STUDIO 1. THE TANK REACTOR: MASS BALANCE.

In a sequence of studio exercises we will study a simple example from chemical reaction engineering. The purpose of these exercises is to demonstrate by detailed instructions how to set up a mathematical model and how to study the model by mathematical analysis and Matlab computation. Note how we start by studying simplified situations and how we calculate exact solutions by hand when it is possible and how we experiment by computing many solutions with Matlab until we understand what is going on.

We begin by recalling how to solve differential equations of first order. Then we introduce the ideal tank reactor.

Important: write a readable report of your work in each studio session. You will need this at the end of the course when you prepare for the written exam; several exam questions will be based directly on the studio work which is only documented in your own notes and the instructions.

Some exercises are called homework in order to save time in the studio classroom.

1. Linear differential equations of first order

Recall that $\frac{d}{dt}\exp(t) = \exp(t)$ and $\exp(0) = 1$. This means that the exponential function $u(t) = \exp(t)$ satisfies the initial-value problem

$$u'(t) = u(t),\ t > 0; \quad u(0) = 1. \tag{1}$$

Let a and u_0 be real numbers and consider the initial-value problem

$$u'(t) = au(t),\ t > 0; \quad u(0) = u_0. \tag{2}$$

The solution is $u(t) = u_0 \exp(at)$. Check this!

Exercise 1. Solve (2) with Matlab: Write the following *function file* `funk1.m`, which defines the right-hand side of the differential equation.

```
function y=funk1(t,u)
global a
y=a*u;
```

Then write the following *script file* `data.m`, which gives default values to the variables that are used.

```
global a
a=1; T=1; u0=1;
```

Finally write the following *script file* `solve1.m`, which solves (2) and plots the solution.

```
[t,u]=ode45('funk1', [0 T], u0);
plot(t,u);
```

Note how the value of a enters into the function via the command `global a`, which must be written both in the function file `funk1.m` and in the script file `data.m`. (Read about "global variables" in `helpdesk`.) Start the computation by typing the following on the Matlab command line:

```
>> data
>> solve1
>> a=-1
>> T=2
>> hold on
>> solve1
```

Compute and observe the solutions for various values of a, positive, negative, and zero. If you type `>> hold on` then Matlab will plot several curves in the same figure. □

Date: March 11, 2003, Niklas Ericsson, Stig Larsson, Mathematics, Chalmers University of Technology.

Now let b be another real number and consider the initial-value problem

$$u'(t) = au(t) + b, \ t > 0; \quad u(0) = u_0. \tag{3}$$

Remember that the solution is given by $u(t) = u_h(t) + u_p(t)$, where $u_h(t) = A\exp(at)$ is a solution of the homogeneous equation $u' - au = 0$ and $u_p(t) = B$ is a particular solution of the inhomogeneous equation $u' - au = b$.

Homework 1. Determine the constants A and B and show that the solution is

$$u(t) = u_0 \exp(at) + \frac{b}{a}(\exp(at) - 1) \quad (\text{if } a \neq 0). \tag{4}$$

What is the solution when $a = 0$? For which values of a does the solution approach an equilibrium $u(t) \to \bar{u}$ as $t \to \infty$? Determine $\bar{u}$. □

Exercise 2. Solve (3) with Matlab: Define b in the file `data.m` and change the global command to `global a b` in both places. Observe what the solutions look like for a positive, negative, and zero. For which values of a does the solution approach an equilibrium $u(t) \to \bar{u}$ as $t \to \infty$? □

Now we consider the situation when $a = a(t)$, $b = b(t)$ are not constant:

$$u'(t) = a(t)u(t) + b(t), \ t > 0; \quad u(0) = u_0. \tag{5}$$

We use the method of *integrating factor*. Write the equation as $u'(t) - a(t)u(t) = b(t)$ and multiply it by the integrating factor $e^{-A(t)}$, where $A(t) = \int_0^t a(r)\,dr$, so that $A'(t) = a(t)$ and A(0)=0. We get

$$\frac{d}{dt}\Big(e^{-A(t)}u(t)\Big) = e^{-A(t)}u'(t) - a(t)e^{-A(t)}u(t) = e^{-A(t)}b(t).$$

