

FINAL EXAMINATION - May 13th, 2020

Chemical Engineering 140

114 Points (+1 for honor code on bCourses quiz)*

Spring 2020

INSTRUCTIONS

You have 205 minutes to complete this exam and submit your answers to Gradescope once downloaded from bCourses (3 hour and 15 minute exam time, 10 minute upload time). If you have trouble uploading to Gradescope, send a pdf file of your solutions to Prof. McCloskey (bmcclosk@berkeley.edu).

Time Penalty: 3 pts. per minute late (e.g., turning in your exam 210 minutes after completing the bCourse quiz will result in a 15 point deduction).

Place name and SID on the first page of your submission.

Open notes and book. Equation solvers (Matlab, Wolfram, Excel, etc.) are allowed.

If you use Matlab or other software to solve a problem, clearly identify the equation, boundary conditions, or other parameters you input into the software and indicate that you used the software to calculate a final answer. No need to submit code with your response.

No internet searches allowed.

Completion on a tablet or on paper is allowable. Please upload your solution in proper order (solution to problem 1 first, problem 2 second, etc.). And on Gradescope, indicate ALL pages that contain ANY part of a solution for each problem.

Show all of your work, keep it legible. BOX ALL ANSWERS if numerical solution or equation is requested.

Read each problem statement carefully, particularly the long ones.

*Extra 5% (5.75 pts) will be added for those who filled out the course survey.

Ideal gas constant:

$R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$; $8.205 \times 10^{-5} \text{ m}^3 \text{ atm mol}^{-1} \text{ K}^{-1}$; $8.314 \times 10^{-2} \text{ L bar mol}^{-1} \text{ K}^{-1}$

Integral Table

$$\int \frac{1}{(x+a)^2} dx = -\frac{1}{x+a}$$

$$\int \frac{1}{a^2+x^2} dx = \frac{1}{a} \tan^{-1} \frac{x}{a}$$

$$\int \frac{x}{a^2+x^2} dx = \frac{1}{2} \ln|a^2+x^2|$$

$$\int \frac{1}{a/x+bx} dx = \frac{1}{2b} \ln(a+bx^2)$$

$$\int x^n dx = \frac{1}{n+1} x^{n+1}$$

$$\int \frac{1}{x} dx = \ln|x|$$

$$\int u dv = uv - \int v du$$

$$\int \frac{1}{ax+b} dx = \frac{1}{a} \ln|ax+b|$$

$$\int e^{ax^2} dx = -\frac{i\sqrt{\pi}}{2\sqrt{a}} \operatorname{erf}(ix\sqrt{a})$$

$$\int e^{-ax^2} dx = \frac{\sqrt{\pi}}{2\sqrt{a}} \operatorname{erf}(x\sqrt{a})$$

$$\int xe^{-ax^2} dx = -\frac{1}{2a} e^{-ax^2}$$

$$\int \ln ax dx = x \ln ax - x$$

$$\int \frac{\ln ax}{x} dx = \frac{1}{2} (\ln ax)^2$$

$$\int \ln(ax+b) dx = \left(x + \frac{b}{a}\right) \ln(ax+b) - x, a \neq 0$$

$$\int \frac{x}{a+bx^2} dx = \frac{1}{2b} \ln(a+bx^2)$$

$$\int e^{ax} dx = \frac{1}{a} e^{ax}$$

$$\int \sqrt{x} e^{ax} dx = \frac{1}{a} \sqrt{x} e^{ax} + \frac{i\sqrt{\pi}}{2a^{3/2}} \operatorname{erf}(i\sqrt{ax}),$$

$$\text{where } \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

$$\int xe^x dx = (x-1)e^x$$

$$\int xe^{ax} dx = \left(\frac{x}{a} - \frac{1}{a^2}\right) e^{ax}$$

$$\int x^2 e^x dx = (x^2 - 2x + 2) e^x$$

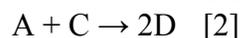
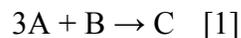
1. [14 pts] Please answer the following True or False questions.
- [2 pt] There is a nonzero enthalpic term for isothermal compression of an ideal gas. (True or False)
 - [2 pt] The Brown number, Br , is defined as

$$Br = \rho V^3 / (w^2 T^8)$$
 where: ρ [=] kg/m^3 , V [=] m/s , w [=] kg , and T [=] K .
 The units of Br are $kg^{-1}K^{-8}s^{-3}$ (True or False).
 - [2 pt] The *bubble-point temperature* of a liquid mixture is the temperature at which the first vapor bubble forms if the mixture is heated at constant volume. (True or False)
 - [2 pt] For liquids and gases, $C_p \approx C_v$ (True or False)
 - [2 pt] ΔH and ΔU are considered state functions. (True or False)
 - [2 pt] For the reaction, $A(g) + B(s) \leftrightarrow 3C(g)$, a decrease in pressure would shift the equilibrium toward more product (to the right). (True or False)
 - [2 pt] The truncated virial equation of state could be recommended to characterize the physical behavior of the nonpolar gas, methane (CH_4). (True or False)

