Master study
Systems and Control Engineering
Department of Technology
Telemark University College
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SCE1106 Control Theory

Task: Chemical reactor modeling

We are in this task going to study the problem of modelling and controlling a chemical reactor. The reaction kinetics for the reactor are given by

$$A \overset{k_1}{\to} B \quad \overset{k_2}{\to} C, \tag{1}$$

$$2A \overset{k_3}{\to} D. \tag{2}$$

Note that there is a 2nd order reaction from substance A to substance D and that the other reactions is of 1st order. The goal is to study and control the product substance B in the reactor. The chemical substances C and D are un-wanted bi-product of the reactions. The control variable to the reactor is the feed-flow (rate of feed flow) u i $[\frac{1}{\text{timer}}]$. The fraction of substance A in the feed-flow, u, is x_{10}. The fractions of substance A and B in the reactor tank are x_1 and x_2, respectively. We see from the reaction kinetics that substances C and D does not influence the substances A and B. The model relationship from the control input, u, to the measurement of the product $y = x_2$ is given by the non-linear, continuous time, state space model

$$\dot{x_1} = -k_1 x_1 - k_3 x_1^2 + (x_{10} - x_1)u, \tag{3}$$

$$\dot{x_2} = k_1 x_1 - k_2 x_2 - x_2 u, \tag{4}$$

$$y = x_2, \tag{5}$$

where the reaction kinetic coefficients are given by $k_1 = 50$, $k_2 = 100$, $k_3 = 10$. The following steady state values for the control variable and the states are given: $x_1 = 2.5$, $x_2 = 1$ and $u = 25$.

a) Compute the steady state value of the fraction of substance A at the inlet to the chemical reactor tank, i.e. compute the steady state value for x_{10}. Tips: put $\dot{x_1} = 0$ and solve for x_{10}.

b) Write a m-file simulator based on the explicit Euler methodin order to simulate the dynamic process model. Use the steady state values as initial/nominal value and simulate the differential equations in time. Check if the states remains constant as a function of time.

c) Simulate the system after a step in the control input from $u = 25$ to $u = 30$ at time instant $t = 0$. The simulation period could be in the interval $0 \leq t \leq 0.1$. The step length in the integration could be fixed to $h = 0.001$. Study the dynamic response from the control input u to the states x_1 and $y = x_2$. What can be said about the responses?

d) We want to held the product substance, $y = x_2$, at a specified reference value, r. Design a PI-controller for the system.

e) Is there possibile to do a better yob with a PID controller. Investigate this..

Remarks: This process may probably have been better controlled by a more advanced model based controller such as an LQ/LQG controller, an MPC controller or a non-linear linearizing controller. Such controllers are analyzed in other courses.

Sketching the solution

The problems are solved in the enclosed MATLAB script **demo_react.m**.

Solution step a) The answer is $x_{10} = 10$.

Solution step b) The step response will be as in Figure 1. As we see there is an inverse response in substance A, i.e. in the state x_2.

Solution step c) Controlling the chemical reactor with a PI controller will be as illustrated in Figure 2 after a step in the reference from $r = 1$ to $r = 1.05$ at time $t = 0$.

Solution step d) Controlling the chemical reactor with a PID controller will be as illustrated in Figure 2 after a step in the reference from $r = 1$ to $r = 1.05$ at time $t = 0$.

