Tutorial sheet solution

(I)

(1) $V = 0.5\, V_{max}$; $S = K_m$

$V = 0.9\, V_{max}$

$0.9 = \frac{S}{K_m + S}$

$S = 10 \cdot K_m$

$V = 0.95\, V_{max}$

$S = 20\, K_m$

(2) $y = 10.525\, x + 1.9631$

$$\frac{1}{V} = \frac{1}{V_{max}} + \frac{K_m}{V_{max}} \frac{1}{S}$$

$$\frac{1}{V_{max}} = 1.9631$$

$V_{max} = 0.509$ μmol/L min

$K_m = 0.509 \times 10.525 = 5.36$ μmol/L

$S_0 = 20$ μmol/L

$$V_{max}\, t = \ln\left(\frac{S_0}{S}\right) K_m + (S_0 - S) \quad \text{or}$$

$$60 \times 0.509 = \ln\left(\frac{20}{S}\right) 5.36 + 20 - S$$

$$\boxed{\ln\left(\frac{20}{S}\right) 5.36 - S - 10.54}$$

Newton's non linear equation sol^n method notes (II)

$$\boxed{f(x) = \ln(20/S)\, 5.36 - S - 10.54}$$

Iteration 1

$S_1 = 1$ $\quad S_1 + \Delta S = 1.001$

$f(S_1) = 4.517$ $\quad f(S_1 + \Delta S) = 4.51176$

$S_2 = 1.86$

Error $= 0.462$

Iteration 2

$S_2 = 1.86$ $\quad S_2 + \Delta S = 1.861$ $\quad f(S_2) = 0.3308$ $\quad f(S_2 + \Delta S) = 0.32695$ $\quad S_3 = 1.946$

Error $= 0.044$

Iteration 3

$S_3 = 1.946$ $\quad S_3 + \Delta S = 1.947$ $\quad f(S_3) = 2.56 \times 10^{-3}$ $\quad f(S_3 + \Delta S) = 1.18 \times 10^{-3}$

$S_4 = 1.9466$ $\quad$ Error $= 3.3 \times 10^{-4}$

③ Tyrosine ⟷ Phenol + pyruvate + ammonium

L-dopa (3 4 dihydroxy L phenylalanine) ⟷ Catechol + pyruvate + ammonium

Total enzyme conc ⇒ 0.85 μg/ml
Pyruvate ⇒ 80mM
NH_4Cl ⇒ 180mM
Phenol ⇒ 50mM

⇒ 2.3mM Tyrosine in 7 minutes

Enzyme activity ⇒ moles of substrate/unit time
1 μmol/min = 1U

Specific activity ⇒ μmol/mg/min (per mg of protein)

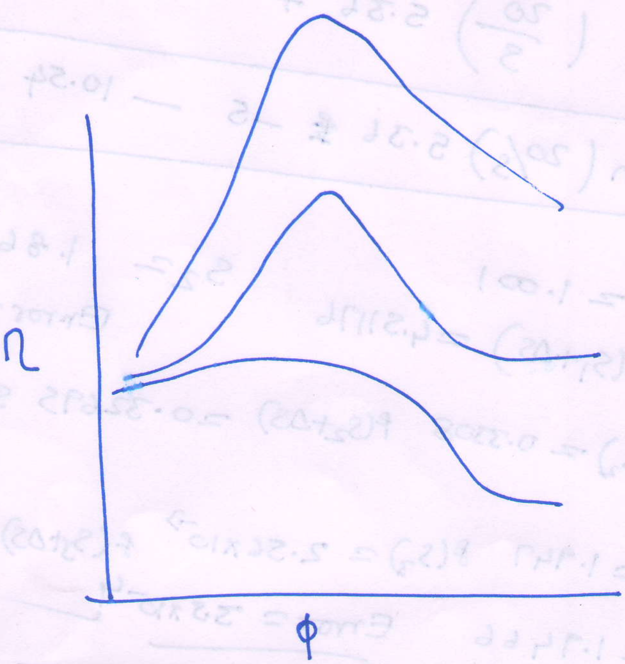
$$\text{Enzyme activity} = \frac{2.3 \times 10^{-3}\,M}{7}$$

