School of Mathematics & Applied Statistics

MATH111: Mathematics Applied Mathematical Modelling 1

Assignment Week 8 Solutions

Spring 2006

1. Give an example of a *linear* differential equation and a *non-linear* differential equation explaining why your equation is linear/non-linear.

   Solution The important part of this question is explaining why your equation is linear or non-linear. There are no marks for providing an example, without justification.

2. Identify if the following differential equations are autonomous or non-autonomous. You *must* justify your answer.

   (a) $\dfrac{\mathrm{d}y}{\mathrm{d}t} = y^2$

   (b) $\dfrac{\mathrm{d}^2t}{\mathrm{d}y^2} = t\dfrac{\mathrm{d}t}{\mathrm{d}y} + \dfrac{1}{t}$

   (c) $\dfrac{\mathrm{d}t}{\mathrm{d}y} = \cos t$

   Solution

   (a) The independent variable is t and the dependent variable is y. The independent variable does not appear explicitly in the equation. Therefore the equation is *autonomous.*

   (b) The independent variable is y and the dependent variable is t. The independent variable does not appear explicitly in the equation. Therefore the equation is *autonomous.*

   (c) The independent variable is t and the dependent variable is y. The independent variable does not appear explicitly in the equation. Therefore the equation is *autonomous.*

3. For two consecutive reactions

$$\mathcal{A} \xrightarrow{k_1} \mathcal{B} \xrightarrow{k_2} \mathcal{C}$$

occurring in a batch reactor the concentrations of the species $\mathcal{A}$ and $\mathcal{B}$ satisfy the differential equations

$$\frac{\mathrm{d}\mathcal{A}}{\mathrm{d}t} = -k_1\mathcal{A}, \qquad \mathcal{A}(0) = C_A, \tag{1}$$

$$\frac{\mathrm{d}\mathcal{B}}{\mathrm{d}t} = k_1\mathcal{A} - k_2\mathcal{B}, \quad \mathcal{B}(0) = 0. \tag{2}$$

The chemical species $\mathcal{A}$ is known as the reactant, the chemical species $\mathcal{B}$ is known as the intermediate product and the chemical species $\mathcal{C}$ is known as the final product.

(a) Solve the system of differential equations to find the concentrations of the reactant and the intermediate product as a function of time.

Solution Equation (1) is an integrable equation and its solution is readily found to be

$$\mathcal{A}(t) = C_A \exp\left[-k_1 t\right].$$

Substituting this expression into equation (2) and re-arranging we obtain

$$\frac{\mathrm{d}\mathcal{B}}{\mathrm{d}t} + k_2\mathcal{B} = k_1 C_A \exp\left[-k_1 t\right], \quad \mathcal{B}(0) = 0.$$

This is a linear equation which can be solved using an integrating factor to obtain

$$\mathcal{B}(t) = \frac{k_1 C_A}{k_2 - k_1}\left(\exp\left[-k_1 t\right] - \exp\left[-k_2 t\right]\right), \tag{3}$$

in which we have assumed that $k_2 \neq k_1$.

(b) In many cases the intermediate product is more valuable than the final product and hence we want to maximise its production. At what time, t_m, should we stop the batch reactor from operating to achieve this aim?

Solution We should stop the batch reactor when the intermediate product has reached its maximum value. This happens when

$$\frac{\mathrm{d}\mathcal{B}}{\mathrm{d}t} = 0.$$

From equation (3) we have

$$\frac{\mathrm{d}\mathcal{B}}{\mathrm{d}t} = \frac{k_1 C_A}{k_2 - k_1}\left(-k_1 \exp\left[-k_1 t\right] + k_2 \exp\left[-k_2 t\right]\right).$$

It follows that

$$t_m = \frac{\ln \frac{k_1}{k_2}}{k_1 - k_2}. \tag{4}$$

(c) Define the fractional yield of the intermediate product by

$$\mathcal{Y}_B = \frac{\mathcal{B}}{C_A}.$$

What is the maximum fractional yield, $\mathcal{Y}_{B,\max}$?

Solution The maximum fractional yield will occur when the concentration of the intermediate product has reached its maximum value. Therefore we substitute the value for t_m, given by equation (4), into equation (3).

