Homework 7 Solutions

Problem 1: Multiple steady states

Problem Statement

Calculate the steady states for the following elementary liquid-phase reaction and data below carried out in a CSTR.

$$A + B \rightarrow 2C$$

Given Variables:

$V = 1L$
$v = 100cm^3/min = 0.1L/min$
$k = 33E + 9exp(-2000(cal/mol)/(RT))$ - k has units of : (L/(mol*min))
$\Delta H_R = -20kcal/mol$
$c_{A0} = 20mol/L$
$c_{B0} = 3mol/L$
$T_0 = 17C$
$T_A = 87C$
$UA = 25cal/(min \times K)$
$\sum \theta_i c_{p,i} \times c_{B0} = 650cal/(L \times K)$

Required:

a) What are the steady state temperatures and conversions for this reactor? Hint: The temperatures will fall between 310K and 375K.
b) Are there unstable steady state values, if so which one(s)?

Solutions

a)

Species mole balance on the CSTR:

$$V = \frac{F_{A0} X_A}{-r_A}$$

$$V = \frac{F_{A0}X_A}{kc_Ac_B} = \frac{F_{A0}X_A}{kc_{A0}^2(1-X_A)(\frac{20}{3}-X_A)}$$

$$V = \frac{v_0X_A}{kc_{A0}(1-X_A)(\frac{20}{3}-X_A)}$$

Energy balance on the CSTR:

$$X_{EB} = \frac{\frac{UA}{F_{A0}}(T-T_a) + \sum\theta_i c_{p,i}(T-T_0)}{-\Delta H_R(T)}$$

Plug X_{EB} into the mole balance for X_A and find the value(s) of T when the Volume is 1L:

T (K)	X
314.3	0.072
340.8	0.470
368.3	0.883

b)

The steady state at T = 340.8K is unstable.

Problem 2: CSTR with multiple steady states

Problem Statement

The elementary liquid phase reaction:

$$A \rightarrow B$$

occurs in a jacketed CSTR. Species A and inert I are fed to the reactor in equimolar amounts. The molar feed rate of A is 80 mol/min.

Given variables:

$F_{A0} = F_I = 80mol/min$
$c_{P,I} = 30cal/(mol \cdot C)$
$c_{p,A} = c_{p,B} = 20cal/(mol \cdot C)$
$UA = 8000cal/(min \cdot C)$
$\Delta H_R = -7500cal/mol$
$k(350K) = 6.6 \times 10^{-3} min^{-1}$
$T_a = 300K$
$E_A = 40,000cal/(mol \cdot K)$
$\tau = 100min$

Required:

a) What is the reactor temperature at a feed temperature of 450K?
b) Plot the reactor temperature as a function of the feed temperature.
c) Suppose that you begin with a feed temperature of 250K, which you slowly increase. What inlet temperature must the reactor be heated before the reactor operates at a high conversion? What are the corresponding temperature and conversion of the fluid in the CSTR just above this inlet temperature?
d) Suppose that the inlet fluid is now heated 5°C above the temperature in part c and is cooled by 20°C where it remains. What will be the conversion?
e) What is the feed temperature which will cause extinction for this reaction system?

Solutions

a) $T_0 = 450K$

Mole balance on species A:

$$V = \frac{F_{A0}X_A}{-r_A} = \frac{c_{A0}v_0X_A}{kc_{A0}(1-X_A)}$$

$$\tau = \frac{X_A}{k(1-X_A)}$$

Energy balance on the CSTR:

$$X_{EB} = \frac{\frac{UA}{F_{A0}}(T-T_a) + \sum \theta_i c_{p,i}(T-T_0)}{-\Delta H_R(T)}$$

$$\sum \theta_i c_{p,i} = \theta_A c_{p,A} + \theta_I c_{p,I} = (1)(20) + (1)(30)$$

$$\Delta c_p = 0$$

$$X_{EB} = \frac{\frac{8000}{80}(T - 300K) + 50(T - 450K)}{-7500}$$

Plug X_{EB} into the mole balance for X_A and find the value(s) of T when the residence time (τ) is 100min:

$$\boxed{T = 399.9K}$$

$$\boxed{X_A = 0.999}$$

b)

Use goalseek to find the steady-state temperature(s) for each inlet temperature.

c)

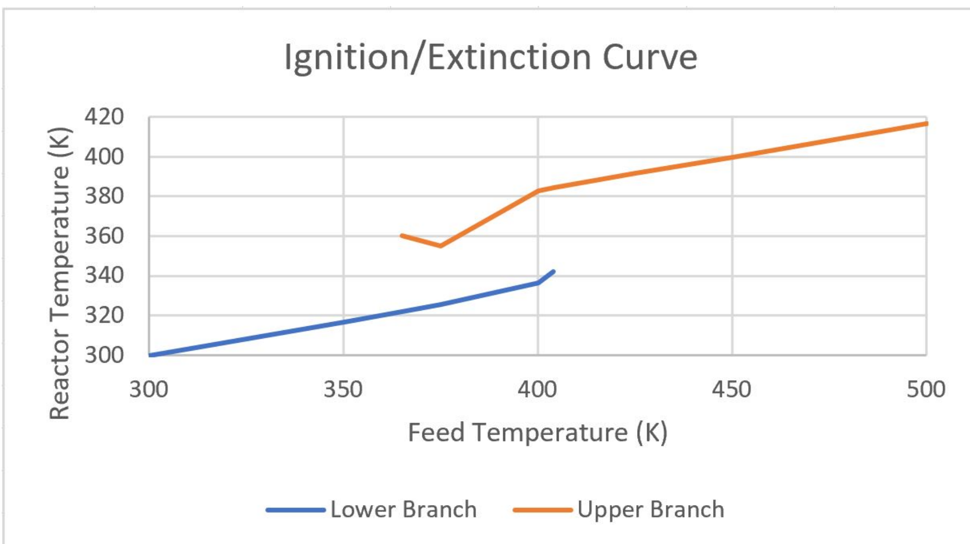
Ignition occurs when $T = 405K$. At $T = 405K$, $T_0 = 384.6K$ & $X_A = 0.991$

d)

