3. Implementing and simulating a system of ODEs in Matlab

Hande Bozkurt, Daria Semenova & Krist V. Gernaey

February 18th 2015

Course 28864: Introduction to Matlab programming

During the previous two exercises you have learned the difference between a Matlab script and a Matlab function. The purpose of this exercise is to get familiar with the functions of Matlab that allow you to simulate a process model consisting of a system of ordinary differential equations (ODEs) using m-files.
At the end of this exercise you should be able to implement and simulate a process model in Matlab using scripts and functions.

Reactions in a CSTR

Assume that you have a continuous stirred-tank reactor (CSTR) with constant volume. In the reactor a first order reaction converts a raw material *A* into an intermediate *I*. An undesired side reaction also takes place that converts *A* into *B*. The other component added to the system, *D*, will react with *I* to produce *P*, the desired product. Simultaneously, *B* will react with *D* to produce the undesired by-product *S*.

The four reactions taking place in the reactor together with their rate expressions are given below.

(1)	$A \rightarrow I$	$r_1 = k_1 C_A$
(2)	$A \rightarrow B$	$r_2 = k_2 C_A$
(3)	$I + D \rightarrow P$	$r_3 = k_3 C_I C_D$
(4)	$B + D \rightarrow S$	$r_4 = k_4 C_D C_B^2$

Where;

$k_1 = 1.25*10^{-2}$	(min^{-1})
$k_2 = 7.5*10^{-3}$	(min^{-1})
$k_3 = 0.265$	($m^3\ mol^{-1}\ min^{-1}$)
$k_4 = 0.15$	($m^6\ mol^{-2}\ min^{-1}$)

The following assumptions are made: (1) the CSTR is perfectly mixed, (2) the mass densities of the feed and product streams are equal and constant, (3) the liquid volume, *V* is constant. The mass balance equation for a component *j* can be written as:

$$V.\frac{dC_j}{dt} = q\left(C_{j,in} - C_j\right) + Vr_j$$

Where;

C_j	the concentration of component j in the reactor
$C_{j,in}$	the concentration of component j in the inflow
q	the flowrate of the inflow and outflow

r the net reaction rate of component j
V the volume of the reactor

The parameters of the system are given in Table 1. The inflow only contains the components *A* and *D*.
Initial conditions were set to 1.252 mol m^{-3} for *A*, 3.131 mol m^{-3} for *B* and 6.52 mol m^{-3} for *I*. The initial concentrations of all other components are set to 0.

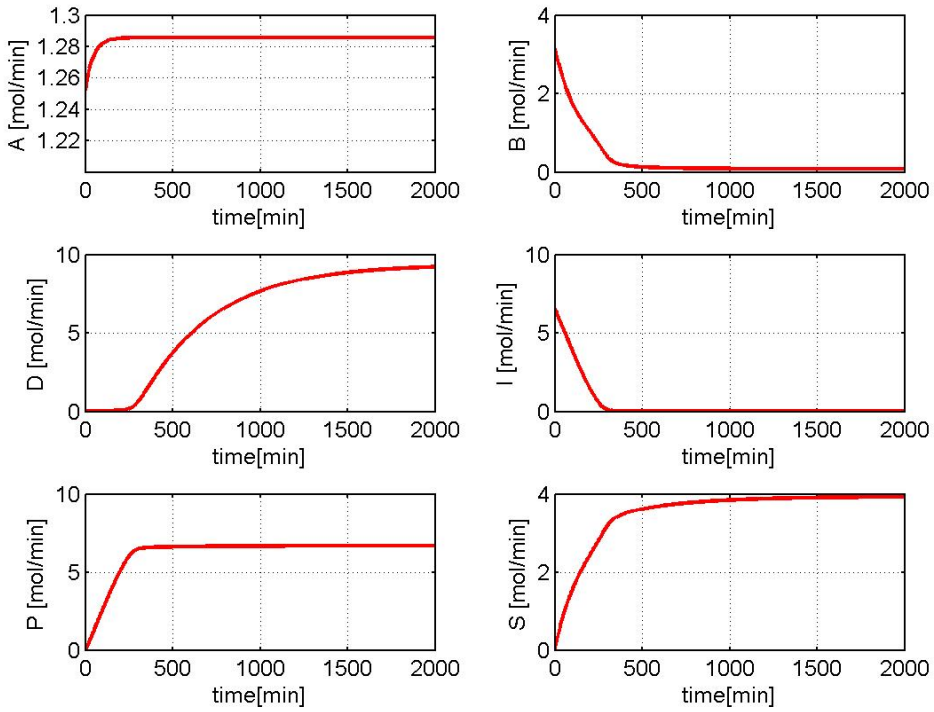
Table 1. Parameters for the model

Parameter	Value	Unit
Volume	800	L
Q	0.032	L sec^{-1}
$C_{A,in}$	0.012	mol L^{-1}
$C_{D,in}$	0.020	mol L^{-1}

When calling the solver make sure to specify the relative tolerance in the options by writing the following statement:

```
options=odeset('RelTol',1e-4);
```

You can use the ode15s solver.
Simulate the system for 2000 minutes. Generate plots for each of the 6 state variables.
Your solution should look as follows – if you get different plots then your ODEs are not implemented correctly.



Handing in:

The script and the function (two Matlab m-files) of the model of the CSTR system for this assignment should be sent as e-mail attachments to kvg@kt.dtu.dk before Wednesday the 25th of February 2015 at 4 pm!

In the email, you clearly list the names and student numbers of the members of your group (maximum 2 persons per group).

To allow automatic sorting of the emails containing your solutions, the subject line of the email should be: 28864-F2015-E3.

For help or questions: dsem@kt.dtu.dk or kvg@kt.dtu.dk