$= 328$ IU/ml

Specific activity ⇒ 328 IU/0.85 μg

⇒ 385.8×10^{3} μmol/mg/min

④



$$\eta = \frac{\text{observed rxn rate}}{\text{maximum rxn rate}}$$

$$\phi = R/3 \sqrt{\frac{V_{max}}{D_{eff}\, K_m}} \quad (\text{sph})$$

↳ Ratio of diffusion + consumption!!

$$\phi = L \sqrt{\frac{V_{max}}{K_m . D_{eff}}}$$

L ↓ thickness

$$\Phi = \frac{\left(\frac{60 x 10^{-4} cm}{3}\right)^2 \left(498 \frac{\mu mols\ ATEE}{\mu mol\ active\ \alpha\text{-}CT.min}\right)\left(1.27 \frac{\mu mols\ active\ \alpha\text{-}CT}{gm}\right)\left(0.41 \frac{gm}{cm^3}\right)}{\left(\frac{3.8 x 10^{-6} cm^2}{sec}\right)\left(\frac{60 sec}{min}\right)\left(1 \frac{\mu mol\ ATEE}{cm^3}\right)} = 4.5$$

This large value of Φ indicates that the reaction rate is diffusion limited.

To calculate the effectiveness factor we need a relationship between Φ and η_I. The dependence of η_I on Φ is shown in Fig. 2.13; however, Fig. 2.13 includes β, which we shall assume is unknown (recall that K_m in β is the intrinsic Michaelis constant of the immobilized enzyme, which may differ from that of the soluble enzyme). Moreover, since the catalyst's overall activity is diffusion limited, K_m cannot be determined in the conventional manner. Nonetheless, we can assume a value of β and use Figure 2.13 to estimate η_I from Φ. This approach will yield an approximate result which, depending on the required accuracy, may be satisfactory. From Fig. 2.13 we see that η_I will fall between about 0.17 and 0.35.

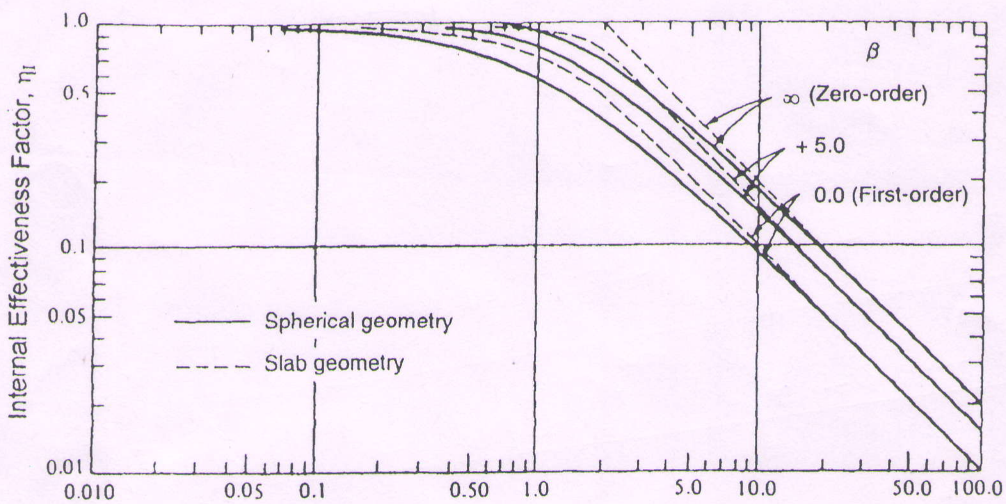


Figure 2.13. *Effectiveness factor, η_I, as a function of the observable modulus, Φ, and the dimensionless substrate concentration, β.*

for problem # 5

substrate inhibited rxn ; more pronounced with pH !!

