CHE401 Exam 2 solution

Question 1

(a)
SUBROUTINE MATRIX(A,B,N,X)
REAL, A(N,N),B(N),X(N),
INTEGER, N
X(1)=B(1)/A(1,1)
DO I=2,N
    SUM=0.0
    DO J=2,N
        SUM=SUM+A(I,J)*X(J)
    ENDDO
    X(I)=B(I)-SUM/A(I,I)
ENDDO
RETURN

(B)

$$\frac{L^i}{L^0} = 1 \times 10^{-1} = 2^{-k}$$

$$Ln(1 \times 10^{-3}) = Ln(2^{-k})$$

$$-6.9 = -kLn(2)$$

$$\frac{-6.9}{0.69} = -k$$

K = 100
Question 2

\[
\frac{dC_A}{dt} = f = F(C_{A_i} - C_A) - \frac{0.05C_A}{0.1 + C_A}
\]

\[x_{i+1/2} = x_i + hf(t_i, x_i)\]

\[\bar{x}_{i+1/2} = f(t_i + \frac{h}{2}, x_{i+1/2})\]

\[x_{i+1} = x_i + h\bar{x}_{i+1/2}\]

Since the independent variable \( t \) does not appear explicitly in the ODE, the algorithm reduces to:

\[x_{i+1/2} = x_i + hf(t_i, x_i)\]

\[x_{i+1} = x_i + hf(x_{i+1/2})\]

Applying the algorithm for the given parameter values gives:

<table>
<thead>
<tr>
<th>( i )</th>
<th>( T )</th>
<th>( C_A )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0.9550</td>
<td>0.0042</td>
</tr>
<tr>
<td>1</td>
<td>0.5000</td>
<td>0.9581</td>
<td>0.0008</td>
</tr>
<tr>
<td>2</td>
<td>1.0000</td>
<td>0.9587</td>
<td>0.00</td>
</tr>
</tbody>
</table>
**Question 3**

(a) BVP because the dependent variable \( x \) is defined on both sides.

(b) Let: \( y_1 = \frac{dx}{dz} \)

then

\[
\begin{align*}
y_2 &= y_1' = y' \\
y_2' &= y''_1 = y''
\end{align*}
\]

Substituting in the original ODE gives:

\[
\frac{dy_1}{dx} = y_2, \quad y_1(0) = y(0) = 3
\]

\[
\frac{dy_2}{dx} = -3y_2 + 10y_1, \quad y_2(0) = y'(0) = z
\]

(c) Applying the finite difference on the original ODE gives:

\[
\frac{x^{i+2} - 2x^{i+1} + x^i}{h^2} + 3\frac{x^{i+1} - x^i}{h} - 10x^i = 0
\]

Multiplying by \( h^2 \) and rearranging gives:

\[
\frac{x^{i+2} - 2x^{i+1} + x^i}{h^2} + 3\frac{x^{i+1} - x^i}{h} - 10x^i = 0
\]

\[
x^{i+2} + (3h - 2)x^{i+1} + (1 - 3h - 10h^2)x^i = 0
\]

Let \( h = 2 \)

\[
x^{i+2} + 4x^{i+1} - 45x^i = 0
\]

\[
i = 0 \quad z = 0 \quad x^2 + 4x^1 - 45x^0 = 0
\]

\[
i = 1 \quad z = 2 \quad x^3 + 4x^2 - 45x^1 = 0
\]

Knowing \( x^0 = 3 \) and \( x^3 = 1 \) the last two equations can be solved simultaneously yield:

\[
x(z=2) = 88.6 \quad \text{and} \quad x(z=4) = 99.5
\]