Assignment 6

(Submission deadline-30 Oct 2020, 5 PM)

1. A first order irreversible reaction A → B is carried out in a packed-bed reactor containing spherical catalyst particles of diameter 3.6 mm. The gas-phase velocity is 150 m/s, entering at a temperature of 300 K. The reaction is considered to be externally mass transfer limited under the operating conditions. If the packed-bed is 0.05 m length, what conversion (percentage) can be expected under isothermal conditions.

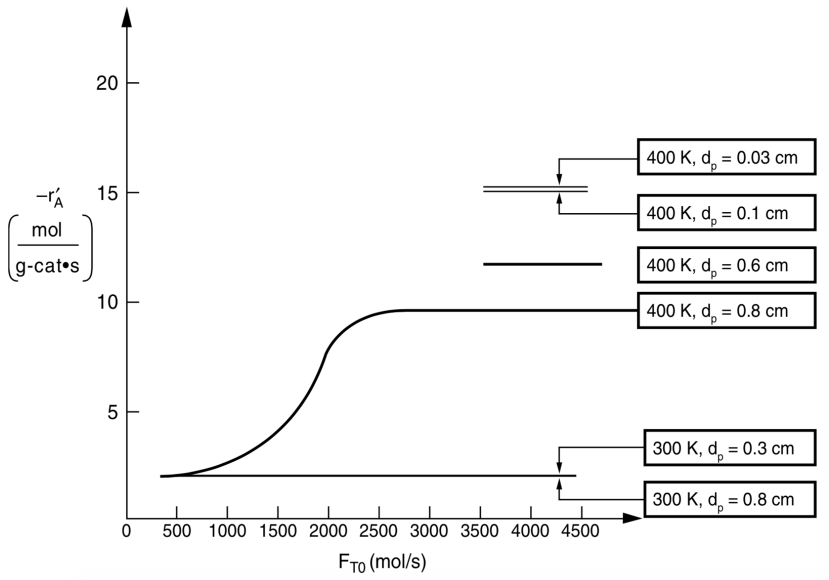
   Data:
   Bed porosity, ϕ = 40%
   Kinematic viscosity at 300 K, $\nu = 4.94\times10^{-5}$ m^2/s
   Diffusivity, $D_{AB} = 1.42\times10^{-4}$ m^2/s

2. Oxygen (pure) is absorbed by xylene in a catalyzed reaction in a mixed-flow reactor. Under constant temperature the following data were obtained.

Stirrer speed (rpm)	*Rate of update of O_2 (mL/hr) for system pressure (abs)*			
	1.2 atm	1.6 atm	2.0 atm	3.0 atm
400	15	31	75	152
800	20	59	102	205
1200	21	62	105	208
1600	21	61	106	207

   (a) What would you conclude about the relative importance of liquid-phase diffusion?
   (b) What is the order of the kinetics of this reaction?

3. The reaction A → B is carried out in a differential packed-bed reactor at different temperatures, flow rates and particle sizes. The results are shown in the figure below.



(a) What regions (i.e conditions, d_p, T, F_{T0}) are external mass transfer-limited?
(b) What regions are reaction rate-limited?
(c) What region is internal-diffusion-controlled?
(d) What is the internal effectiveness factor at T = 400 K and d_p = 0.8 cm?

4. The second-order gas phase decomposition reaction A → B + 2C is carried out in a tubular reactor packed with catalyst pellets <u>0.4 cm</u> in diameter. The reaction <u>is internal diffusion limited</u>. Pure A enters the reactor at a superficial velocity of <u>3 m/s</u>, a temperature of <u>250 °C</u>, and a pressure of <u>500 kPa</u>. Experiments carried out on a smaller pellets where surface reaction is limiting yielded a specific reaction rate of <u>0.05</u> $m^6/(mol.m^2.s)$. Calculate the length of bed necessary to achieve <u>80%</u> conversion.

<u>*Additional information:*</u>
Effective diffusivity (D_e): 2.66×10^{-8} m^2/s
Bed porosity (ϕ): 0.4
Pellet density (ρ_c): 2×10^6 g/m^3
Internal surface area (S): 400 m^2/g.

Some hints:
(i) Use mole balance for PBR for a 2nd order reaction
(ii) Calculate Thiele modulus for 2nd order reaction
(iii) Note that k_2'' is given for 2nd order. Use the relationship $k_{2e} = S\rho_b k_2'$. Note that ρ_b is the bulk density, calculated as: $\rho_b = (1-\phi)\rho_c$
(iv) First ignore the volume change effect on effectiveness factor in your calculations. If you like to include and see the effect, then refer to the paper "*Influence of volume change on gas-phase reactions in porous catalysts*", Journal of Catalysis 4(2), 260 (1965). In this paper an equation is available for effectiveness factor for a 2nd order reaction for very large Thiele modulus:

$$\frac{\eta}{\eta'} = \sqrt{3}\left[\frac{1}{2\epsilon} - \frac{1}{\epsilon^2} + \frac{1}{\epsilon^3}\ln(1+\epsilon)\right]^{1/2}$$

η and η' are effectiveness factor for 'no volume change' and for 'finite volume change' cases, respectively.