e) How would you formulate a suitable optimization problem, and how can you classify it (present a proper mathematical formulation of the optimization problem as discussed in the lecture and specify the dimensions of your functions and variables)?

Objective function : $\max_{x \in [0, 50]} C_b(x)$

Constraints :

→ ODEs

$$\frac{dc_A}{dx} = \frac{A_o}{q}\left[-k_{10}exp\left(\frac{-E_{A_1}}{RT}\right)c_A^{n_1}\right],$$
$$\frac{dc_B}{dx} = \frac{A_o}{q}\left[+k_{10}exp\left(\frac{-E_{A_1}}{RT}\right)c_A^{n_1} - k_{20}exp\left(\frac{-E_{A_2}}{RT}\right)c_B^{n_2} - k_{30}exp\left(\frac{-E_{A_3}}{RT}\right)c_B^{n_3}\right],$$
$$\frac{dc_C}{dx} = \frac{A_o}{q}\left[k_{20}exp\left(\frac{-E_{A_2}}{RT}\right)c_B^{n_2}\right],$$
$$\frac{dc_D}{dx} = \frac{A_o}{q}\left[k_{30}exp\left(\frac{-E_{A_3}}{RT}\right)c_B^{n_3}\right].$$

→ Constants

$c_{A,In} = 12\ \mathrm{mol/m^3}$	$c_{B,In} = c_{C,In} = c_{D,In} = 0\ \mathrm{mol/m^3}$
$k_{10} = 5.4 \cdot 10^{10}\ \mathrm{s^{-1}}$	$E_{A,1} = 7.5 \cdot 10^4\ \mathrm{J/mol}$
$k_{20} = 4.6 \cdot 10^{17}\ \mathrm{s^{-1}}$	$E_{A,2} = 1.2 \cdot 10^5\ \mathrm{J/mol}$
$k_{30} = 5.0 \cdot 10^{7}\ \mathrm{s^{-1}}$	$E_{A,3} = 5.5 \cdot 10^4\ \mathrm{J/mol}$
$n_1 = 1.1$	$n_2 = n_3 = 1$
$R = 8.3145\ \mathrm{J/mol/K}$	$T = 340\ \mathrm{K}$
$A_o = 0.1\ m^2$	$q = 0.12\ \mathrm{m^3/s}$

Classification:

→ Dynamic: Variables change with x.

→ Constrained: ODEs and the axial length of the reactor are constrains.

→ Nonlinear: The solution of the ODE system presents exponential behavior.

→ Continuous: All variables are continuous with regard to x.

→ Global: We want to find the global maximum value for C_b.