II

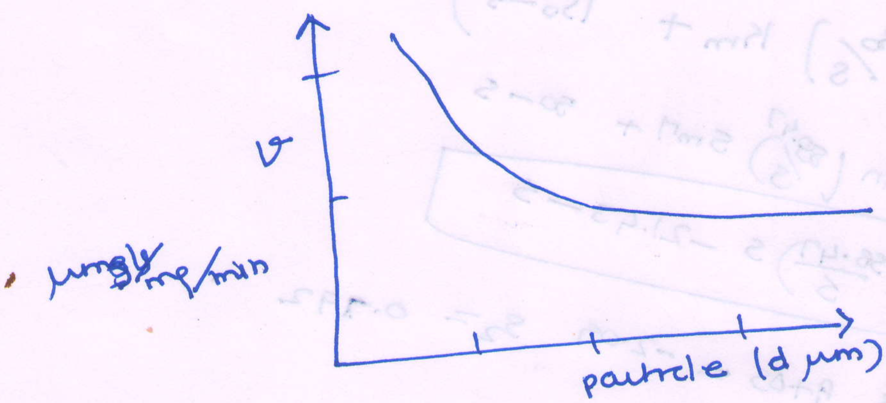
(5) Glucose isomerase

$K_m = 0.209$ M

$S_o = 1.5$ M

$\rho_E = 1.4\ g/cm^3$

$\beta = S_o/K_m = 7.17$



$\phi_{obs} = \frac{v_{obs}}{D_{eff} S_o} \left(\frac{R}{3}\right)^2$

$\phi = \frac{R}{3} \left(\frac{v_{max}}{K_m D_{eff}}\right)^{1/2}$

d	v
100 μm	0.29 μmol/mg/min

Activity (kinetically limited) = 0.3

Activity (diffusion limited) = 0.15

From graph $\beta = 7.17$ & $\eta = 1$

$\boxed{\phi_{obs} \Rightarrow 0.1 \text{ to } 1}$ → From Fig 2.13 in Blood chapter by Clark & Blanch

$\phi_{obs} = \frac{v_{obs}}{D_{eff} S_o} \left(\frac{R}{3}\right)^2$

Use this solve $\boxed{D_{eff}}$

Source of error ⇒ D_{eff} depends on pore size in particle ! as the particle size increase ; it is doubtful the pore ... maintained.

⑥

$S_0 = 2\%\ w/v \Rightarrow 20\ g/L \Rightarrow 58.47\ mM$

$V_{max} = 2\ mmol/min/L$

$K_m = 5mM$

$t = 40$ minutes

$X = ?$

$$V_{max}\, t = \ln\left(\frac{S_0}{S}\right) K_m + (S_0 - S)$$

$$2mM/min \cdot 40 = \ln\left(\frac{58.47}{S}\right) 5mM + 58 - S$$

$$\boxed{f(S) = \ln\left(\frac{58.47}{S}\right) 5 - 21.43 - S}$$

Again using newton's iteration method

$S_1 = 1 \quad S_1 + \Delta S = 1.001 \quad f_1 = -2.08 \quad f_1 + \Delta S = -2.09 \quad S_2 = 0.792$