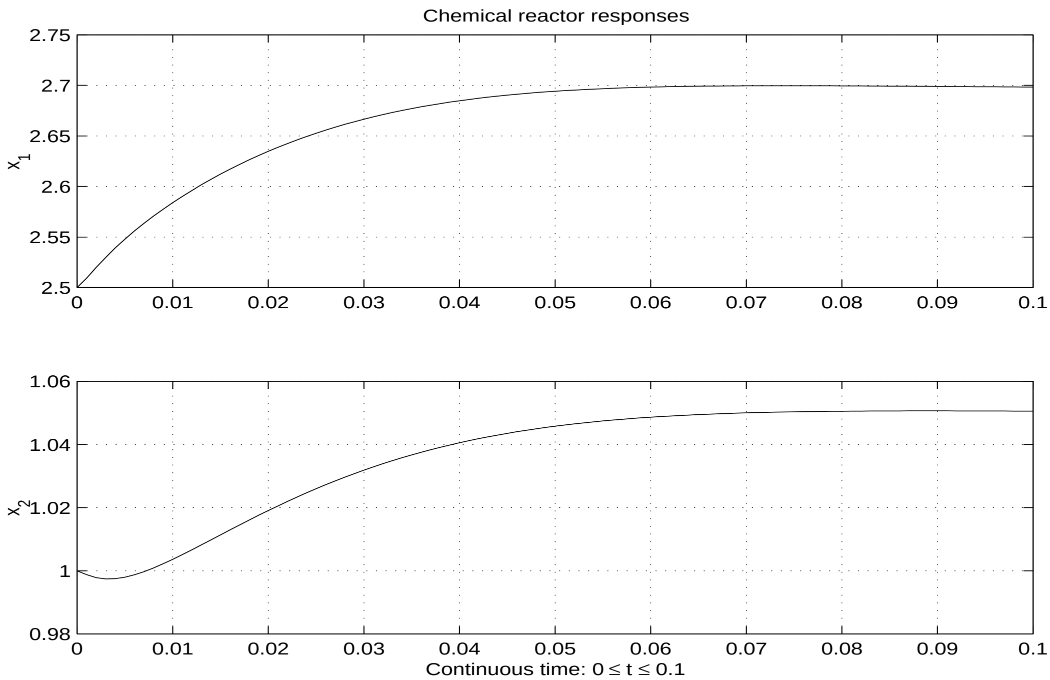

Figure 1: Step response. The figure is generated by the MATLAB file **demo_react.m**.

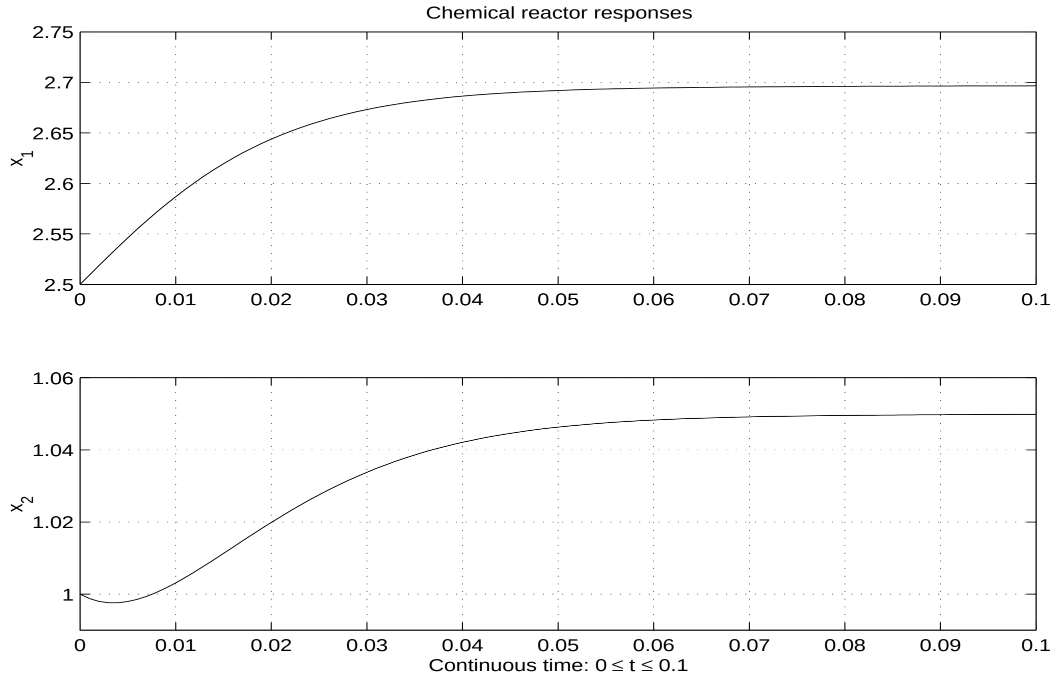

Figure 2: PI-controlling the reactor. The Figure is generated by the MATLAB file **demo_react.m**.

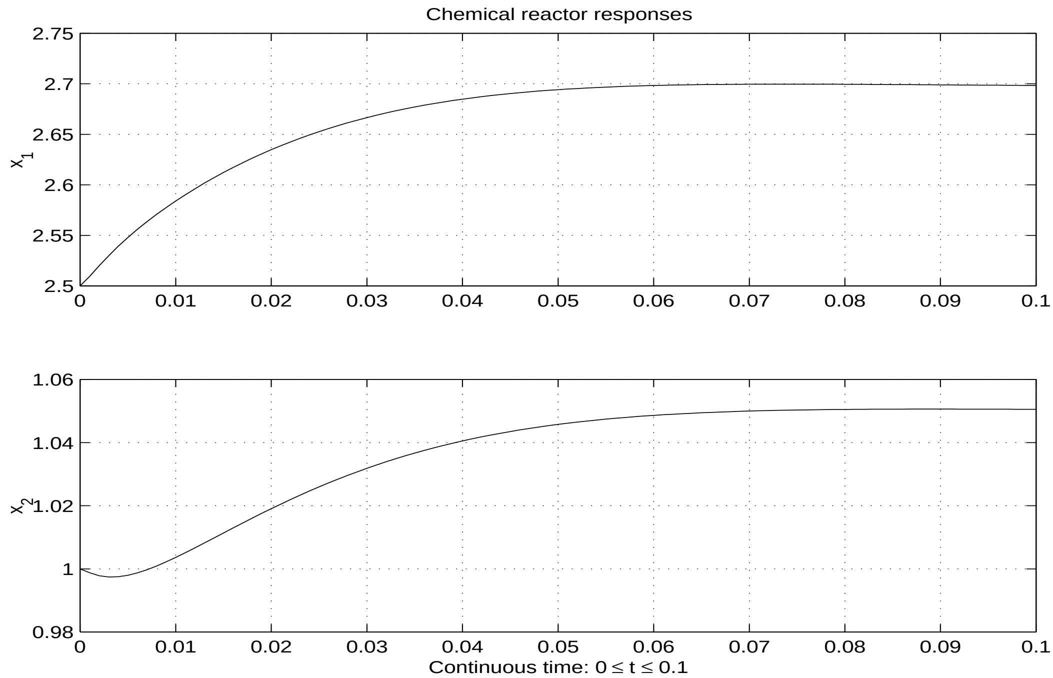

Figure 3: PID-controlling the reactor. The Figure is generated by the MATLAB file **demo_react.m**.

```
% DEMO_REACT.M
% Purpose: Illustrate conventional PID control of a chemical reaktor.
% DDIR 27.03.2001

%% Reaction coefficients.
k1=50; k2=100; k3=10;

%% Nominal process variables.
u=25;                              % Steady state feed flowrate.
x=zeros(2,1);
x(1)=2.5;                          % Steady state concentration of A.
x(2)=1;                            % Steady state concentration of B.
r=1;                               % reference for x_2.

%% Compute concentration of A, x1, at the inlet.
x10= (k1*x(1)+k3*x(1)^2)/u+x(1)   % Compute nominal inlet concentration, x10=C_Ai.

%% Check RHS of dot(x)=f(x,u) if f(x,u)=0.
f=zeros(2,1);
f(1)=-k1*x(1)-k3*x(1)^2+(x10-x(1))*u;
f(2)= k1*x(1)-k2*x(2)-x(2)*u;

h=0.0011; t1=0.1; t=0:h:t1; N=length(t); % Time axis data.

%% Get some parameters from the user
Text=['*** CONTROL OF CHEMICAL REACTOR ***'
      '1 : PI-control                      '
      '2 : Open loop step response in u    '
      '3 : PID control                     '];
disp(Text);
ireg=1;
ireg=dread('Regulert (1) uregulert (2) ',ireg);
if (ireg==1) ~= (ireg==3)
   Kp=25; Ti=10;
   z=25;
   r=1.05;
   r=dread('Spesifiser referanse: r=',r);
   Kp=dread('Kp=',Kp);
   Ti=dread('Ti=',Ti);
   if ireg==3; Td=5; Td=dread('Td=',Td); end
elseif ireg == 2
   u=30;
   u=dread('Sprang i foedepaadrag: u=',u);
end

%% Main simulation loop
X=zeros(N,2); Y=zeros(N,1); U=zeros(N,1);
```

```
D=[0,1]; eold=r-D*x;
for i=1:N
   y=D*x;

   if ireg == 1                          % Discrete PI-controller
      e=r-y;
      u=Kp*e+z;
      z=z+Kp*e/Ti;
   elseif ireg == 2                      % Open loop step response in u.
      u=u;
   elseif ireg ==3
      e=r-y;
      u=Kp*e+z+Kp*Td*(e-eold);
      z=z+Kp*e/Ti;
      eold=e;
   end

   U(i,1)=u; Y(i,1)=y; X(i,:)=x';        % Save variables.

   f(1)=-k1*x(1)-k3*x(1)^2+(x10-x(1))*u; % Update process model.
   f(2)= k1*x(1)-k2*x(2)-x(2)*u;
   x=x+h*f;

end

subplot(211), plot(t,X(:,1)), grid, ylabel('x_1')
title('Chemical reactor responses')
subplot(212), plot(t,X(:,2)), grid, ylabel('x_2')
xlabel('Continuous time: 0 \leq t \leq 0.1')
```