CLL:113-Tut-5(31.8.19)

Multivariate Non-linear Algebraic Equations:

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

$$A \overset{k_1}{\rightarrow} 2B$$

$$A \underset{k_3}{\overset{k_2}{\leftrightarrow}} C$$

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

is given by:

$$F_1 = -C_A + C_{A0} + \left[-K_1 C_A - K_2 C_A^{\frac{3}{2}} + K_3 C_C^2\right]\theta = 0$$

$$F_2 = -C_B + [2K_1 C_A - K_4 C_B^2]\theta = 0$$

$$F_3 = -C_C + \left[K_2 C_A^{\frac{3}{2}} - K_3 C_C^2 + K_4 C_B^2\right]\theta = 0$$

$$F_4 = -C_D + [K_4 C_B^2]\theta = 0$$

Use: 1. The Fixed Point Iteration

2. Newton Raphson Method

And find the concentrations $[C_A\ C_B\ C_C\ C_D]$ for the following situation as a function of iteration

$$K_1 = 1.0\,\frac{1}{\text{s}} \quad K_2 = 0.2\,\frac{\text{lit}^{\frac{1}{2}}}{\text{s}-\text{mol}^{\frac{1}{2}}} \quad K_3 = 0.05\,\frac{\text{lit}}{\text{s}-\text{mol}}$$

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