We integrate from 0 to T:

$$\Big[e^{-A(t)}u(t)\Big]_0^T = \int_0^T e^{-A(t)}b(t)\,dt$$

and hence

$$e^{-A(T)}u(T) - e^{-A(0)}u(0) = \int_0^T e^{-A(t)}b(t)\,dt.$$

Using $A(0) = 0$, $u(0) = u_0$, multiplying by $e^{A(T)}$, and replacing t by s, T by t, we finally get

$$u(t) = u_0 e^{A(t)} + \int_0^t e^{A(t)-A(s)}b(s)\,ds, \quad \text{where } A(t) = \int_0^t a(r)\,dr. \tag{6}$$

Homework 2. Use constant functions $a(t) = a$, $b(t) = b$ in (6) and compute the integrals to obtain (4). □

Exercise 3. Add small time-dependent perturbations to a and b, for example,

$$u'(t) = (a + 0.1\sin(7t))u(t) + (b + 0.1\sin(8t)).$$

Note that this equation is of the form (5) with variable coefficients. Solve the equation with Matlab with the same values of a, b as in Exercise 2. What is the effect of the perturbations? □

2. The tank reactor

In a sequence of studio sessions we will study the ideal mixed tank reactor, see Figure 1. The goal is to design the reactor so that it will operate in a stable way at $(c_f - c)/c_f = 0.5$ ("50 % omsättningsgrad").

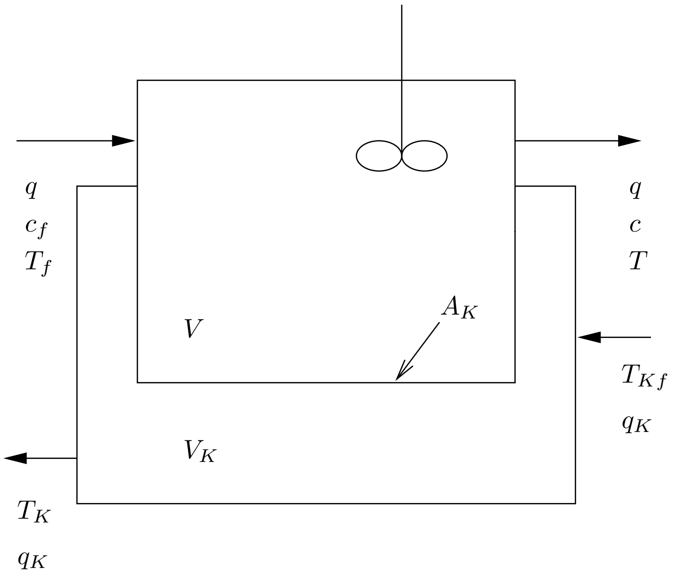

FIGURE 1. The tank reactor.

We will use the following data:

$V = 1.2\ \mathrm{m}^3$ volume of the tank

$c_p = 4.19\ \mathrm{kJ/(kg\ K)}$ heat capacity of the fluid

$\rho = 1000\ \mathrm{kg/m}^3$ density of the fluid

$q_{\mathrm{ref}} = 3.0 \cdot 10^{-4}\ \mathrm{m}^3/\mathrm{s}$ reference flux

$c_f = 5\ \mathrm{kmol/m}^3$ concentration at inflow of the interesting substance

$T_f = 70°\mathrm{C}$ temperature at inflow

$\delta H = -83.7\ \mathrm{kJ/mol}$ heat of reaction

$A_K = 1.0\ \mathrm{m}^2$ area of the cooler

$\kappa = 0.58\ \mathrm{kJ/(m^2\ s\ K)}$ heat transfer coefficient of the cooler

We introduce the following variables:

c $[\mathtt{mol/m}^3]$ concentration in the reactor of the interesting substance

T $[\mathtt{K}]$ temperature in the reactor

q $[\mathtt{m}^3\mathtt{/s}]$ flux through the reactor

T_K, T_{Kf} $[\mathtt{K}]$ temperatures in the cooler and at the cooler inflow

q_K $[\mathtt{m}^3\mathtt{/s}]$ flux through the cooler

V_K $[\mathtt{m}^3]$ volume of the cooler

The reaction is exothermal and of first order with rate of reaction kc $[\mathtt{mol/(m^3s)}]$. The rate coefficient depends on the temperature according to the Arrhenius law:

$$k = k_0 \exp(-E/(RT)) \quad [\mathtt{s}^{-1}] \tag{7}$$

where R $[\mathtt{8.31\ J/(mol\ K)}]$ is the gas constant, E $[\mathtt{J/mol}]$ is the activation energy and k_0 $[\mathtt{s}^{-1}]$ is the rate constant of the reaction. The following rates have been measured:

T [K]	343	353	363	373	383	393	403
k [$\mathtt{s}^{-1}$]	$2.8 \cdot 10^{-5}$	$5.6 \cdot 10^{-5}$	$11.2 \cdot 10^{-5}$	$22.4 \cdot 10^{-5}$	$44.8 \cdot 10^{-5}$	$89.6 \cdot 10^{-5}$	$179.2 \cdot 10^{-5}$

(Based on “Kemisk reaktionsteknik. Övningsuppgifter”, Kemisk reaktionsteknik, CTH 1993, uppgift 7.1.)

