Advanced Numerical Analysis for Chemical Engineering
Quiz-2 (1 hrs.)

1. It is desired to apply the method of finite difference to solve the following PDE

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial z^2}$$

$$\begin{aligned} \text{Boundary Conditions} &: \quad C(0,t) = C(1,t) = 0 \\ \text{Initial Condition} &: \quad C(z,0) = \exp(-0.1z) \end{aligned}$$

where t and z represent dimensionless time and dimensionless length, respectively. Discretize the PDE in the spatial coordinate using the finite difference method and by assuming 3 internal equidistant grid points. Express the resulting system of equations in the following standard form

$$d\mathbf{x}/dt = A\mathbf{x} \text{ with initial condition } \mathbf{x}(0)$$

where

$$\mathbf{x} = \begin{bmatrix} C_1 & C_2 & ... & C_5 \end{bmatrix}^T$$

Note: In your answer, clearly define A matrix and state all elements of the initial condition, $\mathbf{x}(0)$.

2. Consider the PDE given in Q. 1 with the following modified boundary conditions

$$\text{Boundary Conditions}: \frac{dC(0,t)}{dz} = \frac{dC(1,t)}{dz} = 0$$

Descritize (in space) the modified PDE using the method of orthogonal collocations and by assuming two internal collocation points *at* $z_1 = 0.21$ *and* $z_2 = 0.79$. Express the resulting system of DAEs in the following standard form

$$\begin{aligned} d\mathbf{y}/dt &= \mathbf{By} \\ \mathbf{Dy} &= \bar{\mathbf{0}} \\ \mathbf{y}(0) &: \text{Initial Condition} \end{aligned}$$

where

$$\mathbf{y} = \begin{bmatrix} C_1 & C_2 & ... & C_4 \end{bmatrix}^T$$

Note: (a) In your answer, clearly define matrices $\mathbf{B}, \mathbf{D}$ and state all elements of the initial condition, $\mathbf{y}(0)$.(b) The $\mathbf{S}$ and $\mathbf{T}$ matrices corresponding to the given collocation points are as follows

$$\mathbf{S} = \begin{bmatrix} -7 & 8.2 & -2.2 & 1 \\ -2.7 & 1.7 & 1.7 & -0.7 \\ 0.7 & -1.7 & -1.7 & 2.7 \\ -1 & 2.2 & -8.2 & 7 \end{bmatrix}; \quad \mathbf{T} = \begin{bmatrix} 24 & -37.2 & 25.2 & -12 \\ 16.4 & -24 & 12 & -4.4 \\ -4.4 & 12 & -24 & 16.4 \\ -12 & 25.2 & -37.2 & 24 \end{bmatrix}$$