Hence we have

$$\begin{aligned}
\mathcal{Y}_{B,\max} &= \frac{k_1}{k_2 - k_1}\left(\exp\left[\frac{-k_1 \ln \frac{k_1}{k_2}}{k_1 - k_2}\right] - \exp\left[\frac{-k_2 \ln \frac{k_1}{k_2}}{k_1 - k_2}\right]\right),\\
&= \frac{k_1}{k_2 - k_1}\left\{\exp\left[\ln\left(\frac{k_1}{k_2}\right)^{\frac{-k_1}{k_1-k_2}}\right] - \exp\left[\ln\left(\frac{k_1}{k_2}\right)^{\frac{-k_2}{k_1-k_2}}\right]\right\},\\
&= \frac{k_1}{k_2 - k_1}\left[\left(\frac{k_1}{k_2}\right)^{\frac{-k_1}{k_1-k_2}} - \left(\frac{k_1}{k_2}\right)^{\frac{-k_2}{k_1-k_2}}\right],\\
&= \frac{k_1}{k_2 - k_1}\left(\frac{k_1}{k_2}\right)^{\frac{-k_1}{k_1-k_2}}\left[1 - \left(\frac{k_1}{k_2}\right)^{\frac{k_1-k_2}{k_1-k_2}}\right],\\
&= \frac{k_1}{k_2}\left(\frac{k_1}{k_2}\right)^{\frac{-k_1}{k_1-k_2}},\\
&= \left(\frac{k_1}{k_2}\right)^{\frac{-k_2}{k_1-k_2}}.
\end{aligned}$$

4. In section 10.2.1 of the notes we considered the problem of pollutant being dumped at time $t = 0$ into a clean lake into which only fresh water flows. We found that the time taken for the pollutant to reach 5% of its initial value is given by

$$t_{0.05} = \frac{V}{q}\ln 20.$$

In section 10.2.2 we consider the same problem but with a seasonal flowrate. The value of $t_{0.05}$ was found to satisfy the equation

$$\ln(0.05) + \frac{q_0}{V}\left[t_{0.05} + \frac{365\epsilon}{2\pi}\sin\left(\frac{2\pi t_{0.05}}{365}\right)\right] = 0. \tag{5}$$

In the following we take $V = 10^5\mathrm{m}^3$, $q = 5 \times 10^3\mathrm{m}^3\mathrm{hr}^{-1}$ and and $-1 < \epsilon < 1$.

(a) Find $t_{0.05}$ when $\epsilon = 0$.

(b) Find $t_{0.05}$ when $\epsilon = 0.05$.

(c) Draw a graph showing how $t_{0.05}$ depends upon the value for ϵ. Label your axis.

You may find it useful to use the following maple commands: `fsolve` and `implicitplot`.

Solution

(a) $t_{0.05} = 59.9\,\text{hr}$.

(b) $t_{0.05} = 57.5\,\text{hr}$.

(c) See figure 1

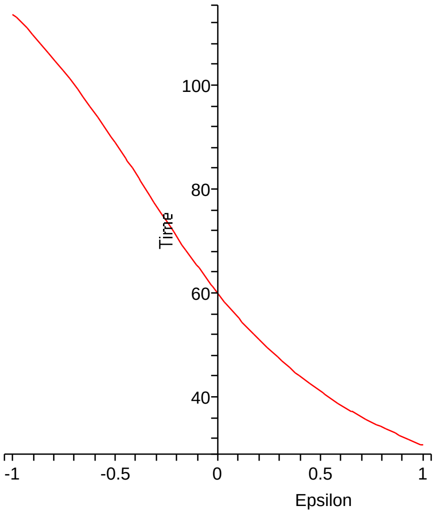

Figure 1: The variation of the time it takes for the pollutant to decrease to 5% of its initial value ($t_{0.05}$) as a function of the half-amplitude of the seasonal flow term (ϵ).

Here's my maple code for this question.

```
# week8-2006.maple
# 05.09.06
#
with(plots):

eqn := ln(0.05) +(q/V)*(t+365*epsilon*sin(2*Pi*t/365)/(2*Pi));

V := 1e5;
q := 5e3;

epsilon := 0;
solve(eqn,t);

epsilon := 0.05;
solve(eqn,t);

epsilon := 'epsilon':

implicitplot(eqn,epsilon=-1..1,t=20..120, grid=[30,30],\
             labeldirections=[horizontal,vertical],\
             labels=["Epsilon","Time"], thickness=1);
```