CEN 786, Spring 2020
Project 4

The following are all adapted from end-of-chapter problems taken from Rawlings and Ekerdt.

1. Rawlings 7.4:

   The following second-order catalytic reaction is currently carried out in a fixed-bed reactor operating isothermally at 650K:

$$A \rightarrow B \text{ with k} = 4.54 \times 10^7 cm^3 mol^{-1} s^{-1}$$

   Pure A is fed to the reactor and a conversion of 93% is achieved at a pressure of 2.0 atm. The catalyst vendor has changed fabrication procedures and has verified that the intrinsic rate constant listed above is unchanged. Note that the volumetric rate calculated with the above rate constant is the rate per volume of catalyst bed. The following data is available:

Property	Old Catalyst	New Catalyst
Effective Diffusivity	0.0095 $\text{cm}^2\ \text{s}^{-1}$	0.0072 $\text{cm}^2\ \text{s}^{-1}$
Particle Density	1.75 g cm^{-3}	1.79 g cm^{-3}
Bed Density	0.84 g cm^{-3}	0.96 g cm^{-3}
Shape	Sphere	Cylinder
Diameter	0.635 cm	0.480 cm
Length	N/A	0.790 cm

   For this problem, you may assume that the surface concentration is always equal to the concentration of species in the bulk fluid (i.e., external diffusion is very fast), that diffusion in either particle only occurs in the radial dimension, and that there is no pressure drop in the reactor.

   Answer the following questions:

   (a) Determine the mass of the old catalyst formulation used in the reactor.

   (b) Determine if the mass of catalyst needs to be changed for the new catalyst to maintain the same conversion of A and production of B

   (c) If the catalyst mass needs to be changed, what is the mass of new catalyst required?.

2. Rawlings 7.5.

   The following catalytic reaction is conducted in a 0.25 cm spherical pellet.

   $$A + B_2 \rightarrow C$$

   The reaction follows a Langmuir-Hinshelwood mechanism in which the rate determining step is the surface reaction between an adsorbed molecule of A and an adsorbed atom of B. Based on this, one can derive an overall rate expression for this reaction:

   $$r = \frac{k_3 K_1 C_A (K_2 C_{B_2})^{\frac{1}{2}} C_m^2}{1 + K_1 C_A + (K_2 C_{B_2})^{1/2} + K_4 C_C}$$

   The following data is also available.

Parameter	Value	Units
K_1	90,100	$cm^3\ mol^{-1}$
K_2	6,500	$cm^3\ mol^{-1}$
K_4	64,400	$cm^3\ mol^{-1}$
T	523	K
D_A	0.045	$cm^2\ s^{-1}$
C_A	$5.83 \times 10^{-}5$	$mol\ cm^{-3}$
C_{B_2}	$1.40 \times 10^{-}4$	$mol\ cm^{-3}$
C_C	$1.17 \times 10^{-}5$	$mol\ cm^{-3}$
k_3	7.41×10^8	$g^2\ mol^{-1}\ cm^{-3}\ s^{-1}$
C_m	1.8×10^{-5}	$mol\ g^{-1}$

   (a) Determine the concentration of A at the center of the catalyst particle.

   (b) Calculate the effectiveness factor for this catalyst at these concentrations.

3. Rawlings 7.6

   A catalytic reaction that is first order in the concentration of A:

   $$A \rightarrow B$$

   is carried out in a spherical pellet with a 0.20 cm radius. The effective diffusivity of A inside of the pellet is 0.015 $cm^2\ s^{-1}$. The rate of reaction at 398 K is 2.63 $\times$ mol cm^{-3} s^{-1} when the concentration of A is 3.25×10^{-5} mol cm^{-3}. The activation energy for this reaction is 20 kcal mol^{-1}.

   Assuming the diffusivity is independent of temperature, what is the rate of reaction at 448K for the same concentration of A?

4. Rawlings 7.8

   The following first-order, gas-phase catalytic reaction is conduced in a fixed-bed reactor:

$$A \rightarrow B$$

   The rate constant is given by:

$$5.74 \times 10^{13}\ exp\left(\frac{-38,000}{RT}\right)\ \mathrm{s}^{-1}$$

   where the units of R are in cal mol^{-1} K^{-1} and Temperature is in Kelvin. The feed consists of pure A at 1.0 atm at 630K and a molar flowrate of 0.5 mol s^{-1}. The catalyst is a cylindrical shaped pellet with a radius of 0.35 cm and a length of 0.5 cm. The catlyst pellet density is 0.84 g cm^{-3}, and the reactor bed density is 0.52 g cm^{-3}. At 630K, the diffusivity in the pellet is 1.40 $\times$ 10^{-3} cm^2 s^{-1}. The reactor operates isothermally and without a pressure drop.

   (a) For the case where diffusion to the pellet surface is infinitely fast (i.e., the surface concentration is equal to the bulk concentration, calculate the mass of catalyst required to achieve 90% conversion of A)

   (b) For the case where the mass transfer coefficient to the external particle surface is 3.75 m/s, calculate the mass of catalyst required to achieve 90% conversion of A. For this example, you may either apply the flux boundary condition at the catalyst surface or solve the external mass transfer problem separately to find the surface concentration as a function of bulk concentration and apply that surface concentration as your boundary condition.

5. Rawlings 7.9

   Estimate the mass of catalyst required in an isothermal fixed bed reactor for the second order reaction:

$$A \rightarrow B$$

   with $r = k_1 C_A^2$ and $k_1 = 1.21 \times 10^5$ cm^3 mol^{-1} s^{-1}

   The feed is pure A at a molar flowrate of 15 mol s^{-1}, the total pressure is 3.0 atm, and the Temperature is 550K. The reactor achieves 90% conversion of A. The catalyst is a hollow cylinder with an outer diameter of 1.3 cm and an inner diameter of 0.5 cm and a length of 0.7 cm. The pellet density is 0.73 g cm^{-3}, and the bed density is 0.58 g cm^{-3}. The diffusivity of A is 0.008 cm^2 s^{-1}, and you may assume it is constant. You may also assume that the reaction is isothermal, there is no pressure drop, and that bulk and surface concentrations of A are equal.