2. [8 pts] Short Answer

- [4 pt] A van der Waals gas is compressed isothermally ($T = 300\text{ K}$) from a molar volume of 2 L/mol to 1 L/mol . If no heat is transferred from or into this closed system, how much work is done on the system? $a = 3.64\text{ L}^2\text{ bar mol}^{-2}$, $b = 0.04267\text{ L mol}^{-1}$. (*Hint: Think about the First Law of Thermodynamics*). Please leave answer in units of L bar mol^{-1}

- [4 pt] The following reactions occur in a vessel:



3 mol of A are initially charged into the vessel. If 1 mol of A remains and 1 mol of D is produced, what is the selectivity of species C over species D?

3. [20 pts] 1.00 mol/s of a mixture of liquid toluene ($z_T = 0.4$; **BP**: 110 °C), benzene ($z_B = 0.15$; **BP**: 80.1 °C), and o-xylene ($z_X = 0.45$; **BP**: 144 °C) are fed into a flash tank, which operates at a total system pressure, P , of 800 mm Hg. The vapor effluent exits the flash tank at $V = 0.3$ mol/s and is in equilibrium with the exiting liquid effluent. For the following problem, assume an ideal solution (e.g. vapor-phase effluent behaves as an ideal gas). **Note**: BP means “boiling point,” z_i is the mol fraction of species i in the feed.

Antoine’s Equation data for benzene, toluene, and o-xylene:

$\log_{10} P_{\text{sat}} \text{ (mm Hg)} = A - B/(T+C)$, where T is in °C

Benzene: $A = 6.89272$, $B = 1203.531$, $C = 219.888$

Toluene: $A = 6.95805$, $B = 1346.773$, $C = 219.693$

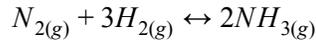
O-xylene: $A = 7.00154$, $B = 1476.393$, $C = 213.872$

- a. [2 pts] Which component dominates in the liquid effluent? Why?

Using appropriate mass balances and an equation solver, find the following:

- b. [10 pts] The temperature, T , of the vapor and liquid effluent.
- c. [8 pts] The molar composition of the vapor effluent and liquid effluent.

4. [39 Points] Questions start on next page. You are helping to design an ammonia synthesis plant. The plant owners want to use the Haber-Bosch Process, where the reaction:



will be carried out in a tubular PBR over an iron catalyst at a pressure of 10 bar. For this problem, it is safe to assume that the PBR temperature is uniform and 400 °C. The PBR is oriented such that it is level with the ground, and for safety purposes, it will be constructed with very rigid walls. Your colleague believes that this reaction will produce a tremendous amount of heat, and they want to use a heat exchanger filled with steam to transfer this heat from the reactor to other parts of the plant to preheat the reactants. The heat exchanger encloses the PBR and will be in intimate contact, such that we can assume no heat generated in the reactor is lost to the environment surrounding the heat exchanger/reactor (see diagram below).

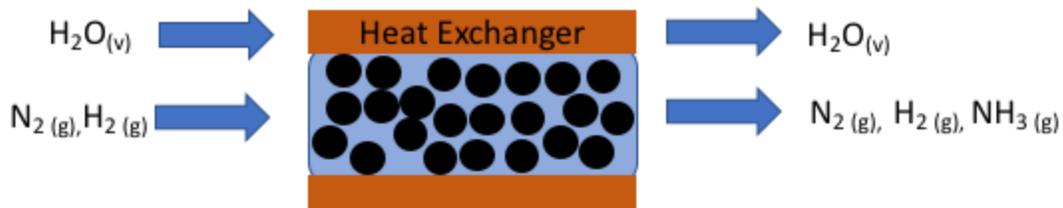


Figure 1: Cross-section of a tubular PBR packed with Fe catalyst particles and fully enclosed by a steam heat exchanger

You may find the following information useful in planning out the design of this system:

Material	\hat{H}_f° * [kJ/mol]	\hat{H} (400°C) ** [kJ/mol]	a x 10 ³	b x 10 ⁵
H ₂	0	10.89	28.84	0.00765
N ₂	0	11.15	29.00	0.2199
NH ₃	-46.2 (g) -67.2 (l)	30.61 (g)	35.15	2.954

* At 25 °C, 1 bar.