$S_2 = 0.792$

$S_3 = 0.690$

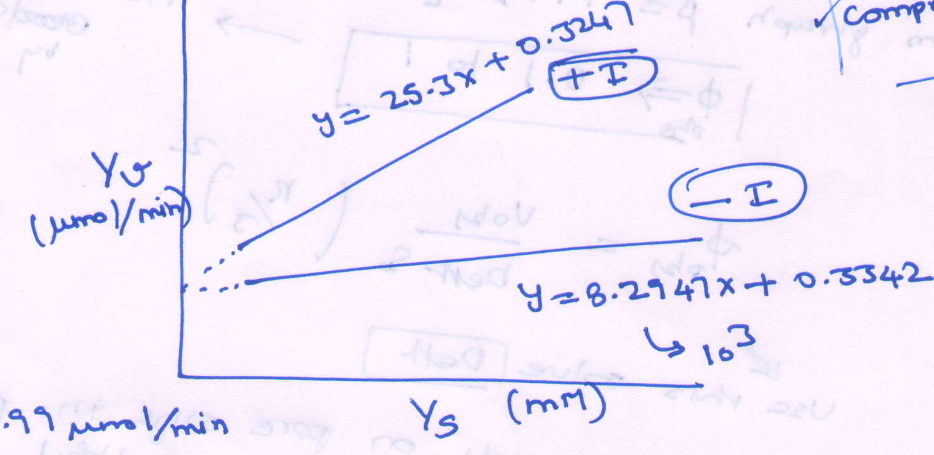
$\therefore \boxed{S = 0.699}$

Reaction proceeds till $S = 0.699$ mM @ 40 min

$$Y_v = \frac{1}{V_{max}} + \frac{K_m}{V_{max}} Y_s$$

⑦

$\boxed{\text{Competitive Inhibition}}$



$V_{max} = 2.99\ \mu mol/min$

$\underline{K_m} = 8.2947 \times 10^3 \Rightarrow 24.8 \times 10^{-3}\ M$ //

8

III

$$\frac{u_{max}}{Vol} \cdot t = S_0 \cdot x - K_m \ln(1-x)$$

$K_m = 2mM$

$u_{max} = 10$ mmol/min $\Rightarrow$ $\cancel{10}$ 2 mmol/L /min

$S_0 = 2M$

$t = 15$ hrs

$$2 \text{ mM} \cdot \text{min}^{-1} \times 15 \times 60 = 2 \cdot x \ln\left(\frac{2 \times 10^3}{S}\right) + 2000 - S$$

$$\cancel{\ln(1-x)} = \cancel{-x} + \cancel{\frac{x^2}{2}} \cancel{- x^3/3}$$

$$f(x) = \ln\left(2000/S\right) 2 + 200 - S$$

Again using newton's nonlinear sol^n

$S_1 = 200$; $S_1 + \Delta S = 200.1$; $f_1 = 4.6$; $f_1 + \Delta S = 4.504$

$\downarrow$

$S_2 = 204.8$

Approx ~ sol^n $\Rightarrow$ $S = 204.8$

$$x = \frac{S_0 - S}{S_0} = \frac{2000 - 204.8}{2000} =$$

$$\boxed{x = 0.8976}$$

9

$$V = \frac{0.128(G) - 0.098(F)}{0.096 + 0.383(G) + 0.25(F)}$$

In CSTR

with 40% conversion

$$\tau_{CSTR} = \frac{V}{S_0 - S}$$

$S = 0.6$

$F = 0.4$

$$\boxed{\tau_{CSTR} = 4.679}$$

In PFR

$$F = S_0 - G$$

$$V = \frac{0.03(S) - 0.098}{0.346 + 0.133(S)}$$

(simplify the eq^n with one variable)

$$\tau = \int_{S_0}^{S} \frac{dS}{V}$$

$$\tau = \int_{S_0}^{S} \frac{0.346 + 0.133(S)}{0.03(S) - 0.098} \, dS$$

Solve ; using integration formula

$$\int \frac{x\,dx}{ax+b} = \frac{x}{a} - \frac{b}{a^2} \ln|ax+b|$$

$$\boxed{\tau_{PFR} = 0.6153}$$

Productivity will be 7.6 times higher in PFR

10

$A_0 = 10\ mM$

$F = 1000\ L/min$ $K_m = 5\ mM$

$v = \frac{v_{max} \cdot A}{K_m + A}$ $X = 0.99$

CSTR

$v_{max} \cdot \tau = K_m \left(\frac{X}{1-X}\right) + X S_0 \Rightarrow$ $\tau = 10.097\ min$

$V_{CSTR} = 10000\ L$

PFR

$\tau \cdot v_{max} = S_0 X - \ln(1-X) K_m$ $\tau = 0.658\ min$

$V_{PFR} = 658\ L$

τ_{CSTR} $\cancel{E/CSTR}$ $\propto$ E_{CSTR}.

V_{PFR}

$v_{max} = K_2 E_0 = 50\ mM/min$.

$K_2 = 50 \times 10^3\ mM/min\ /\ mM(Enz)$

with 10^{-2} mM Enz

$v_{max} = 500\ mM/min$.

$V_{CSTR} = 1000\ L$

$V_{PFR} = 65.8\ L$

To decide reactor type you need to know
- Enzyme cost
- Any inhibitors ?