MM3110 Assignment 4

Ayesha Ulde
MM19B021

September 18, 2021

1 Problem 1

The given ODE

$$\frac{dy}{dt} = yt^3 - 1.5y$$

is a first-order variable-separable ODE. It can be solved analytically as follows:

$$\frac{dy}{dt} = y(t^3 - 1.5)$$

$$\int \frac{dy}{y} = \int (t^3 - 1.5)dt$$

$$ln\, y = \frac{t^4}{4} - 1.5t + ln\, C$$

$$y = C\, e^{0.25t^4 - 1.5t}$$

where C is a constant. Since $y(0) = 1$, $C = 1$.
Therefore, the analytical solution to the given ODE is

$$y = e^{0.25t^4 - 1.5t}$$

Solving the given ODE using the **fourth order Runge-Kutta method** with a step size of 0.05 in MATLAB gives the following solution :

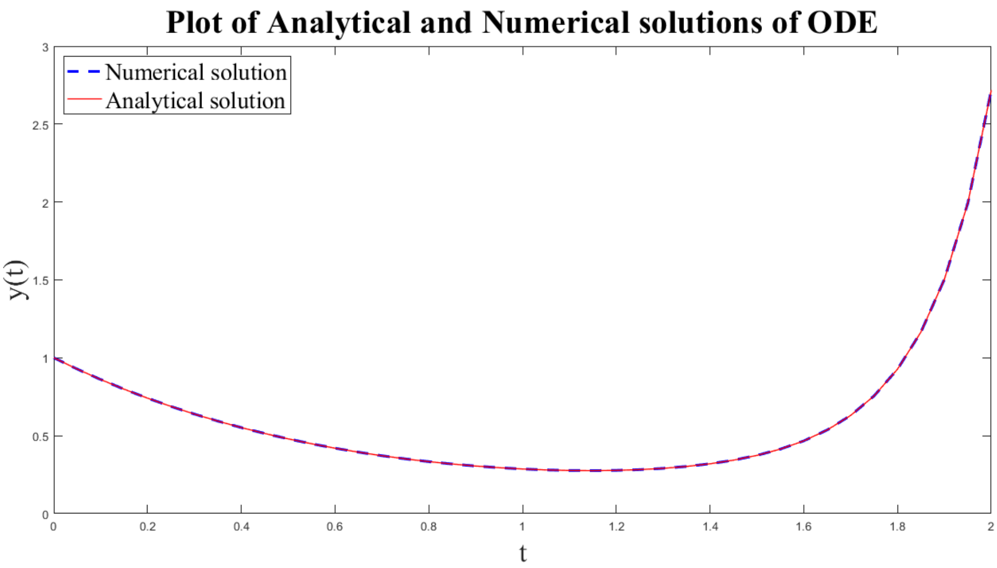

Figure 1: Plot of the analytical and numerical solutions of the ODE given in the problem.

The Runge-Kutta method gives almost 100% accuracy in this case.

2 Problem 2

To solve the given second-order ODE by the **shooting method**, it is converted into two first-order ODEs

$$\frac{dx}{dt} = v$$

$$\frac{dv}{dt} + \frac{c}{m}v - g = 0$$

Then, choosing the step size as 0.25, the above first-order ODEs can be solved using Runge-Kutta method. $x(0)$ is given but $v(0)$ is not, so we give an initial guess for $v(0)$ and refine our guess based to the difference between the output value $v(12)$ and the boundary condition $v(12) = 500\ ms^{-1}$.
Some of the initial guesses for $v(12)$ and the respective output values obtained are given in the table below:

Initial guess for $v(0)$ (in ms^{-1})	**$x(12)$ value obtained (in m)**
100	176.3
200	268.3
300	359.9
400	451.4
450	497.2
453	$499.984 \approx 500$
455	501.8
460	506.4

Since the output value corresponding to $v(0) = 453$ is approximately equal to the boundary condition, we can assume $v(0) = 453\ ms^{-1}$ to find the position and velocity as a function of time. The solutions obtained are plotted below:

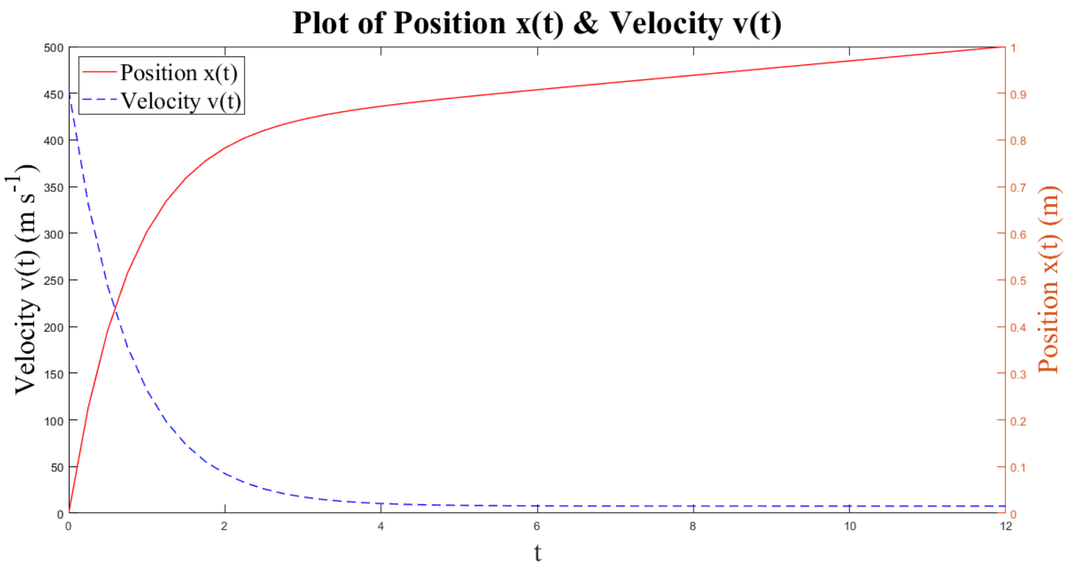

Figure 2: Plot of the position and velocity as a function of time.

