In the reactor the conditions of operations are going to be considered as the following:

$$T = 298.15 \ K$$
$$P = 1 \ atm$$

Joback Method

Boiling temperature estimation

$$T_b = 198 + \sum_k N_k \left(tbk\right)$$

In which N_k is the number of times the contribution appears in thecompound, and tbk is taken form Table 1.

$$T_b = 575.54 \text{ K}$$

Critic temperature estimation

$$T_c = T_b \left[0.584 + 0.965 \left\{ \sum_k N_k \left(tck\right) \right\} - \left\{ \sum_k N_k \left(tck\right) \right\}^2 \right]^{-1}$$

In which N_k is the number of times the contribution appears in the compound, and tck is taken form Table 1.

$$T_c = 785.90 \ K$$

Additional physical consideration

Assuming the virus boiling temperature as thedenaturation temperature of the virus (45°C), we obtain a correction factor. Such consideration results in:

$$T_b = 318.15 \ K$$
$$T_c = 434.43 \ K$$

Sastri Method

Now, we proceed to estimate the thermal conductivity, using the Sastri method.

$$\lambda_L = \lambda_b a^m$$

$$\lambda_b = \sum_k N_k \left(\Delta \lambda_b\right)$$

For alcohols and phenols, a=0.856 and n=1.23. For other compounds, a=0.16and n=0.2. The thermal conductivity at the normal boiling point, b , is determinedwith the group contribution values and corrections in Table 2.

$$\lambda_b = 1943.83 \ \frac{A\,cm^2}{V\,g_{-equiv}}$$

$$T_{b_r} = \frac{T_b}{T_c} = 0.73$$

$$T_r = \frac{T}{T_c} 0.64$$

$$m = 1 - \left(\frac{1 - T_r}{1 - T_{br}} \right)^n = -0.06$$

$$\lambda_-^\circ = 2182.68 \frac{A\,cm^2}{V\,g_{-equiv}}$$

Diffusivity

Diffusion coefficient of ionic $Ag^+$is described by the Nernst equation.

$$D_{AB}^\circ = \frac{RT}{F^2} \frac{\lambda_+^\circ \lambda_-^\circ}{\lambda_+^\circ + \lambda_-^\circ} \frac{|Z_-| + |Z_+|}{|Z_+ Z_-|}$$

Faraday Constant

F =	96488	C/gequiv
R/F^2 =	8.93E-14	

Thermal conductivity

λ_+^0	61.90	Acm^2/Vg_{equiv}
λ_-^0	2182.68	Acm^2/Vg_{equiv}

Valencies

Z_+ =	1.00
Z_- =	1080.00

$\mathscr{D}_{AB}$ = 1.60E-09 m^2/s

Inlet flow

$$F_A = 4\pi {r_1}^2 N_{Ar}|_{r=r1} = \frac{4\pi c D_{AB}}{1/r_1 - 1/r_2} \ln \frac{x_{B2}}{x_{B1}}$$

r_1 =	9.00E-09	M
r_2 =	1.00E-08	M
x_{B1} =	1.80E-09	
x_{B2} =	1.00	
c =	5.54E-08	mol/m3
c_{Ag^+} =	1.00E-16	mol/m3
c_{H2O} =	5.54E-08	mol/m3

F_A =	2.02E-21	mol/s

Concentration within time

Design equations

$$C_i = C_i{}^\circ + \frac{dC_i}{dt}\Delta t$$

and equations showed in the section: Reactor.

Initial conditions at reactor ($C_i{}^\circ$)

$$C_{E_0} = 5.44x10^{-4} mol/L$$

$$C_{S_0} = C_{ES_0} = C_{P_0} = 0$$

Inlet conditions

$$F_A = 2.02x10^{-21} mol/s$$

$$C_s = 1x10^{-4} mol/L$$

Results

Solving our diferential equations by Euler’s method we obtained:

