Kinetics and Reactor Design HW10

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Assigned: April 18, 2023
Due: May 2, 2023

1 Problem Statement

1.1 P12-16$_B$ (a-f)

P12-16$_B$ The elementary reversible liquid-phase reaction

$$A \rightleftarrows B$$

takes place in a CSTR with a heat exchanger. Pure A enters the reactor.

(a) Derive an expression (or set of expressions) to calculate $G(T)$ as a function of the heat of reaction, equilibrium constant, temperature, and so on. Show a sample calculation for $G(T)$ at $T = 400$ K.

(b) What are the steady-state temperatures? (***Ans.:*** 310, 377, 418 K.)

(c) Which steady states are locally stable?

(d) What is the conversion corresponding to the upper steady state?

(e) Vary the ambient temperature T_a and make a plot of the reactor temperature as a function of T_a, identifying the ignition and extinction temperatures.

(f) If the heat exchanger in the reactor suddenly fails (i.e., $UA = 0$), what would be the conversion and the reactor temperature when the new upper steady state is reached? (***Ans.:*** 431 K.)

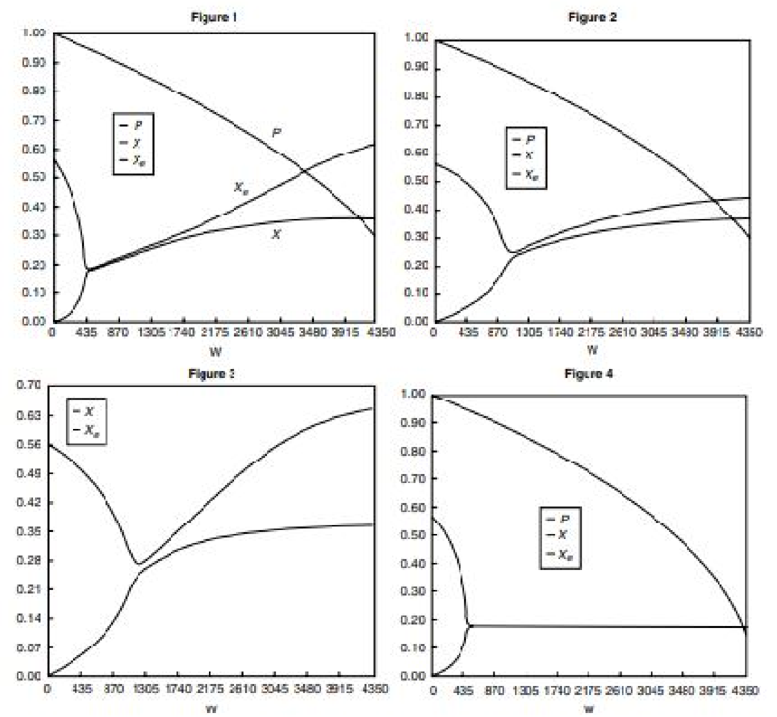
Figure 1

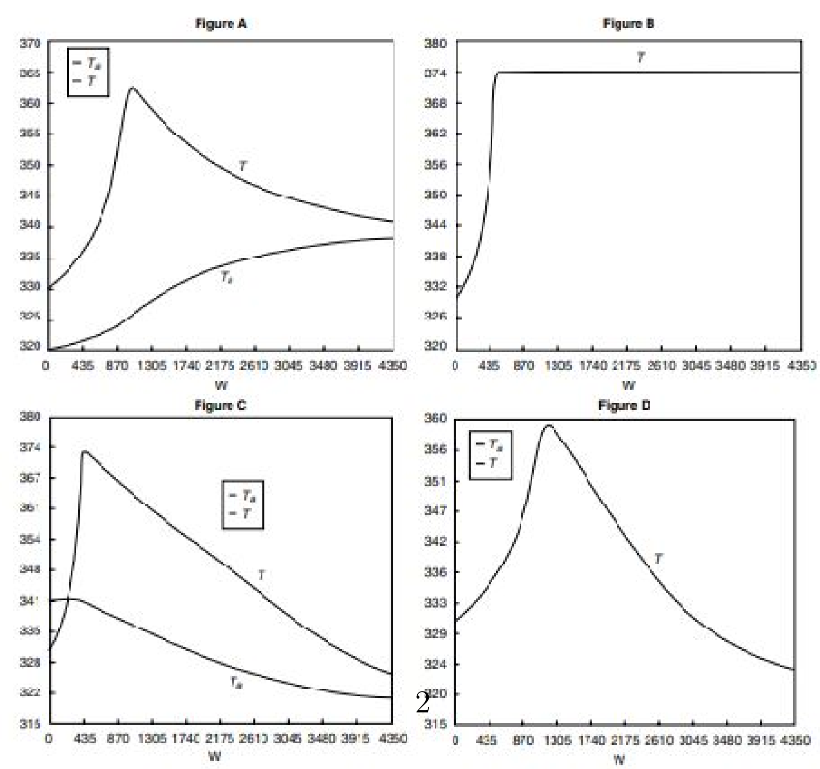
1.2 P12-20$_B$

P12-20$_B$ The reaction

$$A + B \rightleftarrows 2C$$

is carried out in a packed-bed reactor. Match the following temperature and conversion profiles for the four different heat-exchange cases: adiabatic, constant T_a, co-current exchange, and countercurrent exchange.





(a) Figure 1 matches Figure ___
(b) Figure 2 matches Figure ___
(c) Figure 3 matches Figure ___
(d) Figure 4 matches Figure ___

2 Problem Solution

2.1 P12-16$_B$ (a-f)

a)

$$V = \frac{F_{A0}X}{-r_A} = \frac{\nu_0 C_{A0} X}{k[C_A - (C_B/K_e)]} \tag{1}$$
