

CHE 4200 - Product and Process Design

Fall 2018

MIDTERM

This is a closed book and notes examination; one $8\frac{1}{2} \times 11$ inch page of notes (one side only) is allowed. **Please print your name as indicated below and on the last page. Please do NOT write your name or initials anywhere else on the exam except those two noted locations.**

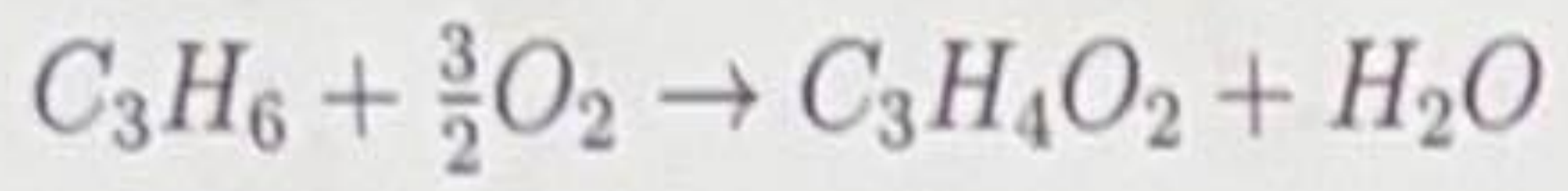
Read all questions carefully; answer them concisely, neatly, and clearly. Define any notation that you introduce. Please show your work clearly. It should be clear to Professor Durand that you understand what you are doing. Show all work on these pages. Use the spaces below the questions and the back of the sheets to show your work. Please use at least 2 significant figures after the decimal point when you are solving numerical problems so that Professor Durand can follow your work. Point values in the left-hand margins are based on 100 points total for the exam.

Good Luck!

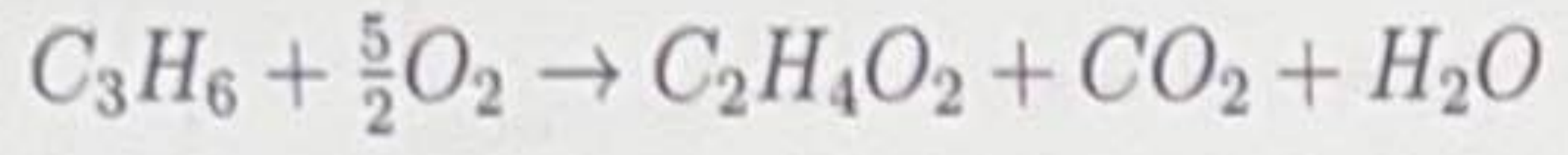
Name:

Neha Bhagirath

40 pts. 1. Your company has learned of a new demand for 60 MM lb/yr of $C_3H_4O_2$. You are assessing the viability of producing this product via the following desired reaction:



However, the following undesired side reaction is also known to occur:



Consider that 50 mol% of the C_3H_6 entering the reactor is converted to products, with 80% of the C_3H_6 that is converted to products reacting in the desired reaction, and 20% of the C_3H_6 that is converted to products reacting in the undesired reaction. Consider 330 days of operation per year and assume that the ratio of the molar flow rate of O_2 entering the reactor to the molar flow rate of C_3H_6 entering the reactor is 7:1. Find the flow rates, in lb/hr, of all species entering and leaving the reactor, of all fresh feeds to the process, and of all recycle streams (assuming that any unreacted reactants are fully recycled).

Use the following table of molecular weights:

$$1 \frac{g}{mol} = 1 \frac{lb}{lbmol}$$

Table 1: Molecular weights.

