MA261 Assignment 4 Part 1 Tom Dalby U1903831.

1.1) i) The two step LMM is convergent if and only if it is consistent and zero-stable.

We have that $y_{n+2} + a y_{n+1} + b y_n = hcf(y_{n+i})$ where $i \in \{0,1,2\}$.

~~To be consistent, we~~

We can rewrite this as $y_{n+2} + a y_{n+1} + b y_n = \cancel{\beta_2} h \sum_{j=0}^{2} \beta_j f(y_{n+j})$ where $\beta_j = 0$ if $j \neq i$, and $\beta_j = C$ if $j = i$.

- The condition for ~~stability~~ consistency is that
  - $b + a + 1 = 0$
  - $\sum_{j=0}^{2} \beta_j = 2 + a$.

But notice regardless of whether $i = 0, 1$ or 2, $\sum_{j=0}^{2} \beta_j = \beta_i = C$, so for all $i \in \{0,1,2\}$, the condition for consistency is,
  - $b + a + 1 = 0$
  - $a + 2 = C$.

- To analyse zero stability recall the first characteristic polynomial for when $i \in \{0,1,2\}$ is
$$\rho(z) = \sum_{j=0}^{2} \alpha_j z^j = b + az + z^2.$$
So ρ is the same regardless of whether $i = 0, 1$ or 2 thus again our choice of i does not matter / the following applies to all three i.

The roots of ρ are $\dfrac{-a \pm \sqrt{a^2 - 4b}}{2}$.

We firstly need at least that $\dfrac{|-a \pm \sqrt{a^2-4b}|}{|2|} \leq |1|$ (there is a second condition needed if the modulus equals 1 but we will worry about this in a bit).

i.e. $|-a \pm \sqrt{a^2 - 4b}| \leq 2$.

Since we are assuming the method is now consistent, so $b = -1 - a$, this becomes $|-a \pm \sqrt{a^2 + 4a + 4}| \leq 2$
$$\Leftrightarrow |-a \pm \sqrt{(a+2)^2}| \leq 2 \Leftrightarrow |-a \pm a + 2| \leq 2.$$

The first roots bounded condition becomes $|-a+a+2| = |2| = 2 \leq 2$. So this root lies on the unit circle, so to ensure zero stability we require that the derivative ρ' at this root is non-zero.

$$\rho'(z) = a + 2z$$

$$\rho'\left(\frac{-a+\sqrt{a^2-4b}}{2}\right) = \rho'\left(\frac{-a+a+2}{2}\right) = \rho'(1) = 2+a \neq 0$$

So $a \neq -2$ necessarily to ensure convergence.

The second roots bounded condition becomes $|-a-a+2| \leq 2$ so $|1-a| \leq 1$, so $0 \leq a \leq 2$.

If $a=0$ or $a=2$, this root also lies on the unit circle, so need to check in both of these cases whether ρ' is zero or not to know whether we can include or must exclude $a=0$ and/or $a=2$.

$$\rho'\left(\frac{-a-\sqrt{a^2-4b}}{2}\right) = \rho'\left(\frac{2-2a}{2}\right) = \rho'(1-a)$$

$$= a+2-2a = 2-a \neq 0$$

So $a \neq 2$ necessarily. Thus the second condition becomes that $0 \leq a < 2$.

So the two conditions for the LMM to be zero stable are that $a \neq -2$ and $0 \leq a < 2$, which can be simplified to $0 \leq a < 2$.

So, for all $i \in \{0,1,2\}$, combining the criteria for consistency and zero stability, the LMM converges if and only if:

1. $0 \leq a < 2$
2. $b = -1-a$
3. $c = 2+a$.

ii) ~~As~~ ~~a~~ For consistency of order 1, we noticed that regardless of the choice of $i \in \{0,1,2\}$ we required

- $b = -1-a$
- $c = 2+a$.

So for each i we will need these two conditions plus the condition for consistency order 2 : $2 + \frac{1}{2}\alpha_1 - 2\beta_2 - \beta_1 = 0$.

$\underline{i=0}$: $y_{n+2} + a y_{n+1} + b y_n = hcf(y_n)$ so $\alpha_1 = a$ $\beta_1 = \beta_2 = 0$ $\beta_0 = c$.

So require $2 + \frac{1}{2}a - 0 - 0 = 2 + \frac{1}{2}a = 0$.

So $a = -4$.
It follows $b = -1 + 4 = 3$ and $c = 2 - 4 = -2$.

So for $i=0$, the LMM is consistent of order 2 if and only if $a = -4$ $b = 3$ and $c = -2$.

$\underline{i=1}$: $y_{n+2} + a y_{n+1} + b y_n = hcf(y_{n+1})$ so $\alpha_1 = a$ $\beta_0 = \beta_2 = 0$ $\beta_1 = c$.