If the feed temperature is 390K after reaching the upper branch, the conversion will be 98%.

e)

The inlet temperature that causes extinction is 363K


Ignition/Extinction Curve
420
400
380
360
340
320
300
Reactor Temperature (K)
300
350
400
450
500
Feed Temperature (K)
Lower Branch
Upper Branch

Problem 3

$$O_2 + 2S \rightleftharpoons 2O\cdot S$$

$$C_3H_6 + O\cdot S \rightleftharpoons C_3H_6O\cdot S$$

$$C_3H_6O\cdot S \longrightarrow C_3H_6O + S$$

a.

$$k_1 (O_2)\frac{(S)^2}{C_T} = k_{-1}\frac{(O\cdot S)^2}{C_T}$$

$$K_1 (O_2)(S)^2 = (O\cdot S)^2$$

$$(S)\sqrt{K_1 (O_2)} = (O\cdot S)$$

PSSH on $(C_3H_6O\cdot S)$

$$0 = k_2 (C_3H_6)(O\cdot S) - k_{-2}(C_3H_6O\cdot S) - k_3 (C_3H_6O\cdot S)$$

$$k_2 (C_3H_6)(O\cdot S) = (k_{-2} + k_3)(C_3H_6O\cdot S)$$

$$\frac{k_2 (C_3H_6)(O\cdot S)}{k_{-2} + k_3} = (C_3H_6O\cdot S)$$

$$\frac{k_2 (C_3H_6)(S)\sqrt{K_1 (O_2)}}{k_{-2} + k_3} = (C_3H_6O\cdot S)$$

$$r = \frac{r_3}{2} = \frac{k_3}{2}(C_3H_6O\cdot S) = \frac{k_3 k_2 (C_3H_6)(S)\sqrt{K_1 (O_2)}}{2(k_{-2} + k_3)}$$

$$C_T = (S) + (O\cdot S) + (C_3H_6O\cdot S)$$

$$C_T = (S) + (S)\sqrt{K_1 (O_2)} + \frac{k_2 (C_3H_6)\sqrt{K_1 (O_2)}}{k_{-2} + k_3}(S)$$

$$(S) = \frac{C_t}{1 + \sqrt{K_1(O_2)} + \frac{k_2(C_3H_6)\sqrt{K_1(O_2)}}{k_{-2} + k_3}}$$

$$r = \frac{k_3 k_2 (C_3H_6)\sqrt{K_1(O_2)}\ C_t}{2(k_{-2} + k_3)\left[1 + \sqrt{K_1(O_2)} + \frac{k_2(C_3H_6)\sqrt{K_1(O_2)}}{k_{-2} + k_3}\right]}$$

b.

$$k_2(C_3H_6)(O \cdot S) = k_{-2}(C_3H_6O \cdot S)$$

$$K_2(C_3H_6)(O \cdot S) = (C_3H_6O \cdot S)$$

$$K_2(C_3H_6)(S)\sqrt{K_1(O_2)} = (C_3H_6O \cdot S)$$

$$r = \frac{k_3}{2}(C_3H_6O \cdot S) = \frac{k_3}{2} K_2 (C_3H_6)\sqrt{K_1(O_2)}(S)$$

$$C_T = (S) + (O \cdot S) + (C_3H_6O \cdot S)$$

$$C_T = (S) + (S)\sqrt{K_1(O_2)} + (S)K_2(C_3H_6)\sqrt{K_1(O_2)}$$

$$(S) = \frac{C_T}{1 + \sqrt{K_1(O_2)} + K_2(C_3H_6)\sqrt{K_1(O_2)}}$$

$$r = \frac{k_3 K_2 (C_3H_6)\sqrt{K_1(O_2)}}{2} \quad \frac{C_t}{1 + \sqrt{K_1(O_2)} + K_2(C_3H_6)\sqrt{K_1(O_2)}}$$

c.

$$C_T = (O \cdot S) = (S)\sqrt{K_1 (O_2)}$$

$$(S) = \frac{C_T}{\sqrt{K_1 (O_2)}}$$

$$r = \frac{k_3}{2} K_2 (C_3H_6) \sqrt{K_1 (O_2)}\ (S)$$

$$r = \frac{k_3}{2} K_2 (C_3H_6)\, C_T$$

$$k_{APP} = \frac{k_3 K_2}{2}$$

$$\frac{d(\ln k_{APP})}{d(1/T)} = \frac{d(\ln k_3)}{d(1/T)} + \frac{d(\ln(K_2))}{d(1/T)}$$

$$\frac{E_{APP}}{\cancel{R}} = \frac{E_3}{\cancel{R}} + \frac{\Delta H_2}{\cancel{R}}$$

$$\Delta H_2 < 0$$

$$E_{APP} < E_3$$