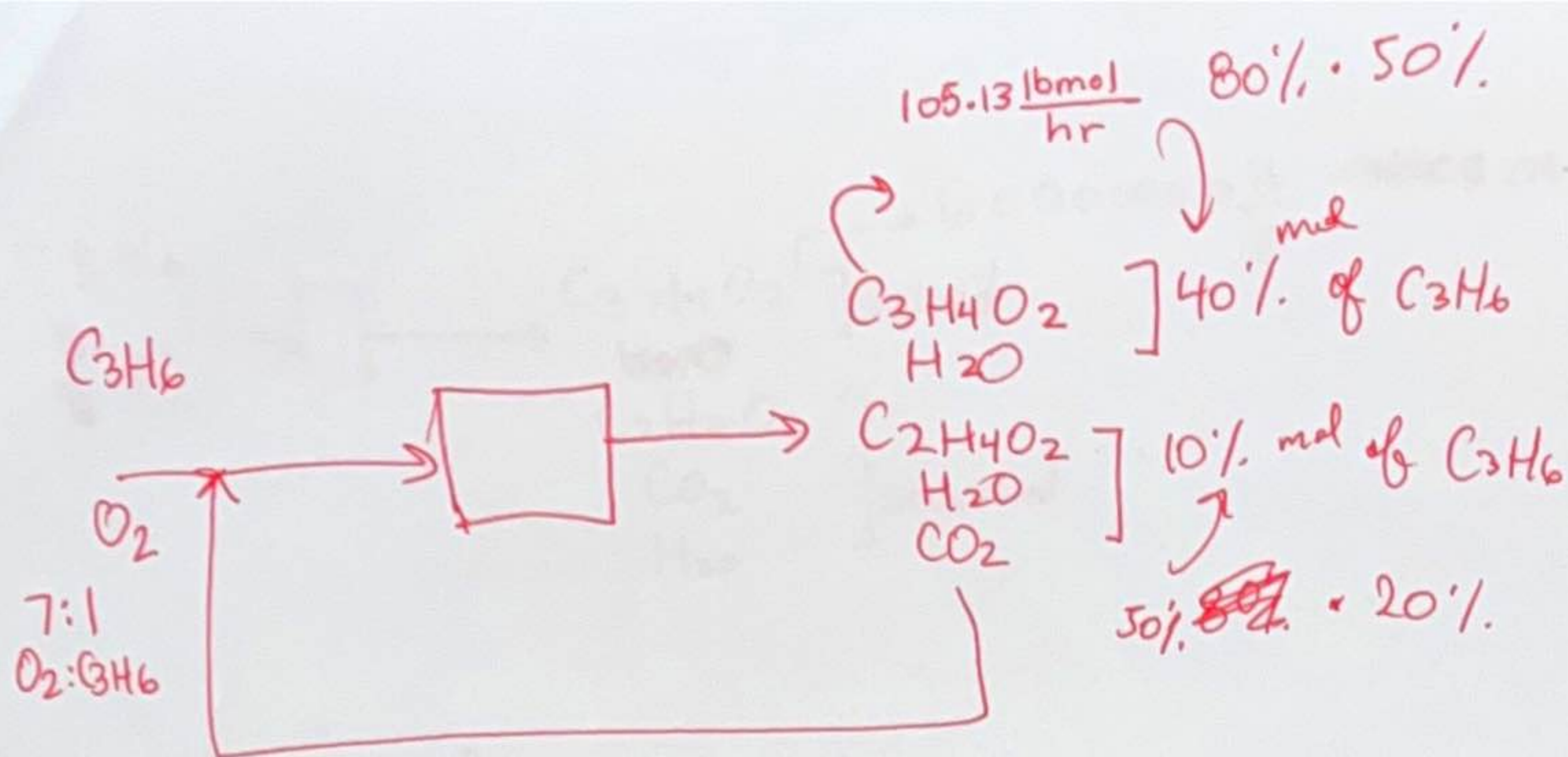
Species	Molecular Weight (g/mol)
C_3H_6	42.08
O_2	32
CO_2	44.01
H_2O	18.01
$C_3H_4O_2$	72.06
$C_2H_4O_2$	60.05

- 1) 4
- 2) 4
- 3) 4
- 4) 4
- 5) 4
- 6) 1
- 7) 1
- 8) 4
- 9) 4
- 10) 4

$$C_3H_4O_2 \rightarrow 60,000,000 \frac{lb}{yr}$$

$$6001.063152 \times \dot{m}_{O_2 out} = 69932.476$$

34/40



$C_3H_4O_2 \text{ out} = H_2O \text{ out} = \text{Stoichiometric amounts} = 105.13 \frac{\text{lbmol}}{\text{hr}}$
From ~~rxn~~ reaction 1