So we require $2 + \frac{1}{2}a - c = 0$
so $c = 2 + \frac{1}{2}a$.
Since $c = 2 + a$ too, it follows $2 + \frac{1}{2}a = 2 + a$ i.e. $a = 0$.
So then $b = -1$ and $c = 2$.
Thus when $i=1$ the LMM is consistent of order 2 iff $a = 0$, $b = -1$ and $c = 2$.

$\underline{i=2}$: $y_{n+2} + a y_{n+1} + b y_n = hcf(y_{n+2})$ so $\alpha_1 = 0$ $\beta_0 = \beta_1 = 0$ $\beta_2 = c$.

So require $2 + \frac{1}{2}a - 2c = 0$
so $c = 1 + \frac{1}{4}a$.
As $c = 2 + a$ also, we need $2 + a = 1 + \frac{1}{4}a$
$\Leftrightarrow \frac{3}{4}a = -1 \Leftrightarrow a = -\frac{4}{3}$.

Then $b = -1 - a = \frac{1}{3}$ and $c = 2 - \frac{4}{3} = \frac{2}{3}$.
So for $i=2$ the LMM is consistent of order 2 iff $a = -\frac{4}{3}$, $b = \frac{1}{3}$ and $c = \frac{2}{3}$.

1.2) A) i) $x(t) = x_0(t) + x_1(t)\varepsilon + O(\varepsilon^2)$.

So $x^2(t) = x_0^2(t) + 2\varepsilon x_0(t)x_1(t) + O(\varepsilon^2)$.

$x'(t) = x_0'(t) + \varepsilon x_1'(t) + O(\varepsilon^2)$

and, $x''(t) = x_0''(t) + \varepsilon x_1''(t) + O(\varepsilon^2)$.

Subbing these into the ODE we get,

$$x_0''(t) + \varepsilon x_1''(t) + O(\varepsilon^2) + x_0(t) + \varepsilon x_1(t) + O(\varepsilon^2)$$
$$+ \varepsilon\left(x_0^2(t) + 2\varepsilon x_0(t)x_1(t) + O(\varepsilon^2) - 1\right)\left(x_0'(t) + \varepsilon x_1'(t) + O(\varepsilon^2)\right) = 0$$

So, $x_0''(t) + x_0(t) + \varepsilon(x_1''(t) + x_1(t)) +$
$\varepsilon\left(x_0'(t)(x_0^2(t) - 1) + O(\varepsilon)\right) + O(\varepsilon^2) = 0$

Then, $x_0''(t) + x_0(t) + \varepsilon\left(x_1''(t) + x_1(t) + x_0'(t)(x_0^2(t) - 1)\right)$
$+ O(\varepsilon^2) = 0$.

Equating the ε^0 and ε^1 parts to 0, we get the following system of ODEs:

- $x_0''(t) + x_0(t) = 0$
- $x_1''(t) + x_1(t) + x_0'(t)(x_0^2(t) - 1) = 0$.

As for the initial conditions, since $x(0) = x_0(0)$, and $x'(0) = 0$, again equating the ε^0 and ε^1 parts to their corresponding components we get:

$$x_0(0) = x(0) \qquad x_0'(0) = 0$$
$$x_1(0) = x_1'(0) = 0.$$

ii) First we solve $x_0''(t) + x_0(t) = 0$ $\quad x_0(0) = x(0) = a$ (call it a for simplicity) and $x_0'(0) = 0$.

As the ~~discriminant~~ roots of $m^2 + 1$ are $\pm i$, we expect $\omega = 1$, i.e.

$x_0(t) = A\cos(t) + B\sin(t)$ for some A, B to be determined.

$x_0(0) = A = a$.

$x_0'(t) = -A\sin(t) + B\cos(t)$. $\quad x_0'(0) = B = 0$.

So $x_0(t) = a\cos(t)$.

We then have $x_1''(t) + x_1(t) = -x_0'(t)\left(x_0^2(t) - 1\right)$

$= a\sin(t)\left(a^2\cos^2(t) - 1\right)$

$= a\sin(t)\left(a^2 - 1 - a^2\sin^2(t)\right)$

$= a^3\sin(t) - a\sin(t) - a^3\sin^3(t).$

$\sin^3(t) = \frac{3}{4}\sin(t) - \frac{1}{4}\sin(3t)$

So $x_1''(t) + x_1(t) = a^3\sin(t) - a\sin(t) - \frac{3}{4}a^3\sin(t) + \frac{1}{4}a^3\sin(3t)$

$= \frac{1}{4}a(a^2 - 4)\sin(t) + \frac{1}{4}a^3\sin(3t).$

We show now that we need the $\sin(t)$ term to disappear or else we end up with the trivial solution, or a non-periodic solution.