$$X[1 + \tau k(1 + (1/K_e))] = \tau k \tag{2}$$
$$X = \frac{\tau k}{1 + \tau k(1 + (1/K_e))} \tag{3}$$
$$G(T) = -\Delta H_{Rx} X = 80000X \tag{4}$$
$$k_1 = 1 \text{ min}^{-1} \text{ at 400K} \tag{5}$$
$$\tau = V/\nu_0 = 10 \text{ min} \tag{6}$$
$$K_C = K_e = 100 \tag{7}$$
$$X = \frac{10}{1 + 10(1.01)} = 0.901 \tag{8}$$
$$G(T) = .901(80000) = 72080 \text{ cal/mol} \tag{9}$$

b)

$$\kappa = \frac{UA}{F_{A0}C_{P_A}} = \frac{3600}{10 \times 40} = 9 \tag{10}$$
$$R(T) = C_{P_A}(1+\kappa)(T - T_C) = 400(T - T_C) \tag{11}$$
$$T_C = \frac{T_0 + \kappa T_a}{1+\kappa} = 310 \tag{12}$$
$$R(T) = 400(T - 310) \tag{13}$$
$$K_C(T) = K_C(400) exp\left[\frac{\Delta H^\circ_{Rx}(T_R)}{R}\left(\frac{1}{400} - \frac{1}{T}\right)\right] \tag{14}$$
$$k(T) = k_1 exp\left[\frac{E}{R}\left(\frac{1}{400} - \frac{1}{T}\right)\right] \tag{15}$$
$$G(T) = -\Delta H^\circ_{Rx}\left[\frac{\tau k(T)}{1 + \tau k(T)\left(\frac{1}{K_C(T)} + 1\right)}\right] \tag{16}$$

Set up G(T) line by finding new K_Cs. Intersection points with R(T): 310K, 380K, 418K.
c) Via the G(T) and R(T) graph, 310K is locally stable lower steady state, and 418 is locally stable higher steady state.
d) R(418) = 400(418 - 310)= 43200. G(418) = 80000X = 43200. X = 0.54.
e) By varying Ta, we move the R(T) line's intercept. At 211K it is tangent near the peak of G(T) therefore that is the extinction temperature. At 365K it is tangent to the near-bottom

of G(T), corresponding to ignition temperature. We know it must be those two because there are no other R(T) lines that lie tangent to G(T) at any point.
f) We set UA to 0 in (10), which subsequently will change R(T). κ is now 0, so R(T) is now 40(T-T_C) instead of 400(T-T_C). Plotting this with G(T) yields a new upper steady state temperature of 443.8K.

