IIT ROPAR
SEMESTER I 2021-22
NUMERICAL SIMULATION LAB (CH230)
Assignment 5 Max Marks: 40

Note: Marks will be awarded for well written codes. Ensure that the files submitted are complete in all respects and only needed to be executed to get the required answers.

1. The concentration of a tracer at the outlet of a reactor is given below.

t, hr	0	1	5.5	10	12	14	16	18	20	24
c, mg/L	1	1.5	2.3	2.1	4	5	5.5	5	3	1.2

The flow rate (m^3/s) for the outlet can be given as follows.

$$Q(t) = 20 + 10\sin\left(\frac{2\pi}{24}(t - 10)\right)$$

Determine the flow weighted average concentration of the tracer leaving the reactor over a 24 hour period.

$$\bar{c} = \frac{\int_0^t Q(t)c(t)dt}{\int_0^t Q(t)dt}$$

(10M)

2. An investigator theorised that the relationship between vision loss (VL) and intraocular pressure P (pressure inside the eye) can be described as

$$VL = A \exp\left(k \int_{25}^{t} (P - 13)\, dt\right)$$

Where VL is the percent vision loss and P is the intraocular pressure (mm Hg), t is the time in years and k and A are constants. Use the data below to determine the constants k and A. (15M)

Patient	**A**		**B**		**C**	
Age at diagnosis	65		43		80	
VL	60		40		30	
	Age, years	***P*, mm Hg**	**Age, years**	***P*, mm Hg**	**Age, years**	***P*, mm Hg**
	25	13	25	11	25	13
	40	15	40	30	40	14
	50	22	41	32	50	15
	60	23	42	33	60	17
	65	24	43	35	80	19

3. The kinetic theory for adsorption of polymers under shear flow near a plane wall leads to the following expression for the steady state concentration C(z) in the wall- normal direction (z axis)

$$C(z) = \exp\left[-\int_z^\infty \frac{L_d}{q^2}\,\mathrm{d}q + 2\varepsilon_s \left\{ \left(\frac{\sigma_s}{z}\right)^6 - \left(\frac{\sigma_s}{z}\right)^{12} \right\} \right]$$

where L_d is a characteristic length scale of polymer migration under shear flow, ε_s is the strength of polymer–wall attraction, and σ_s is a constant. L_d is some function of z, but it is only known numerically. In the far-field limit, you can use treat L_d as a constant, say

L. Then the integral inside the square brackets can be calculated analytically, and you obtain the much simpler expression

$$C(z) = \exp\left[-\frac{L}{z} + 2\varepsilon_s \left\{ \left(\frac{\sigma_s}{z}\right)^6 - \left(\frac{\sigma_s}{z}\right)^{12} \right\} \right]$$

We want to calculate the amount of adsorbed Γ using the relation

$$\Gamma = \int_{z_i}^{z_c} \Big[C(z) - 1 \Big]\,\mathrm{d}z,$$

where z_i is the distance from the wall set by the polymer size and z_c is some distance from the wall.

Determine the value of the above integral with ε_s =4, σ_s = 2; L =0.5, z_i =0.5 and z_c =10 using the multiple application trapezoidal rule. Plot the value of the integral with the number of segments n =1,2 ..60. Explain the nature of the plot observed. What would be the value of the integrand if the quad command is used? (15M)