** Referenced to \hat{H} of each gas at 25 °C, 1 bar.

Where $\hat{C}_p(T) = a + bT$ [=] $\frac{kJ}{mol K}$

\hat{H} [kJ/kg] for superheated steam at various temperatures and relevant pressures, referenced to liquid water at 0 °C:

	200°C	300°C	400°C	500°C	600°C	700°C
1 bar	2875	3074	3278	3488	3705	3928
10 bar	2827	3052	3264	3478	3697	3923

- (a) [5 pts] Before you get started designing the heat exchanger, you want to be sure that it is even necessary. Is your colleague correct; will this reaction produce heat? If so, how much (in kJ/ mol N₂) at standard conditions (defined for this problem as 25 °C, 1 bar)? If it does produce heat, your colleague wants to lower the reactor temperature as much as possible to shift the reaction further toward ammonia production. Is this a good idea? Why or why not?
- (b) [5 pts] To properly design the heat exchanger, you need to account for all possible energy losses in the system. Neglecting friction, and without doing any calculations, what is the overall energy balance of the PBR once it has reached steady-state operation? What about the heat exchanger? How are these 2 energy balances connected?
- (c) [5 pts] The PBR is sized such that the outlet percent conversion of N₂ is 50%. Assuming a stoichiometric feed of N₂ and H₂ at 400 °C and 10 bar, what is the necessary feed rate of each species to produce 100 mol NH₃/hr?
- (d) [10 pts] If the reactor feed and outlet stream are at 400 °C and 10 bar, and using the conversion and production rates provided in part c, how much heat will be produced in kJ/ hr (i.e., what is ΔH_{rxn} at 400 °C)? Pressure effects can be assumed to be negligible.
- (e) [10 pts] Your colleague also suggests that 5 kg/hr of superheated steam entering at 10 bar and 200°C and leaving at 1 bar is sufficient to remove all of the heat from the reactor. Are they correct? *Hint:* consider what the maximum outlet temperature of the steam could be given the operation of the reactor. What is the minimum flow rate of steam needed (in kg/hr) to ensure all of the heat generated in the reactor is removed?
- (f) [4 pts] The temperature of the heat exchanger can be approximated as the linear average of the inlet and outlet steam temperatures, and the heat exchanger is designed to have an average heat transfer coefficient between it and the reactor of $h = 0.05 \text{ kW m}^{-2} \text{ K}^{-1}$. Assuming that the outlet steam temperature is the temperature of the reactor, what is the necessary contact surface area needed between the heat exchanger and reactor?

5. [33 pts] Transient filling of a tank with compressed gas.

A 100 m³ rigid tank at 25 °C initially contains 1 atm of argon (MW= 40 g/mol). I want to know how long it will take to fill the tank with an additional 1000 kg of argon. Assume for this problem isothermal operation (25 °C). The inlet valve to the tank operates in a way such that when it is opened, the flow rate into the tank is inversely proportional to the pressure of the tank, i.e., $\dot{n} = k/P$, where \dot{n} is in mol/s, P is the pressure in the tank (in atm), and k is given by the valve manufacturer as 50 (mol atm)/s. Argon can be treated as an ideal gas under these conditions (ideal gas constant provided on the first page). All pressures are absolute. Integral identities from the table on the second page will be valuable here.

- [3 pts] What is the final pressure, in atm, of the tank assuming no leaks occur and the 1000 kg of Ar is added isothermally?
- [5 pts] Set up, but do not solve, a differential equation that describes the accumulation of either mols or kg of Ar in the tank as a function of time. Your answer should only contain constants and the total moles of gas in the tank at any given time, $N(t)$. State the initial condition.
- [5 pts] Integrating your answer from part b, how long, in seconds, does it take to fill the tank with 1000 kg Ar?

Immediately after transferring the 1000 kg of Ar to the tank, I notice that the pressure gauge reads 6.8 atm (absolute), which is below the value I expected (as calculated in part b). I suspect that the tank is leaking. It is known that any leak rate will be proportional to the pressure in the tank, so $\dot{n}_{leak} = \alpha P$, where α is proportionality constant related to the size of the leak (ideally, $\alpha = 0$ mol s⁻¹ atm⁻¹).

- [5 pts] Set up a new mass or mol balance for Ar in the tank during the filling process, including the leak. What are the initial *and* final conditions for this balance?
- [9 pts] Integrate this balance and solve the resulting nonlinear equation to find the value for α (in mol s⁻¹ atm⁻¹).
- [6 pts] Using the value of α calculated in part f., from the end of filling (i.e., when the inlet valve is shut off), how long would it take to lose an additional 500 kg of Ar from the leak? If you can't find a value for α in part f., just use 1 mol/(s atm).