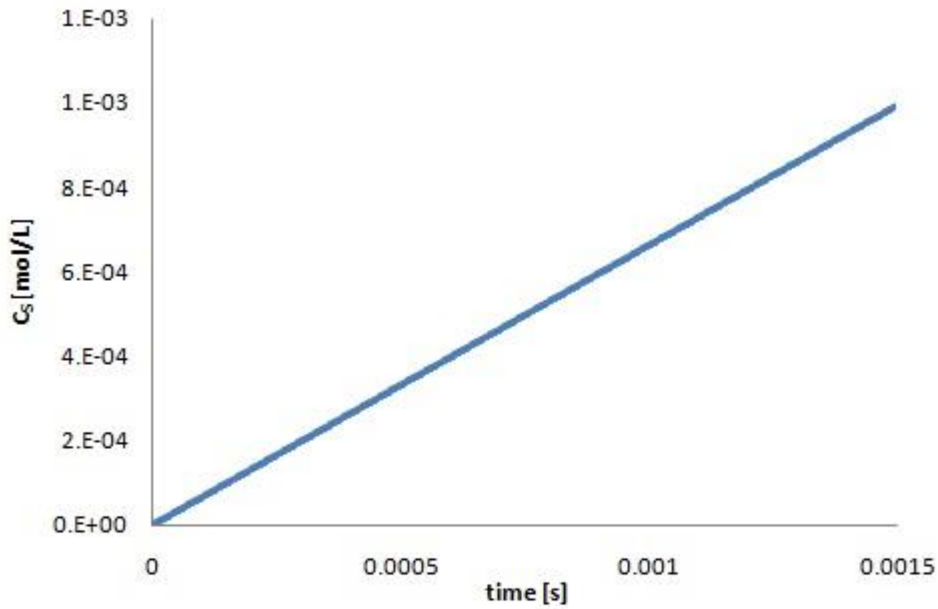

Figure 1.- Substrate concentration within time

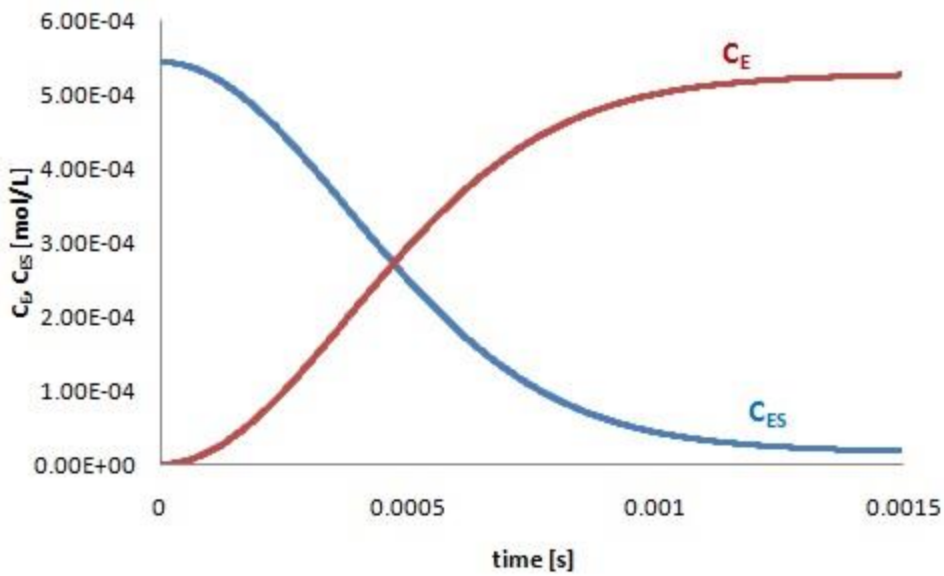

Figure 2.- Enzyme and Enzyme-Substrate concentrations within time

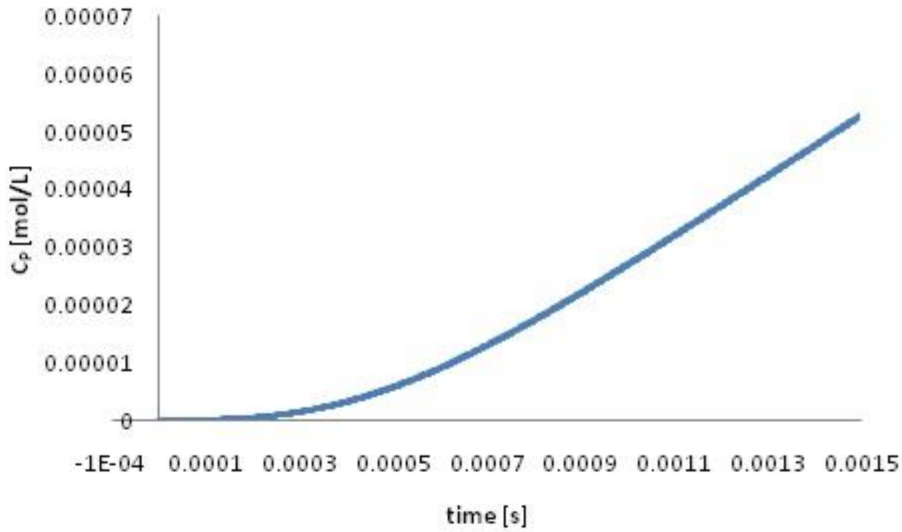

Figure 3.- Product concentration within time