$C_3H_4O_2 \text{ out} = 105.13 \frac{\text{lbmol}}{\text{hr}} \cdot 72.06 \frac{\text{lb}}{\text{lbmol}} = 7575.6678 \frac{\text{lb}}{\text{hr out}}$

$H_2O \text{ out from reaction 1: } 105.13 \frac{\text{lbmol}}{\text{hr}} \cdot 18.01 \frac{\text{lb}}{\text{lbmol}} = 1893.3913 \frac{\text{lb}}{\text{hr out}}$

40% mol of ^{C₃H₆ reacted} C₃H₄O₂ out is $105.13 \frac{\text{lbmol}}{\text{hr}}$ (which is C₃H₄O₂ out)

100% mol C₃H₆ into reactor

$100\% \text{ mol } C_3H_6 \text{ into reactor} = \frac{105.13}{4} \times 10 = 262.825 \frac{\text{lbmol}}{\text{hr}}$ in $\cdot 42.08 \frac{\text{lb}}{\text{lbmol}} = 11059.676$

$O_2 \text{ into reactor} \rightarrow 7 \cdot 262.825 = 1839.775 \frac{\text{lbmol}}{\text{hr}} \cdot 32 \frac{\text{lb}}{\text{lbmol}} = 58872.8 \frac{\text{lb}}{\text{hr}}$ into reactor

50% unreacted C₃H₆ in recycle $\rightarrow 262.825 \cdot 0.5 = 131.4125 \frac{\text{lbmol}}{\text{hr}} \cdot 42.08 \frac{\text{lb}}{\text{lbmol}} = 5529.838$

10% mol of C₃H₆ into reactor goes to CO₂, H₂O, C₂H₄O₂ $\frac{\text{lb}}{\text{hr}}$ recycle stream out of reactor

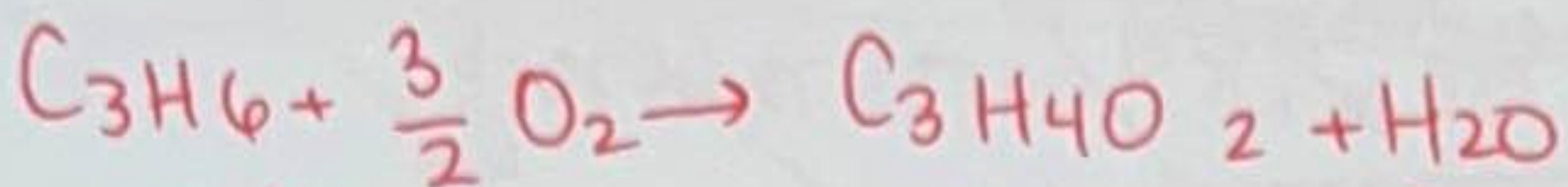
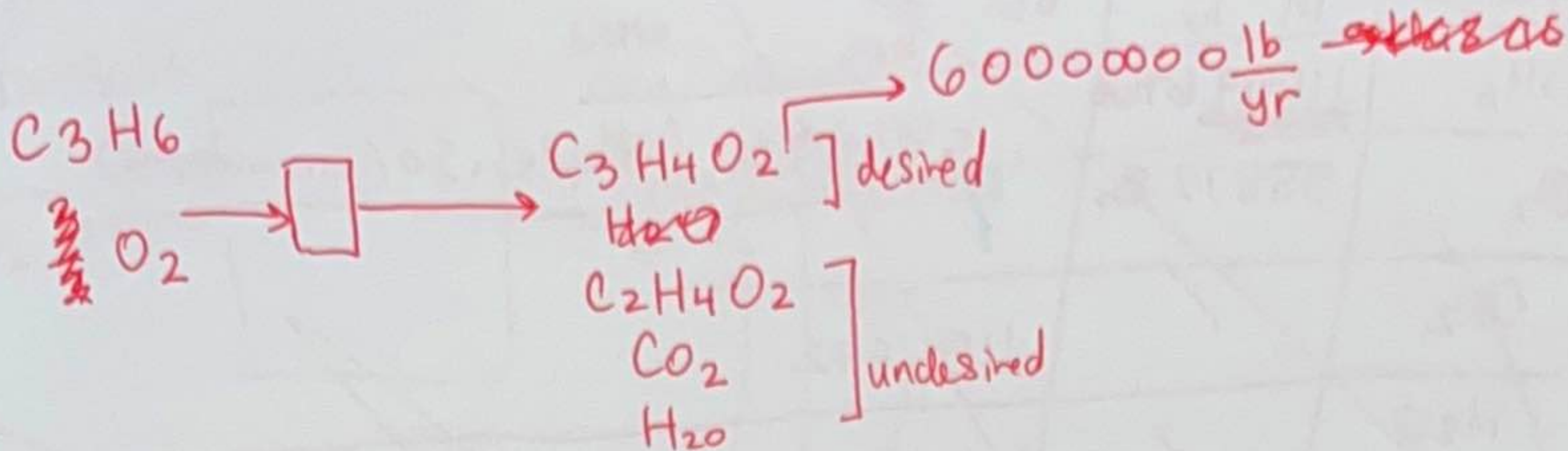
$.10 \cdot 262.825 = 26.2825 \frac{\text{lbmol}}{\text{hr}}$

