Chemical Reaction Engineering—Homework #8

Due: Online submission on Canvas, **Wednesday, April 1, 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: Synthesis of TBA

t-Butyl alcohol is used in place of lead additives in gasoline (*Ind. Eng. Chem. Res.* 1988, 27, 2224). t-Butyl alcohol (TBA) is formed over an Amberlyst-15 catalyst by the liquid-phase hydrogenation of isobutene (I). Generally, hydrocarbons, water (W), and solid catalysts comprise the system. Given the following reaction mechanism, derive a rate law for the disappearance of I by using the assumptions in parts a-d.

$I + S \leftrightarrow I \cdot S$	k_1, k_{-1}
$W + S \leftrightarrow W \cdot S$	k_2, k_{-2}
$W \cdot S + I \cdot S \leftrightarrow TBA \cdot S + S$	k_3, k_{-3}
$TBA \cdot S \leftrightarrow TBA + S$	k_4, k_{-4} and $K_{TBA} = k_{-4}/k_4$

a. The surface reaction is rate-limiting. Assume all other steps are QE.

b. The adsorption of isobutane is rate-limiting. Assume all other steps are QE.

c. Eley-Rideal kinetics are followed and the surface reaction is rate limiting. The following mechanism is followed. Assume steps 1 and 3 are QE.

$I + S \leftrightarrow I \cdot S$	k_1, k_{-1}
$I \cdot S + W \leftrightarrow TBA \cdot S$	k_2, k_{-2}
$TBA \cdot S \leftrightarrow TBA + S$	k_3, k_{-3} and $K_{TBA} = k_{-3}/k_3$

d. Isobutene and water are adsorbed onto different sites. The surface reaction is rate limiting and TBA is not on the surface. Assume all other steps are QE. There is also not a need to divide by the total number of sites in the rate expression for this part.

$I + S_1 \leftrightarrow I \cdot S_1$	k_1, k_{-1}
$W + S_2 \leftrightarrow W \cdot S_2$	k_2, k_{-2}
$I \cdot S_1 + W \cdot S_2 \leftrightarrow TBA + S_1 + S_2$	k_3, k_{-3}

Problem 2: External Mass Transfer Limitations in a PBR

The irreversible gas-phase reaction A → B is carried out in an isobaric PBR packed with catalyst particles. The reaction is first order in the concentration of A on the catalyst surface:

$$-r_{AS}' = k'C_{AS}$$

The feed consists of 50 mol % A and 50 mol% inert and enters the reactor at a temperature of 300K. The entering volumetric flow rate is 10 L/s. The relationship between the Sherwood number and the Reynolds number is:

$$Sh = 100\ Re^{1/2}$$

The entering concentration of A is 1.0 M. Assume that the reaction is external mass transfer limited.

a. If the reactor is operating isothermally, what is the catalyst weight necessary for 60% conversion of A? [900 kg]

b. If the reaction is operating adiabatically, what is the catalyst weight necessary for 60% conversion of A? [500 kg]

<u>Additional information:</u>
Kinematic viscosity: 0.02 cm^2/s
Particle diameter: 0.1 cm
Superficial velocity: 10 cm/s
Catalyst surface area/mass of catalyst bed: 60 cm^2/g cat
Diffusivity of A: 0.01 cm^2/s
Heat of reaction: -10000 cal/mol A
Heat capacity of A: 25 cal/(mol K)
Heat capacity of B: 25 cal/(mol K)
Heat capacity of inerts: 75 cal/(mol K)
k′ at 300K = 0.01 cm^3/(g cat *s)
E = 4000 cal/mol