Let $Y_1(t)$ solve $x_1''(t) + x_1(t) = \frac{1}{4}a(a^2-4)\sin(t).$

The general solution then is

$\frac{1}{2}t\tilde{F}(t) + C_1\cos(t) + C_2\sin(t)$, where $\tilde{F}' = \frac{1}{4}a(a^2-4)\sin(t).$

$= -\frac{a^3}{24}t\cos(3t) - \frac{1}{8}t\left(4a(a^2-1) - 3a^2\right)\cos(t) + C_1\cos(t) + C_2\sin(t).$

$-\frac{a^3}{24}t\cos(3t)$ is not periodic, due to t constantly changing its amplitude, unless $a = 0$. If $a = 0$, $x_0(t) = 0$ and $x_1(t) = 0$ so we get the trivial solution (unsure if classed as periodic?).

So to find the non-trivial periodic solutions, we require that $a \neq 0$ and $\frac{1}{4}a(a^2-4)\sin(t) = 0$ (the trivial function).

This then implies $x(0) = a = \pm 2$ (so then $a^2 - 4 = 0$).

If this is the case, we get

$x_1''(t) + x_1(t) = \frac{1}{4}a^3\sin(3t)$, $\omega = 3.$

Thus we expect $x_1(t) = \frac{1}{1-9} \times \frac{1}{4}a^3\sin(3t) + C_1\cos(t) + C_2\sin(t)$

$= -\frac{1}{32}a^3\sin(3t) + C_1\cos(t) + C_2\sin(t).$

$x_1(0) = 0 = C_1$. $\quad x_1'(t) = -\frac{3}{32}a^3\cos(3t) + C_2\sin(t).$

$x_1'(0) = 0 = -\frac{3}{32}a^3 + C_2$. $\quad C_2 = \frac{3}{32}a^3$

So therefore $x_1(t) = \frac{3}{32}a^3\sin(t) - \frac{1}{32}a^3\sin(3t).$

So if $a = x(0) \in \{-2, 2\}$, we get the non-trivial periodic solutions:

$$x_0(t) = a\cos(t) \quad , \quad x_1(t) = \frac{1}{32}a^3(3\sin(t) - \sin(3t))$$

Otherwise, for any other a, the only periodic solution is the trivial solution, i.e.

$x_0(t) = x_1(t) = 0 \ \forall t$.

B) i) $\tau = t\omega$; $\quad x(t) = y(\tau) = y(\omega t)$.

So $x'(t) = \omega y'(\omega t) = \omega y'(\tau)$.

$x''(t) = \omega^2 y''(\omega t) = \omega^2 y''(\tau)$.

So subbing into the ODE we get

$$\omega^2 y''(\tau) + y(\tau) + \varepsilon(y^2(\tau) - 1)\omega y'(\tau) = 0.$$

$$y(0) = x(0) \quad y'(0) = x'(0) = 0.$$

ii) Now using $y(\tau) = y_0(\tau) + \varepsilon y_1(\tau) + O(\varepsilon^2)$

and $\omega = 1 + \varepsilon\omega_1 + O(\varepsilon^2)$, the ODE becomes

$$(1 + \varepsilon\omega_1 + O(\varepsilon^2))^2(y_0''(\tau) + \varepsilon y_1''(\tau) + O(\varepsilon^2)) + y_0(\tau) + \varepsilon y_1(\tau) + O(\varepsilon^2)$$

$$+ \varepsilon(y_0^2(\tau) + 2\varepsilon y_0(\tau)y_1(\tau) + O(\varepsilon^2) - 1)(1 + \varepsilon\omega_1 + O(\varepsilon^2))$$
$$(y_0'(\tau) + \varepsilon y_1'(\tau) + O(\varepsilon^2))$$

$$= (1 + 2\varepsilon\omega_1 + O(\varepsilon^2))(y_0''(\tau) + \varepsilon y_1''(\tau) + O(\varepsilon^2)) + y_0(\tau) + \varepsilon y_1(\tau) + O(\varepsilon^2)$$

$$+ \varepsilon((y_0^2(\tau) - 1)y_0'(\tau) + O(\varepsilon))$$

$$= y_0''(\tau) + \varepsilon y_1''(\tau) + 2\varepsilon\omega_1 y_0''(\tau) + y_0(\tau) + \varepsilon y_1(\tau)$$
$$+ \varepsilon y_0'(\tau)(y_0^2(\tau) - 1) + O(\varepsilon^2)$$

$$= y_0''(\tau) + y_0(\tau) + \varepsilon(y_1''(\tau) + y_1(\tau) + y_0'(\tau)(y_0^2(\tau) - 1)$$
$$+ 2\omega_1 y_0''(\tau)) + O(\varepsilon^2). = 0.$$