CO₂ $\rightarrow 26.2825 \frac{\text{lbmol}}{\text{hr}} \cdot 44.01 \frac{\text{lb}}{\text{lbmol}} = 1156.692 \frac{\text{lb}}{\text{hr out}}$

H₂O $\rightarrow 26.2825 \frac{\text{lbmol}}{\text{hr}} \cdot 18.01 \frac{\text{lb}}{\text{lbmol}} = 473.347 \frac{\text{lb}}{\text{hr out}} + 1893.39 \frac{\text{lb}}{\text{hr from rxn 1 out}} = 2366.737 \frac{\text{lb}}{\text{hr out}}$

C₂H₄O₂ $\rightarrow 26.2825 \frac{\text{lbmol}}{\text{hr}} \cdot 60.05 \frac{\text{lb}}{\text{lbmol}} = 1578.26 \frac{\text{lb}}{\text{hr out}}$

C₃H₆ feed fresh $\rightarrow 11059.676 - 5529.838 = 5529.838 \frac{\text{lb}}{\text{hr}}$ in (w/o recycle)



50%
converted

80%

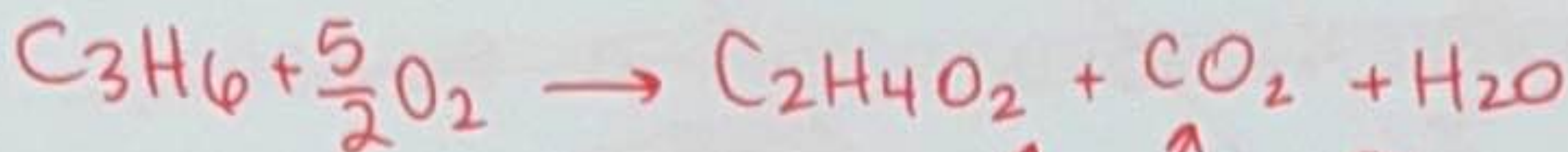
80%

of
50%

of
50%

= 40%

= 40%



20%

of
50%

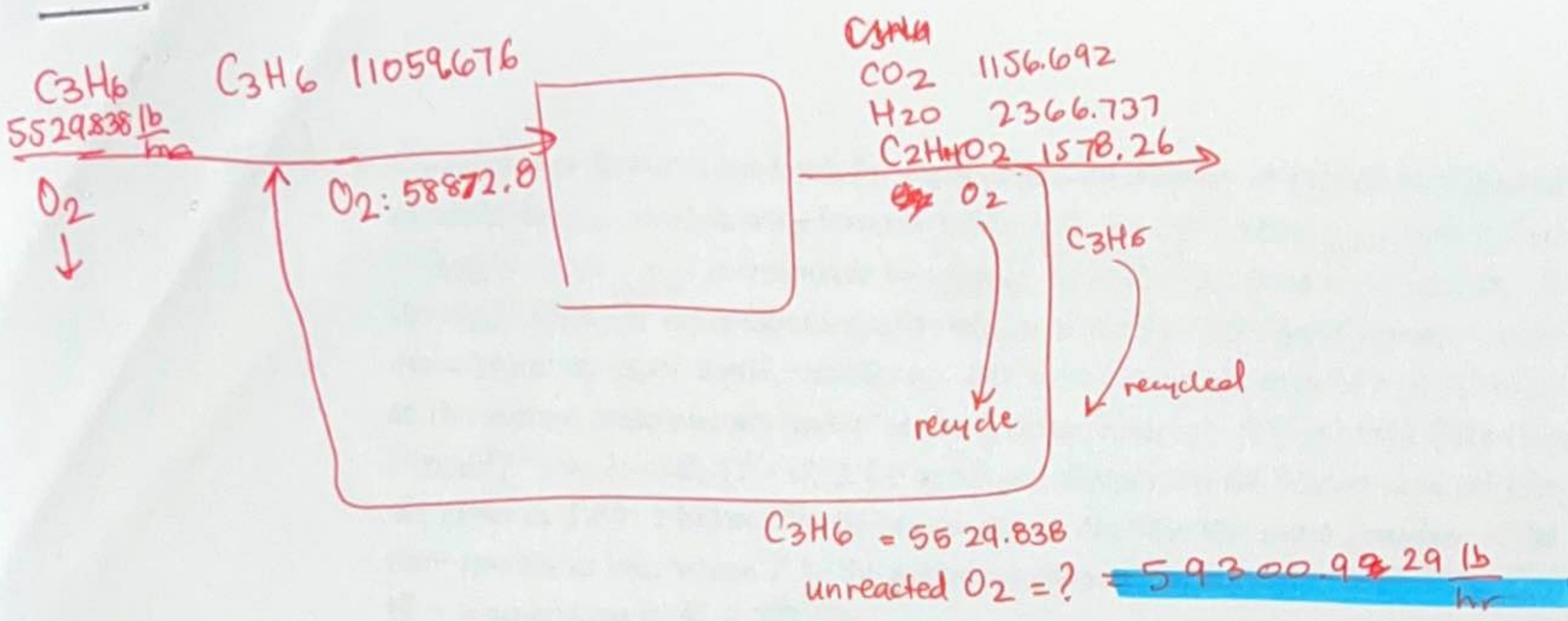
$$\frac{60000000 \frac{lb}{yr}}{330 \text{ days}} \times \frac{1 \text{ yr}}{330 \text{ days}} \times \frac{1 \text{ day}}{24 \text{ hrs}} \times \frac{1 \text{ lb mol}}{7206 \text{ lb}} = 105.13 \frac{\text{lb mol}}{\text{hr}}$$

$C_3H_4O_2$ out
 and H_2O out
 \downarrow
 $105.13 \frac{\text{lb mol}}{\text{hr}} \times 159 \frac{\text{lb}}{\text{lb mol}}$

105.13 * is 40% that is converted,

$$1 \text{ g/mol} = 1 \frac{\text{lb}}{\text{lb mol}}$$

(all lb/hr)



Mass balance

~~5529.838 + O₂ in w/o recycle = 1156.692 + 2366.737 + 1578.26~~

