Problem 3

Compound A diffuses through a 4-cm long tube and reacts as it diffuses. The equation governing diffusion with reaction is

$$D\,\frac{d^2A}{dx^2} - kA = 0.$$

At one end of the tube, there is a large source of A at a concentration of 0.1 M. At the other end of the tube there is an adsorbent material that quickly absorbs any A, making the concentration 0 M. If D = 1.5 × 10−6cm2/s, k = 5 × 10-6s−1, compute the concentration of A as a function of distance in the tube. Solve using the shooting method or finite difference method.

Description of Problem:

The problem described involves the diffusion of a chemical species, denoted as "A," through a 4-centimeter-long tube. The diffusion of A is accompanied by a chemical reaction, and this diffusion-reaction process is governed by the following differential equation:

$$D\,\frac{d^2A}{dx^2} - kA = 0.$$

Where:

- D is the diffusion coefficient of A, equal to $1.5 \times 10^{-6} cm^2/s$.
- k is the rate constant for the chemical reaction, equal to $5 \times 10^{-6} s^{-1}$.
- x is the distance along the tube (measured in centimeters).
- A(x) represents the concentration of A at position x.

The boundary conditions for this problem are as follows:

1. At one end of the tube (x = 0), there is a large source of A, and the initial concentration is 0.1 M (Molar).
2. At the other end of the tube (x = 4 cm), there is an adsorbent material that quickly absorbs any A, effectively making the concentration of A at that end 0 M (completely absorbed).

Procedure:

We will solve the problem using finite difference method, which is used to solve bounded value problems(BVP's) where we will have some boundary conditions. The boundary conditions in this problem are A(0)=0.1M and A(4)=0M.

To solve this problem by numeric methods, we will need to divide the interval [0,4] in N equal parts.

Hence the step size will be $h = \frac{(0+4)}{N} = \frac{4}{N}$.

Then we will use the formula of finite difference to approximate the ODE

$$\boxed{\frac{d^2y}{dx^2} = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}}$$

The solution of the above form will form a tri-diagonal system, which can be easily solved using TDMA to get values of y at different values of x.

Now, according to the given problem

$$D\,\frac{d^2A}{dx^2} - kA = 0.$$

with x ranging from [0,4].

Let the step size be equal to h=0.01

The boundary conditions provided are as follows A(0) = 0.1 and A(4) = 0. Also the values of the constants, $D = 1.5 \times 10^{-6}\, cm^2 s^{-1}$ and $k = 5 \times 10^{-6} s^{-1}$.

$$\frac{d^2A}{dx^2} = \frac{A_{i+1} - 2A_i + A_{i-1}}{h^2}$$

Substituting this in the main equation we get

$$\Rightarrow D\left(\frac{A_{i+1}-2A_i+A_{i-1}}{h^2}\right) - kA_i = 0$$

$$\Rightarrow DA_{i-1} - (2D + kh^2)A_i + DA_{i+1} = 0$$

For i=0 $\quad A_0 = 0.1$

For i=1 $\quad 0.1D - (2D + kh^2)A_1 + DA_2 = 0.$

For i=2 to n-2 $\quad DA_{i-1} - (2D + kh^2)A_i + DA_{i+1} = 0$

For i=n-1 $\quad DA_{n-2} - (2D + kh^2)A_{n-1} + DA_n = 0$

For i=n $\quad A_n = 0$

Now, these equations will form Tri-diagonal-system which can be easily solved using TDMA

Output Plot: