Advanced Numerical Analysis for Chemical Engineering
Programming Quiz B (2 hrs 30 minutes)

Integration Method: Runge-Kutta 4'th Order

Given ODE-IVP

$$\begin{aligned}\frac{d\mathbf{x}}{dt} &= \mathbf{F}(\mathbf{x},t)\\ \mathbf{x}(0) &= \mathbf{x}_0\end{aligned}$$

where $\mathbf{x} \in R^n$ and $F(\mathbf{x},t)$ is a $n \times 1$ function vector.

Runge-Kutta 4'th order method

$$\mathbf{x}(n+1) = \mathbf{x}(n) + \frac{h}{6}\left(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4\right)$$

$$\begin{aligned}\mathbf{k}_1 &= \mathbf{F}\left(t_n, \mathbf{x}(n)\right) = \mathbf{F}(n)\\ \mathbf{k}_2 &= \mathbf{F}\left(t_n + \frac{h}{2}, \mathbf{x}(n) + \frac{h}{2}\mathbf{k}_1\right)\\ \mathbf{k}_3 &= \mathbf{F}\left(t_n + \frac{h}{2}, \mathbf{x}(n) + \frac{h}{2}\mathbf{k}_2\right)\\ \mathbf{k}_4 &= \mathbf{F}\left(t_n + h, \mathbf{x}(n) + h\mathbf{k}_3\right)\end{aligned}$$

Note that $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$ and $\mathbf{k}_4$ are $n \times 1$ function vectors.

Problem: Continuous Fermenter

Consider a continuously operated fermenter described by the following set of ODEs

$$\begin{aligned}\frac{dX}{dt} &= -DX + \mu(S,P)X\\ \frac{dS}{dt} &= D(23.4 - S) - \frac{1}{Y_{X/S}}\mu(S,P)X\\ \frac{dP}{dt} &= -DP + (\alpha\mu(S,P) + \beta)X\end{aligned}$$

where X represents effluent cell-mass or biomass concentration, S represents substrate concentration and P denotes product concentration. The model parameters are given as

$$\begin{aligned}\mu(S,P) &= \frac{0.48(1 - \frac{P}{50})S}{1.2 + S + \frac{S^2}{22}}\\ Y_{X/S} &= 0.4\ ;\ \ \alpha = 2.2\ ;\ \ \beta = 0.2\ ;\ \ D = 0.1736\end{aligned}$$

Integrate the above system of equations starting from initial state

$$\mathbf{x}(\mathbf{0}) = \begin{bmatrix} X(0) & S(0) & P(0)\end{bmatrix}^T = \begin{bmatrix} 7.30 & 5.14 & 25\end{bmatrix}^T$$

from $t = 0$ to $t = 30$ with integration step size $h = 0.5$. Plot $X(t)$ v/s time, $S(t)$ v/s time and $P(t)$ v/s time in three separate figures.