~~O₂ →~~

For every 1 mol C₃H₆ reacted
 For every 5/2 mols O₂ reacted, 1 mol CO₂ is made

~~2628 lbmol/hr~~ of CO₂ are made = ~~10.512 mols~~

~~5/2~~

Mass balance on recycle point

~~(5529.838 + O₂) + (5529.838 + O₂) = 58872.8 + 11059.676~~

~~O₂ = 29436.4~~

Reactor MB

11059.676 + 58872.8 = 1156.692 + 2366.737 + 1578.26 + (O₂ ~~react~~ recycle)

recycle = (5529.838 + O₂) ⇒ O₂ = 59300.929 lb/hr

getting negative O₂ mols into fresh feed

25 pts ✓ 2. Consider that Raoult's law holds for vapor-liquid equilibrium of a mixture of benzene and toluene (i.e., the following formula holds: $y_i P = x_i P_i^{sat}$, where $i = 1$ corresponds to benzene and $i = 2$ corresponds to toluene, x_i is the mol fraction of species i in the liquid phase at vapor-liquid equilibrium, y_i is the mol fraction of species i in the vapor phase at vapor-liquid equilibrium, P_i^{sat} is the vapor pressure of pure species i at the system temperature, and P is the system pressure). The Antoine Equation ($\log_{10}(P_i^{sat}) = A_i - (B_i/(T + C_i))$), for which the parameters for benzene and toluene are given in Table 2 below, can be considered to describe the vapor pressure of the pure species in bar, where T is the system temperature in Kelvin (temperature in $^{\circ}C =$ temperature in $^{\circ}F + 273.15$).

