School of Mathematics & Applied Statistics

MATH111: Mathematics Applied Mathematical Modelling 1

Assignment Week 8 Solutions

Spring 2006

1. Give an example of a \textit{linear} differential equation and a \textit{non-linear} differential equation explaining why your equation is linear/non-linear.

\textbf{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 \textit{must} justify your answer.

(a) \( \frac{dy}{dt} = y^2 \)

(b) \( \frac{d^2t}{dy^2} = t \frac{dt}{dy} + \frac{1}{t} \)

(c) \( \frac{dt}{dy} = \cos t \)

\textbf{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 \textit{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 \textit{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 \textit{autonomous}.

3. For two consecutive reactions

\[ A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} C \]

occurring in a batch reactor the concentrations of the species \( A \) and \( B \) satisfy the differential equations

\begin{align*}
\frac{dA}{dt} &= -k_1A, \quad A(0) = C_A, \quad (1) \\
\frac{dB}{dt} &= k_1A - k_2B, \quad B(0) = 0. \quad (2)
\end{align*}

The chemical species \( A \) is known as the reactant, the chemical species \( B \) is known as the intermediate product and the chemical species \( C \) 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.

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

\[ A(t) = C_A \exp[-k_1t]. \]

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

\[ \frac{dB}{dt} + k_2B = k_1C_A \exp[-k_1t], \quad B(0) = 0. \]

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

\[ B(t) = \frac{k_1C_A}{k_2 - k_1} \left( \exp[-k_1t] - \exp[-k_2t] \right), \quad (3) \]

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

\[
\frac{dB}{dt} = 0.
\]

From equation (3) we have

\[
\frac{dB}{dt} = \frac{k_1 C_A}{k_2 - k_1} \left( -k_1 \exp[-k_1 t] + k_2 \exp[-k_2 t] \right).
\]

It follows that

\[
t_m = \frac{\ln \left( \frac{k_1}{k_2} \right)}{k_1 - k_2}, \tag{4}
\]

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

\[
\mathcal{Y}_B = \frac{B}{C_A}.
\]

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

\[
\mathcal{Y}_{B,max} = \frac{k_1}{k_2 - k_1} \left( \exp \left[ -k_1 \ln \frac{k_1}{k_2} \right] - \exp \left[ -k_2 \ln \frac{k_1}{k_2} \right] \right),
\]

\[
= \frac{k_1}{k_2 - k_1} \left\{ \exp \left[ \ln \left( \frac{k_1}{k_2} \right)^{\frac{k_2}{k_1 + k_2}} \right] - \exp \left[ \ln \left( \frac{k_1}{k_2} \right)^{\frac{k_1}{k_1 + k_2}} \right] \right\},
\]

\[
= \frac{k_1}{k_2 - k_1} \left\{ \left( \frac{k_1}{k_2} \right)^{\frac{k_2}{k_1 + k_2}} - \left( \frac{k_1}{k_2} \right)^{\frac{k_1}{k_1 + k_2}} \right\},
\]

\[
= \frac{k_1}{k_2} \left( \frac{k_1}{k_2} \right)^{\frac{k_2}{k_1 + k_2}} \left[ 1 - \left( \frac{k_1}{k_2} \right)^{\frac{k_1}{k_1 + k_2}} \right],
\]

\[
= \frac{k_1}{k_2} \left( \frac{k_1}{k_2} \right)^{\frac{k_2}{k_1 + k_2}},
\]

\[
\mathcal{Y}_{B,max} = \left( \frac{k_1}{k_2} \right)^{\frac{k_2}{k_1 + k_2}}.
\]

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

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

In the following we take \( V = 10^6 \text{m}^3 \), \( q = 5 \times 10^3 \text{m}^3 \text{hr}^{-1} \) 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 $\epsilon$. Label your axis.

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

**Solution**

(a) $t_{0.05} = 59.9$ hr.
(b) $t_{0.05} = 57.5$ hr.
(c) See figure 1

![Graph](image)

**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 ($\epsilon$).

Here’s my Maple code for this question.

```maple
# 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);
```