So equating ε components we get the following two ODEs:

$$y_0''(\tau) + y_0(\tau) = 0$$
$$y_1''(\tau) + y_1(\tau) = -y_0'(\tau)(y_0^2(\tau)-1) - 2\omega_1 y_0''(\tau).$$

with initial conditions: $y_0(0) = x_0(0) = a$ (we call it a for simplicity)
$y_0'(0) = 0$
$y_1(0) = y_1'(0) = 0.$

(ii) Just as in part A, we expect $y_0(t) = A\cos t + B\sin t$

Then, $y_0(0) = a = A.$
$y_0'(t) = -a\sin t + B\cos t$
$y_0'(0) = 0 = B.$
So $y_0(t) = a\cos(t).$

So $y_1''(\tau) + y_1(\tau) = a\sin(\tau)(a^2\cos^2(\tau)-1) + 2\omega_1 a\cos(\tau)$
$= a\sin(\tau)(a^2 - 1 - a^2\sin^2(\tau)) + 2\omega_1 a\cos(\tau)$
$= a^3\sin(\tau) - a\sin(\tau) - a^3\sin^3(\tau) + 2\omega_1 a\cos(\tau).$

$\sin^3(\tau) = \frac{3}{4}\sin(\tau) - \frac{1}{4}\sin(3\tau)$ so,

$$y_1''(\tau) + y_1(\tau) = \frac{1}{4}a^3\sin(\tau) - a\sin(\tau) + \frac{1}{4}a^3\sin(3\tau) + 2\omega_1 a\cos(\tau).$$

Let $Y_1(t)$ denote the solution to ~~$\frac{1}{4}a^3$ si~~
$$y_1''(\tau) + y_1(\tau) = \frac{1}{4}a(a^2-4)\sin(\tau) + 2\omega_1 a\cos(\tau)$$

and $Y_2(\tau)$ denote the solution to
$$y_1''(\tau) + y_1(\tau) = \frac{a^3}{4}\sin(3\tau).$$

Then the actual solution $y_1(\tau) = Y_1(\tau) + Y_2(\tau).$

Let $\tilde{F}(\tau) = -\frac{1}{4}a(a^2-4)\cos(\tau) + 2\omega_1 a\sin(\tau)$

Then, $\tilde{F}'(\tau) = \frac{1}{4}a(a^2-4)\sin(\tau) + 2\omega_1 a\cos(\tau)$.

So $Y_1(\tau) = -\frac{1}{8}a(a^2-4)\tau\cos(\tau) + \omega_1 a\tau\sin(\tau) + C_1\cos(\tau) + C_2\sin(\tau)$

$-\frac{1}{8}a(a^2-4)\tau\cos(\tau) + \omega_1 a\tau\sin(\tau)$ is not periodic unless we force it to be 0.

If $a=0$, then $y_0(\tau) = a\cos(\tau) = 0$ $\forall\tau$, and $y_1(\tau)=0$ too (can see why from the ODE) thus we end up with y being the trivial function.

So assuming $a\neq 0$, this forces $\omega_1 = 0$ so $\omega_1 a\tau\sin(\tau)$ vanishes.

To ensure the $-\frac{1}{8}a(a^2-4)\tau\cos(\tau)$ term vanishes $\forall\tau$, we need $a^2-4=0$ i.e. $a=\pm 2$.

Given this then, $Y_1(\tau) = C_1\cos(\tau) + C_2\sin(\tau)$.

$$Y_2(\tau) = \frac{1}{1-9}\left(\frac{1}{4}a^3\sin(3\tau)\right) + C_3\cos(\tau) + C_4\sin(\tau)$$

$$= -\frac{1}{32}a^3\sin(3\tau) + C_3\cos(\tau) + C_4\sin(\tau).$$

$$\begin{aligned}\text{So } y_1(\tau) &= Y_1(\tau) + Y_2(\tau)\\ &= -\frac{1}{32}a^3\sin(3\tau) + A\cos(\tau) + B\sin(\tau)\end{aligned}$$

$$(A = C_1 + C_3,\ B = C_2 + C_4).$$

$y_1(0) = A = 0$

$y_1'(\tau) = -\frac{3}{32}a^3\cos(3\tau) + B\cos(\tau)$

$y_1'(0) = 0 = -\frac{3}{32}a^3 + B$ $\quad B = \frac{3}{32}a^3$

$y_1(\tau) = \frac{1}{32}a^3(3\cos(\tau) - \cos(3\tau))$.

So if $a=\pm 2$*, we get the periodic solutions: $y_0(\tau) = a\cos(\tau)$ and $y_1(\tau) = \frac{1}{32}a^3(3\cos(\tau) - \cos(3\tau))$. For any a, the zero function is also a periodic solution.

