

**CBE 60546
Fall 2021
Final Exam
12/13/21**

1. Methane oxidation over a palladium catalyst. (100 points)

A 8 cm long, 1 cm internal diameter tube, packed with alumina particles is used as a reactor for the the oxidation of methane. A 5 cm portion of the tube is packed with a catalyst, which is 0.5 wt% Pd on alumina. This is a similar set up to an experiment in the CBE 40459 Lab.

The oxygen mole fraction is kept at 0.3. Helium and methane make up the remaining feed.

The inlet and outlet concentration measurements are made external to the reactor, at 298K and 1 ATM. Inside the reactor is kept at chosen fixed temperatures and (nominally) 1 ATM. The ideal gas law is applicable.

All gases except helium can be assumed to have a heat capacity of $7/2 R$ (~29 J/mol-K). Helium will be close to 21 J/mol/K. The heat of (complete) combustion of methane (at 298 K) is 800 kJ/mol.

These data are for a single pass through the reactor.

Feed Flow (298K, 1 ATM)	Reactor Temp	Inlet Methane mole fraction (298K, 1 ATM)	Exit methane mole fraction (298 K,1 ATM)
1.5 cm ³ /s	505 K	0.01	0.006
1.5 cm ³ /s	515 K	0.01	0.005
1.5 cm ³ /s	525 K	0.01	0.0028

- At 505K, if a first order reaction is assumed, what is the apparent first order rate constant, based on the volume of the reactor packed with catalyst?
- Based on the data in the table, what is a (rough) approximation for the activation energy for this reaction assuming that kinetics are 1st order in methane and that O₂ is in great excess?
- The reactor configuration allows for recycle. If the flow rate in the recycle stream is 10 cm³/s, at 505K, what will the concentration of the exit stream be?
- To keep the reaction zone at 505K, what is the rate of heat removal/addition necessary for the reactor running at a single pass?
- Suppose that there was no cooling? What would be the maximum possible temperature increase for the gas mixture?
- To keep the reaction zone at 505K, what is the rate of heat removal/addition necessary for the reactor running with the recycle stream at 10 cm³/s?
- Suppose that you run the reactor in recycle mode and you find that the rate is more sensitive to temperature change than the data in the table. What could be going on?

Some additional data are available...

Feed Flow (298K, 1 ATM)	Reactor Temp	Inlet Methane mole fraction (298K, 1 ATM)	Exit methane mole fraction (298 K, 1 ATM)
1.5 cm ³ /s	505 K	0.01	0.006
1.5 cm ³ /s	505 K	0.02	0.011
1.5 cm ³ /s	505 K	0.03	0.0162
1.5 cm ³ /s	505 K	0.04	0.0176

Using standard, but simplified assumptions about the reaction, i.e., methane and O₂ both adsorb (O₂ → 2 O on the surface) and the reaction occurs on the surface, the following expression has been proposed for methane oxidation on palladium. Note that *₀ is the total reactive site density on the catalyst surface.

$$\frac{k K_1 [\text{CH}_4] (K_2 [\text{O}_2])^{1/2} [*_0]^2}{(1 + K_1 [\text{CH}_4] + (K_2 [\text{O}_2])^{1/2})^2}$$

- j. What range of reaction orders for methane could be produced by this expression?
- k. Explain if/how the data can be rationalized in terms of this rate expression.
- l. The catalyst particles in the reactor have a diameter of 0.1 cm. At the reaction temperature, the average diffusivity of the gases inside the particle is about 0.002 cm²/s. Is diffusion resistance inside the particles limiting the reaction?
- m. Suppose that the particles are replaced by larger particles of 0.3 cm diameter. Quantify any change in the likely reaction performance of the reactor.
- n. Comment *qualitatively* on the statement: “the pressure inside the reactor is roughly uniform at 1 ATM”.

It turns out that water actually inhibits this reaction and so the kinetic expression needs further modification. You can read about this in a paper by Cybulski, Smeltz, Zvinenvich, Gounder, Delgass and Ribiero in *Chemical Engineering Education* (2016).

2. Power expenditure by a flying insect. (30 points)

The typical power consumption for a flying insect of the size of a “Yellowjacket” is about $1W/g$, almost all of which is used for flying. These creatures weigh about $0.1g$.

On October 10, 2019, during some serious halloween decorating, a wayward Yellowjacket managed to sting Professor McCready on the ear. (Fortunately only part of a possible venom dose.)

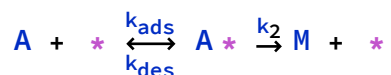


The temperature was $74F$. Most likely the offending insect flew approximately 2 meters from the nest in the ground to the ear.

Such an event could almost certainly not have occurred the previous week when the temperature was $58 F$. Explain quantitatively.

3. Analysis of a sequential reaction (50 points)

Consider a reaction scheme we have seen before for $A \rightarrow M$ using a catalyst on a surface.



It is not too hard to show that the rate for this reaction sequence is

$$r = \frac{k_2 K_{ads} [A] [*]_0}{1 + \frac{k_2}{k_{des}} + K_{ads} [A]}$$

where
$$K_{ads} \equiv \frac{k_{ads}}{k_{des}}$$

- For which values of which parameters could the initial adsorption step be close to equilibrium?
- Adsorption experiments have provided a value of 10 l/mol for K_{ads} , also $k_{des} = 0.1/s$. Use these rate data to “estimate” k_2 and $[*]_0$.

[A] (mol/l)	r mol/(l-s)
2	2
1	1.9
0.01	0.1

- Suppose that an inert, B , is present that can also reversibly adsorb on the surface as



Explain why this inert will affect the observed reaction rate of $A \rightarrow M$.

4. Conversion of fruit juice using an immobilized enzyme catalyst. (50 points)



APPLIED FOOD BIOTECHNOLOGY, 2019, 6 (2): 119-126
 Journal homepage: www.journals.sbmu.ac.ir/afb

Research Article

pISSN: 2345-5357
 eISSN: 2423-4214

Effective Diffusivity Coefficients for Degradation of Pectin in Guava (*Psidium guajava L.*) Pulp Using Immobilized Pectinase

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This paper states the desirability of fruit juices, compared to jellies, jams, etc. (which generally have significant added sugar) from a nutrition standpoint, but that pulpy fruits (e.g., bananas) cannot directly be juiced by squeezing the fruit. In such cases enzymes, such as pectinase, are used to break down the pulp to produce a pourable juice. As “luck” would have it (to enable this exam question!), for ease of processing, the enzyme is often immobilized in porous, spherical beads.

In this problem you need to estimate the effective diffusion coefficient of pectin inside the porous beads in which the enzyme pectinase is immobilized. Only limited information is available. You may need to use some judicious approximation to get an answer.

It is expected that the enzyme catalyzed reaction can be modeled with Monod kinetics as

$$\text{rate} = \frac{V_{\max} C_s}{K_m + C_s}$$

The available data are:

Cs (wt % pectin /volume)	D _p (particle diameter) (mm)	Rate (wt % pectin /volume)/s
1.783	Free enzyme	4.33 X 10 ⁻⁴
1.783	1.9	2.2 X 10 ⁻⁴
1.783	2.5	1.6 X 10 ⁻⁴
1.783	3.4	1.1 X 10 ⁻⁴

Provide an estimate of the diffusion coefficient.