\end{equation*}
$$

gives the LQ-optimal control

$$
\begin{equation*}
u_{k}=u_{k-1}+G_{1} \Delta x_{k}+G_{2}\left(y_{k-1}-r\right) \tag{26}
\end{equation*}
$$

where

$$
G_{1}=\left[\begin{array}{ll}
-23.4261 & -84.5791 \tag{27}
\end{array}\right], G 2=-20.0581
$$

Simulation results after changes in the reference signal $r$ are illustrated in Figure 1.


Figure 1: Simulation of the chemical reactor in Example ?? with LQ-optimal control. This figure is generated by the MATLAB file dlq_ex3_du.m.