Table 2: Antoine equation parameters for benzene and toluene.

i	A_i	B_i	C_i
1	4.73	1660.65	-1.46
2	4.08	1346.38	-53.51

15 pts. (a) Would a flash drum at 116 C and 2 bar be a reasonable option for separating benzene and toluene if it is desired to obtain both in a pure form? Why or why not? Justify based on a computation of the mol fractions of the species in the vapor and liquid phases at the proposed flash drum operating conditions. Your answer must include both a computational component and a text-based justification that uses the computational result to make a design judgment.

(See attached page)

$$\log_{10} P_1^{\text{sat}} = A - \frac{B}{T+C}$$

$A = 4.73$
 $B = 1660.65$
 $C = -1.46$
 $116 + 273.15 = 389.15$

benzene $P_1^{\text{sat}} = 2.79$ bar

$$\log_{10} P_2^{\text{sat}} = A - \frac{B}{T+C}$$

$A = 4.08$
 $B = 1346.38$
 $C = -53.51$
 $116 + 273.15 = 389.15$

toluene $P_2^{\text{sat}} = 0.6686$ bar
 1.171 bar

$$y_1 + y_2 = 1 \quad X_1 + X_2 = 1$$

$$y_1 P = X_1 P_1^{\text{sat}}$$

$$y_2 P = X_2 P_2^{\text{sat}}$$

If $P = 2$ bar

If $P = 2$ bar

$$(1 - y_2) P = (1 - X_2) P_1^{\text{sat}}$$

$$y_2 P = X_2 P_2^{\text{sat}}$$

But then the liquid stream ~~is~~ has almost equimolar amount so this flash would not be a good option

$$\textcircled{1} 2 - 2y_2 = 2.79 - 2.79X_2$$

$$\textcircled{2} 2y_2 = 1.171X_2$$

$$y_2 = 0.5855X_2$$

Sub in to $\textcircled{1}$

$$2 - 2(0.5855X_2) = 2.79 - 2.79X_2$$

$$2 - 1.171X_2 = 2.79 - 2.79X_2$$

$$X_2 \quad 2 - 2.79 = -1.619X_2$$

$$+0.79 = 1.619X_2$$

$$X_2 = 0.48$$

$$X_1 = 1 - X_2 = 0.52$$

$$y_2 = 0.5855X_2 = 0.28$$

4

$$y_1 = 1 - y_2 = 0.71896$$

If there are subsequent separations occurring, the vapor fraction could be separated further ~~but~~ ~~to do so~~ ~~because~~ since the vapor stream does have 0.718 mol fraction benzene.

Would not

A flash drum ~~would~~ be a reasonable option at this P and T because ~~there are~~ in the vapor stream there is a fraction of 0.28 mol toluene and 0.718 benzene.

however there is 0.48 mol fraction toluene in the liquid stream, and 0.52 mol fraction benzene in the liquid stream. This flash did not help in separating the components to a high degree. ~~So if one stage separation is so~~ So if no subsequent separations are occurring, it is not a good option because the vapor or liquid stream both ~~is not~~ are not very pure in one component.

10 pts.

(b) Now consider that you would like to pump toluene at 10 C and 1.01325 bar to 20 bar. Consider that the manufacturer has provided the required net positive-suction head (NPSH) as 5 ft. Is the available NPSH greater than the manufacturer's value? Consider that the head increase is due only to a change in pressure across the pump, and that the density of the toluene at the pump inlet conditions is 48.3 lb/ft³. (Relevant conversion factors: 1 bar = 2088.55 psf)

NPSH = liquid P @ inlet - vapor pressure as head
 $1.01325 \times 2088.55 = 2116.223 \text{ lb/ft}^2$

NPSH = $\frac{\text{Suction pressure} - \text{vapor pressure}}{\text{liquid density}}$
 → Antoine's at 10°C → 283.15K
 $33.4168 \frac{\text{lb}}{\text{ft}^2}$

$48.3 \frac{\text{lb}}{\text{ft}^3}$
 NPSH = 43.12 ft

NPSH > 5ft?