*and $\omega_1 = 0$

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MA261 Modelling and Differential Equations Assignment Sheet 4

2.1)
The code for this question can be found in the file named “Q1.py” and is a modified version of the code given on Moodle.

We were unable to get the estimates for the period to within 1e-4 of the value given in the question’s preamble of 162.64.

The results we observed were

	Fixed	Built-in
Explicit	162.84125	162.85539
Implicit	162.65000	162.83026

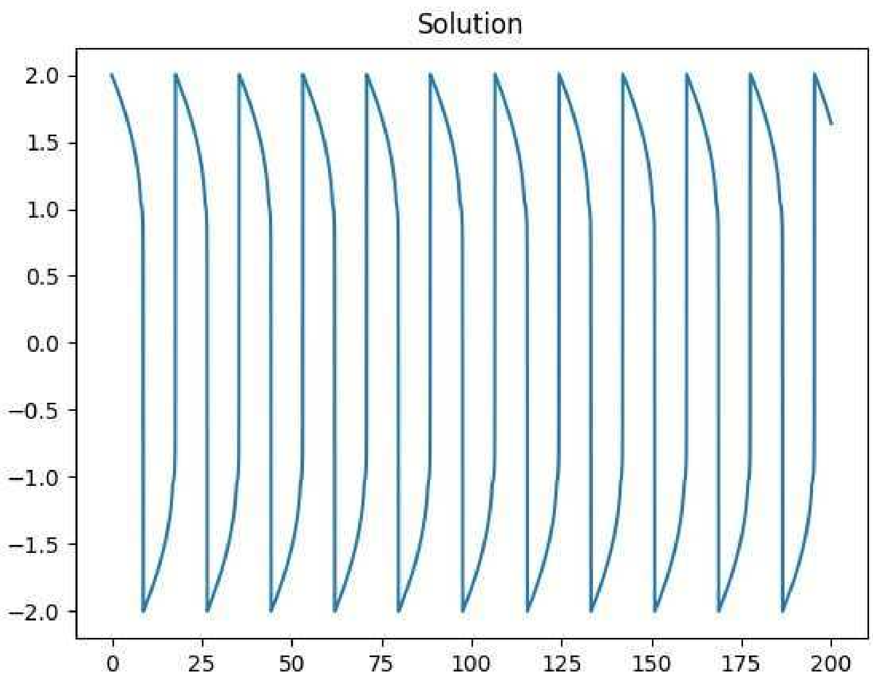
These were achieved with a value of “*N_0*” of 3200 and a tolerance of 1e-7 in both for the explicit methods. For the implicit methods we had a value of “*N_0”* of 320 and a tolerance of 1e-7.

In all cases, the graphs looked virtually identical, with no noticeable differences between them.

2.2)
The code for this question can be found in the file named “Q2.py” and is a modified version of the code given on Moodle. Note that there is some code duplication between “Q1.py” and “Q2.py” however, we felt that each question ought to have its own self-contained script.

For the explicit method, we estimated the period as 152.44236 when “*N_0”* was 3200. Although interestingly, we found that the period was 163.79753 when “*N_0*” was 400.

The code for the implicit method does not work from some reason and produces a “squashed” solution which is demonstrated in the picture below



2.3) (ii) $A \xrightarrow{k_1} X,\ B + X \xrightarrow{k_2} Y + D,\ 2X + Y \xrightarrow{k_3} 3X$

$X \xrightarrow{k_4} E$

A, B, D, E are constant

Let the reactant vector be

$y = (X, Y)^T$

From the notes, we see that the speed vector for such a system of reactions would be

$$w(y) = \begin{pmatrix} k_1 A \\ k_2 B X \\ k_3 X^2 Y \\ k_4 X \end{pmatrix}$$

~~The~~ From the notes, we see that the stoichiometry matrix for X and Y ~~would is~~ for such a system of reactions would be.

$$\Gamma = \begin{pmatrix} 1 & 0 \\ -1 & 1 \\ 1 & -1 \\ -1 & 0 \end{pmatrix} \quad \text{so } \Gamma^T = \begin{pmatrix} 1 & -1 & 1 & -1 \\ 0 & 1 & -1 & 0 \end{pmatrix}$$

So $\dot{y} = \Gamma^T w(y)$

$$\text{So } \begin{pmatrix} \dot{X} \\ \dot{Y} \end{pmatrix} = \begin{pmatrix} 1 & -1 & 1 & -1 \\ 0 & 1 & -1 & 0 \end{pmatrix} \begin{pmatrix} k_1 A \\ k_2 B X \\ k_3 X^2 Y \\ k_4 X \end{pmatrix}$$

