CLL:113-Tut-4(4.10.20)

Multivariate Non-linear Algebraic Equations:

Q1. The mass balance equations for the following reactions taking place in a CSTR:

$$A \xrightarrow{k_1} 2B$$

$$A \xrightarrow{k_2} C$$

$$k_3$$

$$B \stackrel{k_4}{\rightarrow} D + C$$

is given by:

$$F_{1} = -C_{A} + C_{A0} + \left[-K_{1}C_{A} - K_{2}C_{A}^{\frac{3}{2}} + K_{3}C_{C}^{2} \right] \theta = 0$$

$$F_{2} = -C_{B} + \left[2K_{1}C_{A} - K_{4}C_{B}^{2} \right] \theta = 0$$

$$F_{3} = -C_{C} + \left[K_{2}C_{A}^{\frac{3}{2}} - K_{3}C_{C}^{2} + K_{4}C_{B}^{2} \right] \theta = 0$$

$$F_{4} = -C_{D} + \left[K_{4}C_{B}^{2} \right] \theta = 0$$

Use Newton Raphson Method and find the concentrations $\begin{bmatrix} C_A \ C_B \ C_C \ C_D \end{bmatrix}$ for the following situation as a function of iteration

$$K_1 = 1.0 \frac{1}{s}$$

$$K_2 = 0.2 \frac{\text{lit}^{\frac{1}{2}}}{\text{s} - \text{mol}^{\frac{1}{2}}} \quad K_3 = 0.05 \frac{\text{lit}}{\text{s} - \text{mol}}$$

$$K_4 = 0.4 \frac{\text{lit}}{\text{s - mol}} \theta = 2s C_{A0} = 1 \text{ mol/lit}$$