CHE401 Exam 2 solution

Question 1

(a)

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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
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(B)

$$\frac{L^k}{L^0} = 1\times10^{-3} = 2^{-k}$$

$$Ln(1\times10^{-3}) = Ln(2^{-k})$$

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

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

K = 100

<u>Question 2</u>

$$\frac{dC_A}{dt} \equiv f = F(C_{Af} - C_A) - \frac{0.05C_A}{0.1 + C_A}$$

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

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:

i	T	C_A	$f(x)$
0	0	0.9550	0.0042
1	0.5000	0.9581	0.0008
2	1.0000	0.9587	0.00

Question 3

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

Let: $y_1 = dx/dz$
then

$y_2 = y'_1 = y'$
$y'_2 = y''_1 = y''$

Substituting in the original ODE gives:

$$\frac{dy_1}{dx} = y_2 \qquad y_1(0) = y(0) = 3$$
$$\frac{dy_2}{dx} = -3y_2 + 10y_1 \qquad y_2(0) = y'(0) = z$$

(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 z=0 $$x^2 + 4x^1 - 45x^0 = 0$$

i=1 z=2 $$x^3 + 4x^2 - 45x^1 = 0$$

knowing x^0 = 3 and x^3 = 1the last tow equations can be solved simultaneously yield:

$x(z=2) = 88.6$ and $x(z=4) = 99.5$