

ABE370 Test 1

Problem 1 (30 points)

Solution Problem 1

the rate of reaction model for a 2nd order reaction is $dC/dt = -k C^2$

Solving for this gives, $1/C - 1/C_0 = kt$

solving this for C_0

$$C_{\min} := 0.1 \frac{\text{mg}}{\text{mL}} \quad k_{\text{acid}} := 0.07 \frac{\text{mL}}{\text{mg} \cdot \text{day}} \quad \text{shelf_time} := 90 \text{ day}$$

$$C_{\text{initial}} := \frac{1}{\frac{1}{C_{\min}} - k_{\text{acid}} \cdot \text{shelf_time}}$$

$$C_{\text{initial}} = 0.27 \frac{\text{mg}}{\text{mL}}$$

Problem 2 (30 points)

Solution Problem 2

The reaction rate equation for a 3rd order reaction is

$$-dC/dt = kC^3$$

the solution to this is

$$CA_0 := 300 \frac{\text{mol}}{\text{L}} \quad k := 5.26 \cdot 10^{-6} \cdot \frac{\text{L}^2}{\text{mol}^2 \cdot \text{min}}$$

$$CA(t) := \frac{CA_0^2}{\sqrt{1 + 2 \cdot CA_0^2 \cdot k \cdot t}}$$

$$t := 10 \text{ min}$$

$$CA(t) = 92.723 \frac{\text{mol}}{\text{L}}$$

a. $XA := \frac{CA_0 - CA(t)}{CA_0}$ $XA = 0.691$

b. Based on the reaction stoichiometry, every mol of A reacted produces 2 moles of B.

$$Cb(t) := 2 \cdot (CA_0 - CA(t))$$
$$Cb(t) = 414.553 \frac{\text{mol}}{\text{L}}$$

Problem 3 (40 points)

A. Using the proposed mechanism, write the differential rate equations for A, B, C, AB* and ABB*.

$$d[A]/dt = -k_1[A][B] + k_2[AB^*]$$

$$d[B]/dt = -k_1[A][B] + k_2[AB^*] - k_3[AB^*][B] + k_4[ABB^*]$$

$$d[C]/dt = k_4[ABB^*]$$

$$d[AB^*]/dt = k_1[A][B] - k_2[AB^*] - k_3[AB^*][B]$$

$$d[ABB^*]/dt = k_3[AB^*][B] - k_4[ABB^*]$$

B. Assuming AB* and ABB* are transition intermediates whose concentrations are at steady state, derive the rates of reaction of A, B and C. Be sure to compare your rates so they satisfy the mass balance requirements of the reaction!

First, solve for [AB*] and [ABB*] using their rate equations:

$$d[AB^*]/dt = k_1[A][B] - k_2[AB^*] - k_3[AB^*][B] = 0$$

solving for [AB*],

$$[AB^*] = \frac{k_1[A][B]}{k_2 + k_3[B]}$$

$$d[ABB^*]/dt = k_3[AB^*][B] - k_4[ABB^*] = 0$$

solving for [ABB*],

$$[ABB^*] = \frac{k_3[AB^*][B]}{k_4} = \frac{k_1 k_3 [A][B]^2}{k_2 k_4 + k_3 k_4 [B]}$$

Plug these results into the rate equations for A, B and C

$$d[A]/dt = -k_1[A][B] + k_2[AB^*] = -k_1[A][B] + \frac{k_2 k_1 [A][B]}{k_2 + k_3[B]}$$

$$= \frac{-k_1[A][B](k_2 + k_3[B]) + k_2 k_1 [A][B]}{k_2 + k_3[B]} = \frac{-k_1 k_3 [A][B]^2}{k_2 + k_3[B]}$$

$$d[B]/dt = -k_1[A][B] + k_2[AB^*] - k_3[AB^*][B] + k_4[ABB^*]$$

$$k_2 k_1 [A][B] - k_3 k_1 [A][B]^2 + k_4 k_1 k_3 [A][B]^2$$

$$= -k_1[A][B] + \frac{k_2}{k_2 + k_3[B]} - \frac{k_2}{k_2 + k_3[B]} + \frac{k_2 k_4}{k_2 k_4 + k_3 k_4 [B]}$$

$$= \frac{-k_1 k_3 [A][B]^2}{k_2 + k_3[B]}$$

$$d[C]/dt = k_4[ABB^*] = \frac{k_4 k_1 k_3 [A][B]^2}{k_2 k_4 + k_3 k_4 [B]} = \frac{k_1 k_3 [A][B]^2}{k_2 + k_3[B]}$$

Since the overall reaction stoichiometry is $A + B = C$, then $d[A]/dt = d[B]/dt = -d[C]/dt$. This is consistent with the derived rate equations.

C. Explain how the rate of formation of C behaves/changes with respect to changes in the concentration of B at high B concentrations, i.e. is it not a function of [B]; increases linearly with [B]; faster than linear?

$$d[C]/dt = \frac{-k_1 k_3 [A][B]^2}{k_2 + k_3[B]}$$

$$\text{At high [B], } k_3[B] \gg k_2, \text{ so } d[C]/dt = \frac{-k_1 k_3 [A][B]^2}{k_3[B]} = -k_1 [A][B]$$

So the rate of reaction would increase linearly with increases in [B].