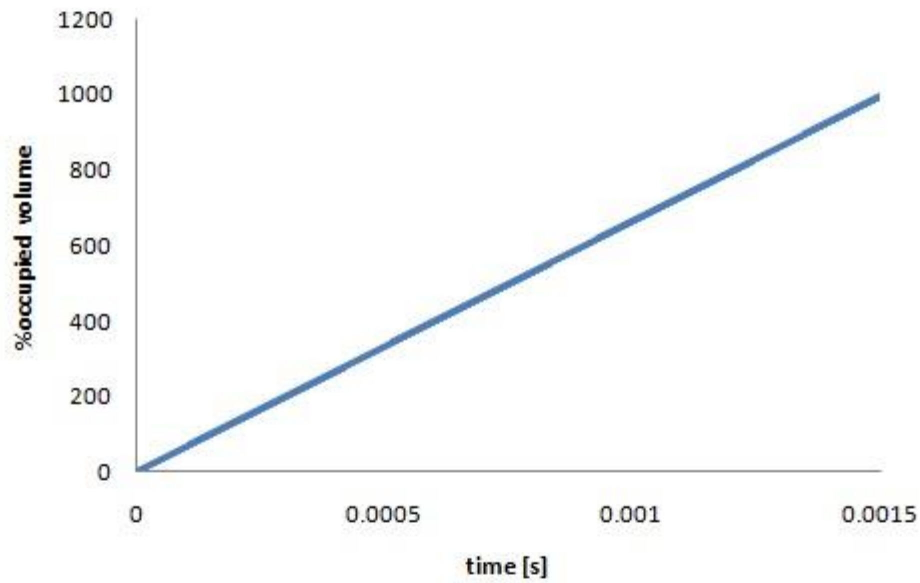

Figure 4.- Percentage of occupied volume in reactor within time

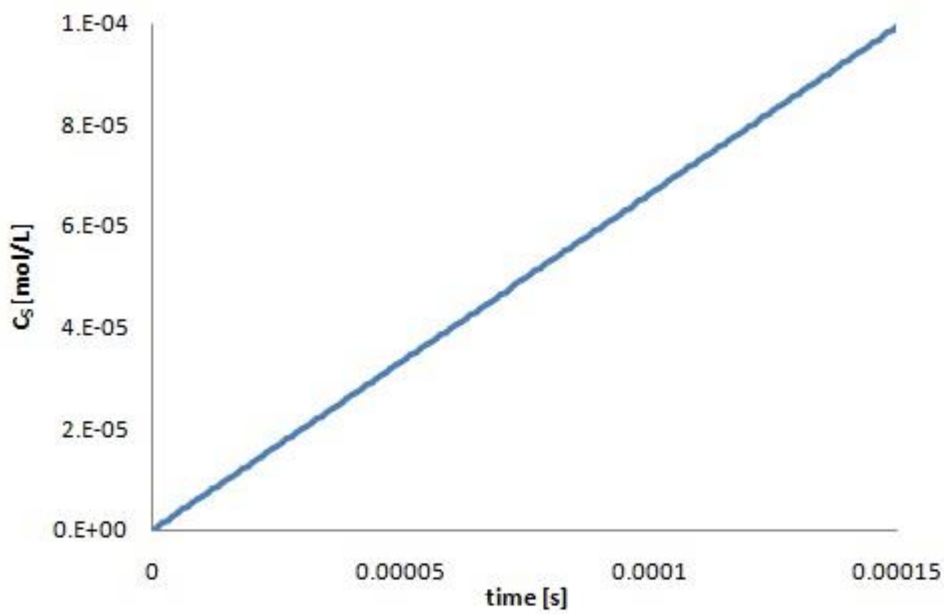

Figure 5.- Substrate concentration within time at 100%volume capacity

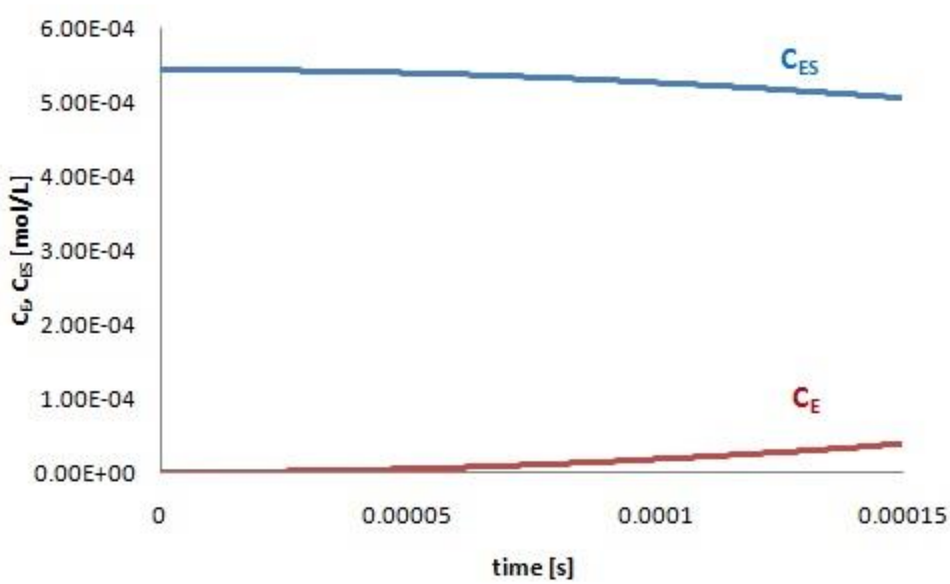