So $\begin{pmatrix} \dot{X} \\ \dot{Y} \end{pmatrix} = \begin{pmatrix} k_1 A - k_2 BX + k_3 X^2 Y - k_4 X \\ k_2 BX - k_3 X^2 Y \end{pmatrix}$

(ii) $[\dot{X}] = \frac{mole}{l \cdot s}$

For the first ODE to be dimensionally homogeneous, we require

$[k_1 A] = \frac{mole}{l \cdot s}$

$LHS = [k_1] \cdot [A] = [k_1] \cdot \frac{mole}{l}$

So require $[k_1] = \frac{1}{s}$

We also require

$[k_2 BX] = \frac{mole}{l \cdot s}$

$LHS = [k_2] \cdot [B] \cdot [X]$

$= [k_2] \cdot \frac{mole^2}{l^2}$

So require $[k_2] = \frac{l}{mole \cdot s}$

We also require

$$[k_3 X^2 Y] = \frac{mole}{l \cdot s}$$

$$LHS = [k_3] \cdot \frac{mole^3}{l^3}$$

So require $[k_3] = \frac{l^2}{mole^2 \cdot s}$

Finally, we require

$$[k_4 X] = \frac{mole}{l \cdot s}$$

$$LHS = [k_4] \cdot [X]$$

$$= [k_4] \cdot \frac{mole}{l}$$

So require $[k_4] = \frac{1}{s}$

Now, just need to check that k_2 and B_3 satisfy dimensional homogeneity in the 2^{nd} equation

$$[k_2 B X] = [k_2][B][X]$$

$$= \frac{l}{mole \cdot s} \cdot \frac{mole^2}{l^2}$$

$$= \frac{mole}{l \cdot s}$$ exactly as required

Finally, need to check

$$[k_3 X^2 Y] = [k_3] \cdot [X]^2 \cdot [Y]$$

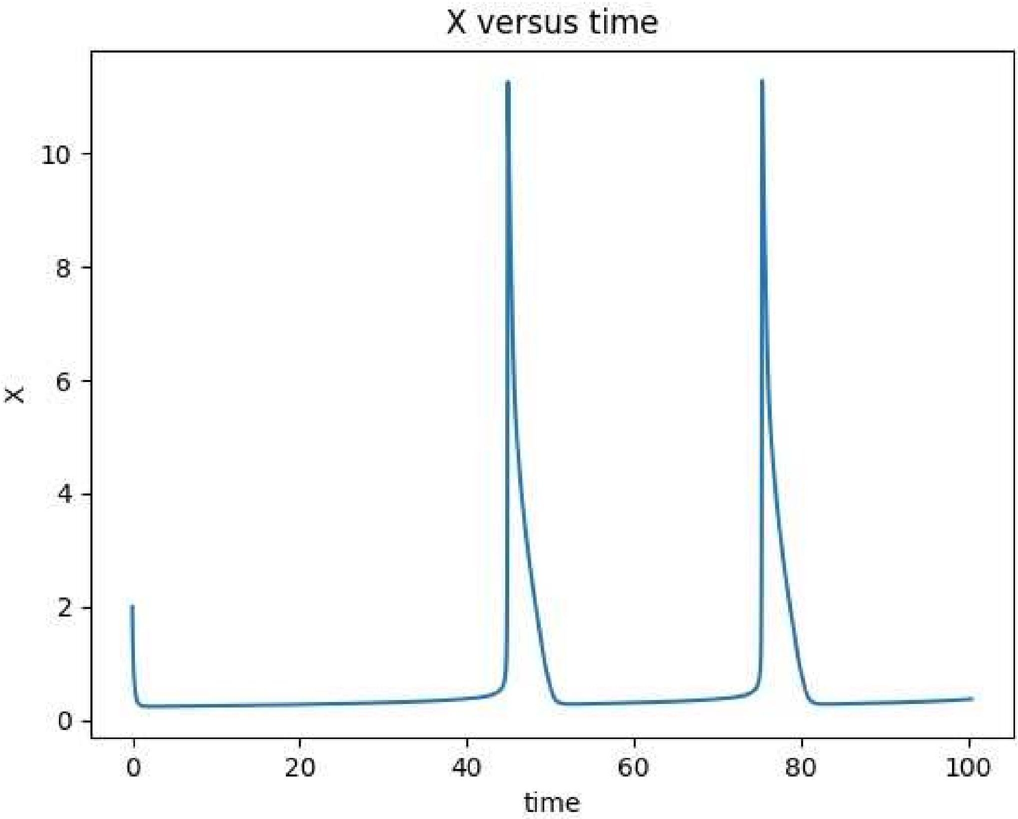
$$= \frac{l^2}{mole^2 \cdot s} * \frac{mole^2}{l^2} * \frac{mole}{l}$$

