Chemical Reaction Engineering—Homework #7

Due: Online submission on Canvas, **Wednesday, March 25, 2020, at 11:59pm.**

No late submissions will be accepted.

Problems that require a numeric answer should have 3 significant figures.
Units, where required, are shown in blue. Please use these units.

Problem 1: Multiple steady states

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

$$A + B \rightarrow 2C$$

V = 1 L

k = 33E+9 exp(-20000(cal/mol)/(RT))
k has units of : (L/(mol*min))

$-\Delta H_R$ = 20 kcal/mol
c_{B0} = 3 mol/L
T_0 = 17 deg C
A = 250 cm^2
$\Sigma\Theta_i\, c_{p,i} * c_{B0}$ = 650 cal/(L*K)

c_{A0} = 20 mol/L
v = 100 cm^3/min
U = 0.1 cal/(cm^2 * min * K)
T_a = 87 deg C

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)?

Problem 2: CSTR with multiple steady states

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.

Information:

$c_{P,I} = 30$ cal/(mol °C)	$c_{P,A} = c_{P,B} = 20$ cal/(mol °C)
$UA = 8000$ cal/(min °C)	$\Delta H_R = -7500$ cal/mol
$k = 6.6 \times 10\text{-}3$ min^{-1} at 350 K	$T_a = 300$K
$E_a = 40{,}000$ cal/(mol K)	$\tau = 100$ min

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?

Problem 3: Propylene oxidation

Propylene oxidation to acetone is believed to proceed via the following elementary steps.

$O_2 + 2\,S \leftrightarrow 2\,O \cdot S$	with rate constants k_1, k_{-1}
$C_3H_6 + O \cdot S \leftrightarrow C_3H_6O \cdot S$	with rate constants k_2, k_{-2}
$C_3H_6O \cdot S \rightarrow C_3H_6O + S$	with rate constant k_3

a. Find the overall rate expression if step 1 is QE.
b. Find the overall rate expression if step 1 and step 2 are QE.
c. Write the apparent rate constant (k_{app}) and the apparent activation energy (E_{app}) for the mechanism in part b if $O \cdot S$ is the MASI.