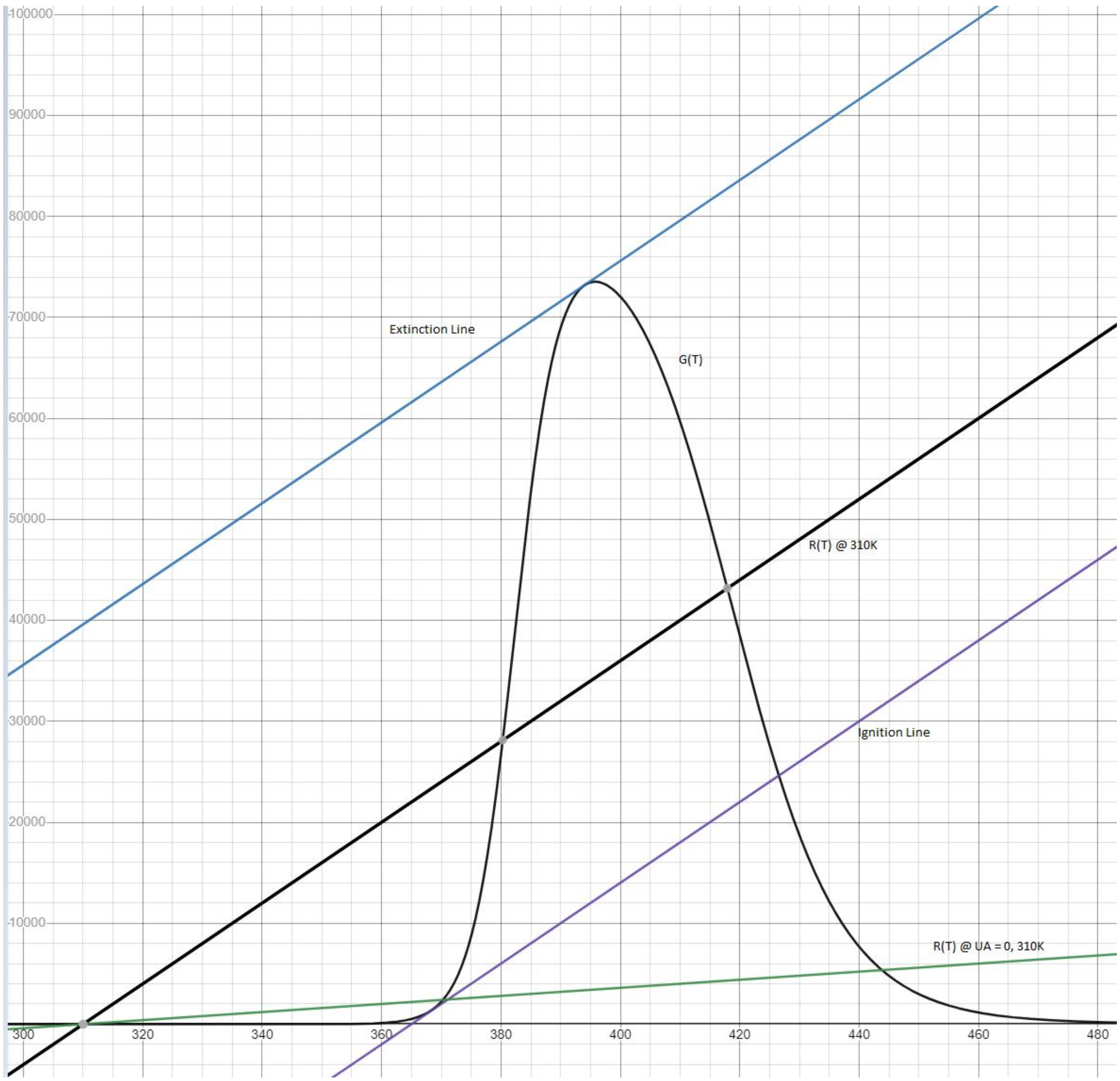


Figure 3: My Desmos plots for parts b, c, d, e, f

2.2 P12-20$_B$

Thought process: Figure A is co-current, B is adiabatic, C is counter-current, D is constant Ta. No pressure drop in Figure 1 so that matches to constant Ta (D). Perfect convergence, straight line between Xe and X in Figure 4 so that matches to adiabatic (B). Figure 1 converges close to the start of the PBR and then Xe and X separate out. This might indicate counter-current flow (C) as that is around when Ta = T. This leaves Figure 2 to match with (A), co-current flow.