Figure 6.- Enzyme and Enzyme-Substrate concentrations within time at 100%volume capacity

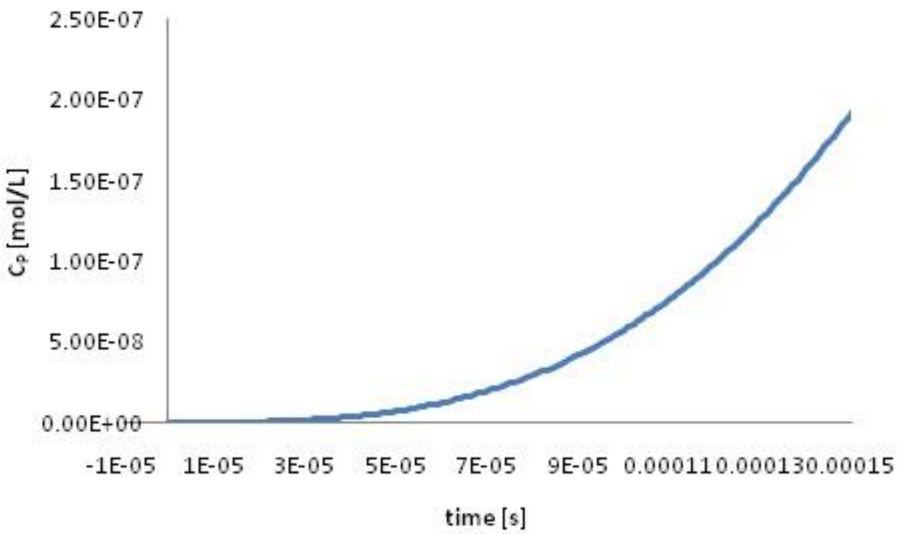

Figure 7.- Product concentration within time at 100%volume capacity

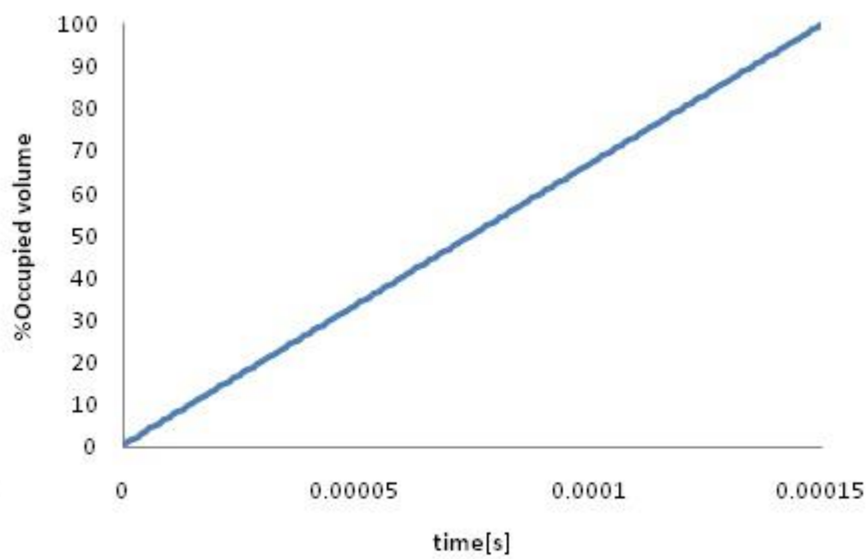

Figure 8.- Percentage of occupied volume in reactor within time at 100%volume capacity