TMA681 Tillämpad matematik K, 2001

# STUDIO 1. THE TANK REACTOR: MASS BALANCE.

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

(MA2 9.2) 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 is written both in the function file `funk1.m` and in the main program `data.m`. Start the computation by typing the following on the Matlab command line:

```
>> data
>> solve1
>> a=-1
>> T=2
>> 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.

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 (MA2 10.5) 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 $u' - au = b$.

---

*Date*: March 28, 2001, Niklas Ericsson, Stig Larsson, Mathematics, Chalmers University of Technology.

**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* (MA2 9.2). Write the equation as $u' - a(t)u = b(t)$ and multiply it by the integrating factor $e^{-A(t)}$, where $A(t) = \int_0^t a(s)\,ds$, 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

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

**Exercise 3.** Solve (5) with Matlab. Use, for example, $a = \pm 1$, $b(t) = 1 + 0.1\sin(7t)$.

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

## 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").

We will use the following data:

$V = 1.2$ m$^3$ volume of the tank

$c_p = 4.19$ kJ/(kg K) heat capacity of the fluid

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

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

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

$T_f = 70°$C temperature at inflow

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

$A_K = 1.0$ m$^2$ area of the cooler

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

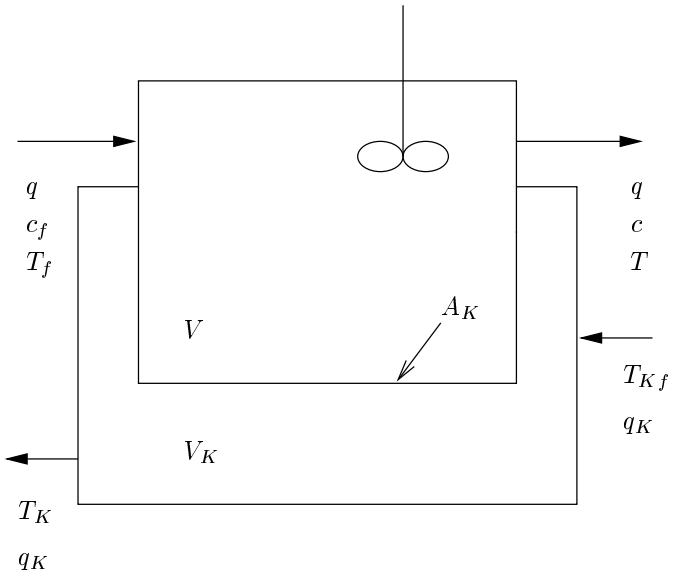


FIGURE 1. The tank reactor.

We introduce the following variables:

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

$T$ [K] temperature in the reactor

$q$ [m$^3$/s] flux through the reactor

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

$q_K$ [m$^3$/s] flux through the cooler

$V_K$ [m$^3$] volume of the cooler

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

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

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

| $T$ [K] | 343 | 353 | 363 | 373 | 383 | 393 | 403 |
|---|---|---|---|---|---|---|---|
| $k$ [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

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

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

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

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;
```

**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 $\bar{X}$. Explain what happens in the extreme cases $\bar{X} = 0$, $\bar{X} = 1$. Insert the command `Xbar=.5;` in the file `data.m` and the formula for `Ubar` in the file `solve1.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 `[m^3/s]`).

Next week 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.