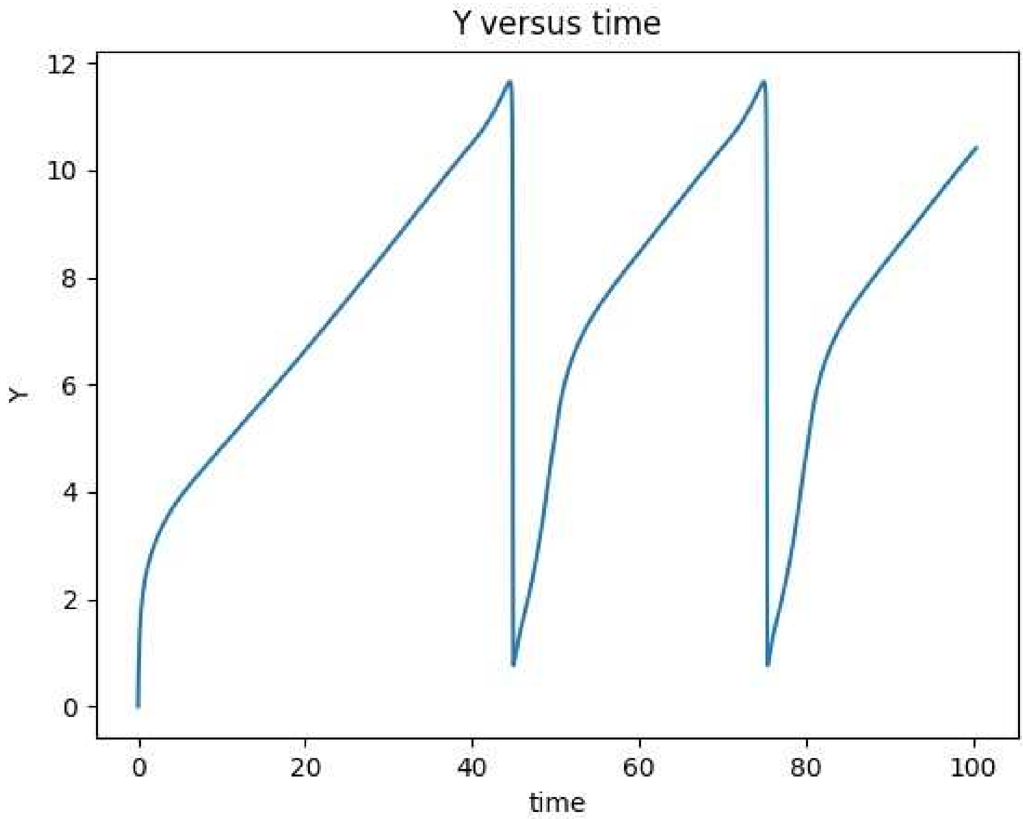
$$= \frac{mole}{l \cdot s}$$ exactly as required.

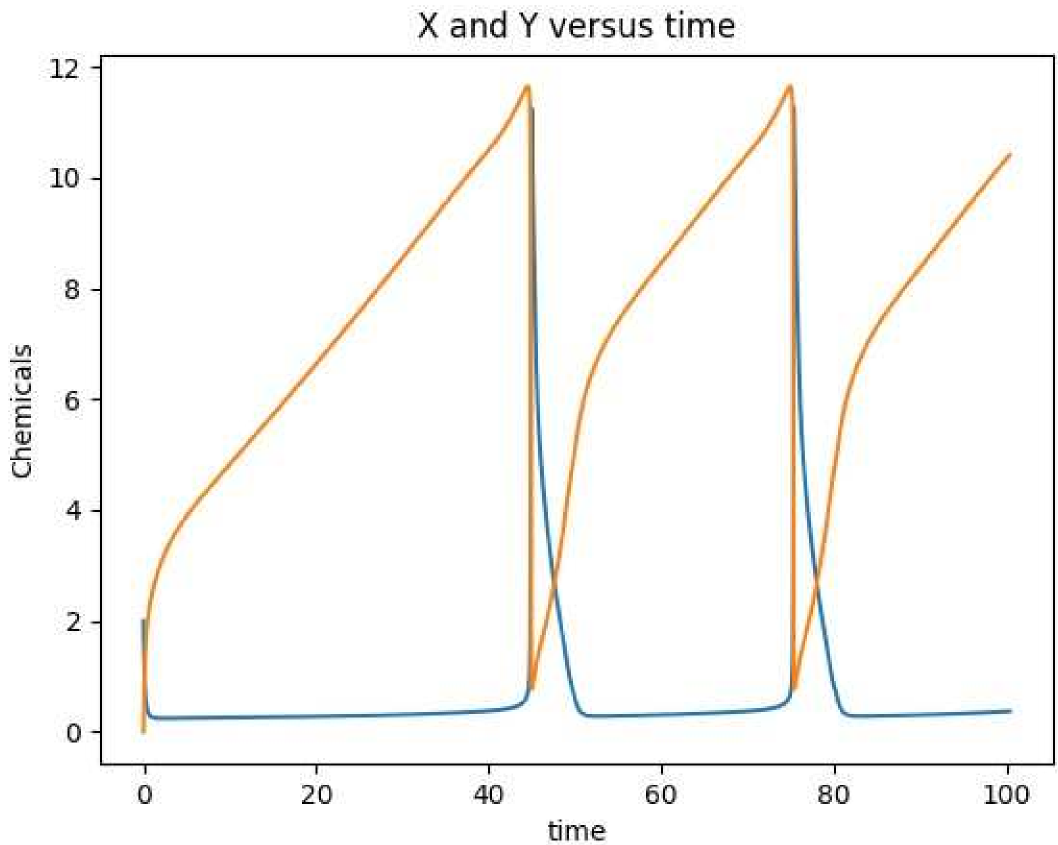
So with the units of k_1, k_2, k_3, k_4 specified earlier, the system of ODEs is indeed dimensionally homogeneous.