3 Problem 3

To find the concentrations from times 0 to 3 s, we set

$$f_a(c_a, c_b, c_c) = 10c_ac_c + c_b$$

$$f_b(c_a, c_b, c_c) = 10c_ac_c - c_b$$

$$f_c(c_a, c_b, c_c) = -10c_ac_c + c_b - 2c_c$$

Setting $h = 0.05\dot{s}$, we can solve the given three first-order ODEs simultaneously using **Euler's method** as follows:

$$c_a^{i+1} = c_a^i + hf_a(c_a^i, c_b^i, c_c^i)$$
$$c_b^{i+1} = c_b^i + hf_b(c_a^i, c_b^i, c_c^i)$$
$$c_c^{i+1} = c_c^i + hf_c(c_a^i, c_b^i, c_c^i)$$

Using the initial condition $c_a^0 = 50$, $cb^0 = 0$ & $c_c^0 = 40$, and iterating in steps of 0.05s from 0 to 3 s, we get the following concentrations of three reactants:

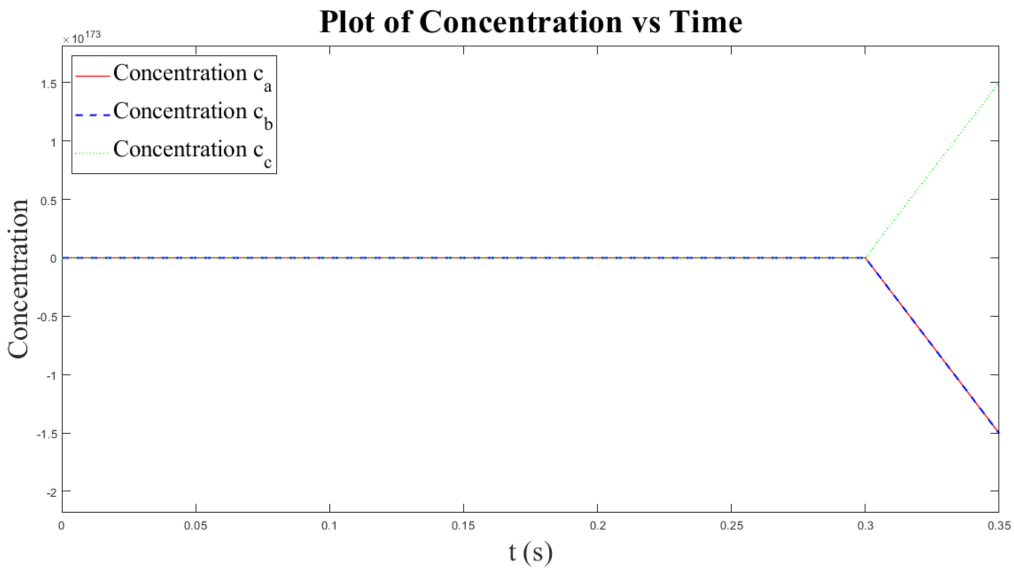

Figure 3: Plot of concentration of reactants a, b & c from times 0 to 3 s.

It can observed that after time exceeds 0.35 s,

$$c_a \to -\infty$$

$$c_b \to -\infty$$

$$c_c \to \infty$$

4 Problem 4

For a particle in an infinite square well, the potential energy is infinitely large outside the region $0 < x < L$, and zero within that region. Hence, the particle is confined within the box. The **1D time-independent Schrodinger wave equation** for the particle within the box is given by

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{1}$$

Since V(x) is zero inside the box,

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{2}$$

Setting

$$k^2 = \frac{2mE}{\hbar^2}$$

Equation (2) can be rewritten as

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \tag{3}$$

The analytical solutions for equation (3) under the boundary conditions that at $x = 0$ and $x = L$, $\psi(x) = 0$ give

$$k = \frac{n\pi}{L},\ n = 1, 2, 3, ...$$

Therefore,

$$E \equiv E_n = n^2 \frac{\hbar^2 \pi^2}{2mL^2},\ n = 1, 2, 3, ...$$

Ground state energy is given by setting $n = 1$:

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$

For a 0.5 nm wide well,

$$E_1 = 2.4123 \times 10^{-19}\ J$$

To solve equation (3) numerically, the **Finite difference method** can be used. Substituting a central finite-divided difference approximation for the second derivative

$$\frac{\psi_{i+1} - \psi_i + \psi_{i-1}}{h^2} + k^2 \psi_i = 0$$

where h is length of the segment. The above equation can also be expressed as

$$\psi_{i-1} - (2 - h^2 k^2)\psi_i + \psi_{i+1} = 0 \tag{4}$$

Dividing the width of the well into 5 segments, h = 0.1 nm and $\psi_0 = 0$ & $\psi_5 = 0$. Solving i = 1, 2, 3 & 4 in equation (4), we get a set of equations which can be solved by the matrix representation method, which can be done in MATLAB by using the *equationsToMatrix* function in the Symbolic Math Toolbox. Of the solutions obtained, the smallest value will give us the ground state solution, which is $2.33 \times 10^{-19}\ J$. The numerical solution $2.33 \times 10^{-19}\ J$ is, therefore, quite close to the analytical solution $2.4123 \times 10^{-19}\ J$. Hence, it is possible to solve such a system using a numerical approach as well.