2.1. **Mass balance.** When we build a *mathematical model* for the tank reactor it is important not to consider all aspects at once. We therefore begin by making a big simplification: we assume that the rate coefficient k is constant, for example, $k =??$ corresponding to $T =??$ (choose a value from the table). Recall that k depends strongly on T, see (7), so this is not very realistic, but it will be a good starting point for our investigation.

The mass balance equation is

$$V\frac{dc}{dt} = q(c_f - c) - ckV. \quad \texttt{[mol/s]}$$

This equation says that the rate of change of the total amount of the interesting substance is equal to the influx minus the outflux minus the reaction rate. In order to make the equation dimensionless we divide by $q_{\text{ref}}c_f$ `[mol/s]`. We get

$$\frac{V}{q_{\text{ref}}}\frac{d}{dt}\Big(\frac{c}{c_f}\Big) = \frac{q}{q_{\text{ref}}}\Big(1 - \frac{c}{c_f}\Big) - \frac{c}{c_f}k\frac{V}{q_{\text{ref}}}. \tag{8}$$

We introduce $\tau = V/q_{\text{ref}}$ `[s]` (“uppehållstid”) and the dimensionless variables

$$\begin{aligned} s &= t/\tau \text{ (dimensionless time)},\\ X &= c/c_f \text{ (dimensionless concentration)},\\ U &= q/q_{\text{ref}} \text{ (dimensionless flux)}. \end{aligned}$$

Then, by the chain rule,

$$\frac{dX}{ds} = \frac{dX}{dt}\frac{dt}{ds} = \tau\frac{dX}{dt} = \frac{V}{q_{\text{ref}}}\frac{d}{dt}\Big(\frac{c}{c_f}\Big),$$

and (8) becomes

$$\frac{dX}{ds} = U(1 - X) - Xk\tau,$$

that is,

$$\frac{dX}{ds} = -(k\tau + U)X + U; \quad X(0) = X_0. \tag{9}$$

Note that this is of the form (5) with $a = -(k\tau + U)$ and $b = U$.

Exercise 4. Change your Matlab programs from part 1 so that they solve (9). Let first U be equal to a constant value $\bar{U}$. Does the solution $X(s)$ approach an equilibrium $\bar{X}$ as $s \to \infty$? Hint: Begin the file `data.m` by

```
global ktau Ubar
V=1.2;   qref=3.0e-4;
k=?? ;
tau=V/qref;   ktau=k*tau;
Ubar=1;  % equilibrium value of U
```

Change also the function file `funk1.m` to a file `tank.m` beginning with

```
function y=tank(s,X)
global ktau Ubar
U=Ubar;
y=??  % enter the expression for the right-hand side
```

□

Exercise 5. Recall that we want the reactor to operate at $(c_f - c)/c_f = 0.5$, i.e., at $\bar{X} = 0.5$. Determine $\bar{U}$ so that this is achieved. Hint: the equation for $\bar{X}$, $\bar{U}$ is obtained by setting $\frac{dX}{ds} = 0$ in (9), i.e.,

$$-(k\tau + \bar{U})\bar{X} + \bar{U} = 0. \tag{10}$$

Find a formula for $\bar{U}$ in terms of $k\tau$ and $\bar{X}$. Insert the command `Xbar=.5;` and the formula for `Ubar` in the file `data.m`. □

Exercise 6. We now investigate if the operating point $\bar{X} = 0.5$ is stable with respect to changes of the initial value X_0. Set $U = \bar{U}$ and solve (9) with Matlab with several initial values X_0. Is it stable? □

Exercise 7. We next investigate if the operating point $\bar{X} = 0.5$ is stable with respect to changes of the flux U. Set $X_0 = \bar{X} = 0.5$ and solve (9) with Matlab with, for example, $U(s) = \bar{U} + 0.1\sin(7s)$. Is it stable? □

Exercise 8. Finally, compute the required flux $\bar{q}$ (in dimensional units `[m³/s]`). □

Next studio session we will include the temperature dependence in k and we will see that the operating point $\bar{X} = 0.5$ is *not* always stable then.