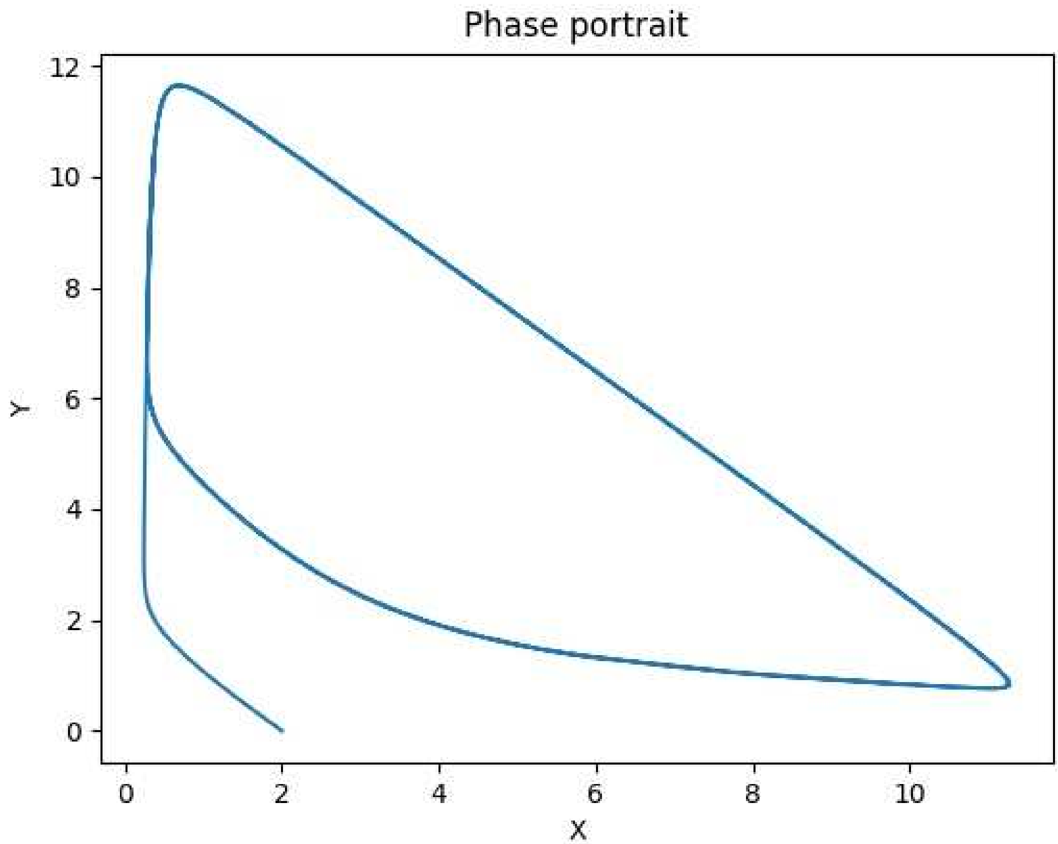
2.3)
The code for this question can be found in the file “Q3.py” and is a very slight modification of “Q2.py”. However, we felt that each question ought to have its own self-contained script and therefore decided to duplicate the code.

We decided to produce graphs showing the variation of the same quantities as as in the assignment. We produced following graphs:




Y versus time
Y
time
0
2
4
6
8
10
12
0
20
40
60
80
100


X and Y versus time
Chemicals
time
0
2
4
6
8
10
12
0
20
40
60
80
100


Phase portrait
Y
X
12
10
8
6
4
2
0
0
2
4
6
8
10