P = 1.01325 bar

T = 10 + 273.15 = 283.15K

$\log_{10} P_1^* (\text{toluene}) = 4.08 - \frac{1346.38}{283.15 - 53.51}$

$P_1^* = 0.016 \text{ bar} \times 2088.55 = 33.4168 \text{ psf } \frac{\text{lb}}{\text{ft}^2}$

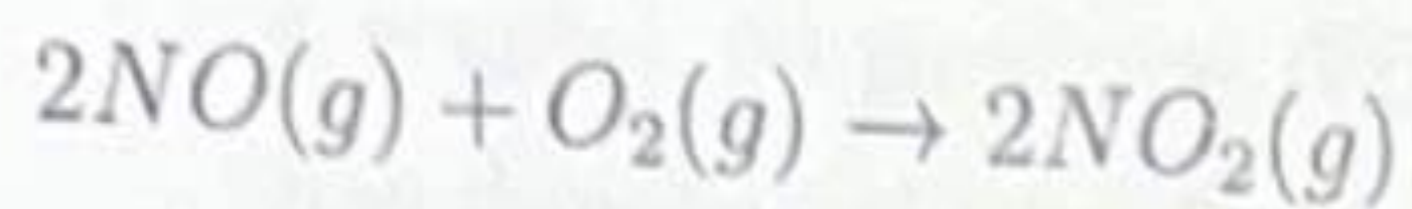
1) 2
 2) 2
 3) 1
 4) 1
 5) 1
 6) 3

10/10

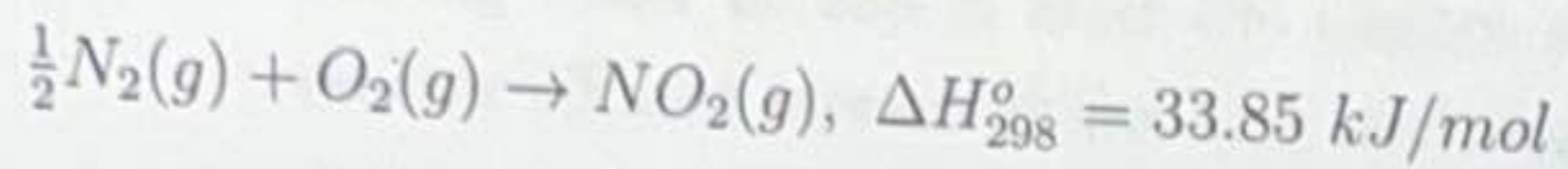
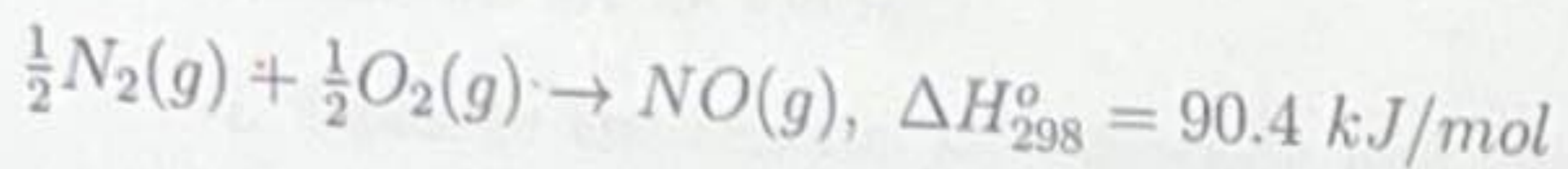
$\frac{\text{lb}}{\text{ft}^2} \div \frac{\text{lb}}{\text{ft}^3} \rightarrow \frac{\text{lb}}{\text{ft}^2} \cdot \frac{\text{ft}^3}{\text{lb}} \rightarrow \text{ft}$

∴ Yes, the available NPSH (43.12 ft) is greater than the manufacturer's value of 5ft.

10 pts. ✓ 3. Consider the following reaction:



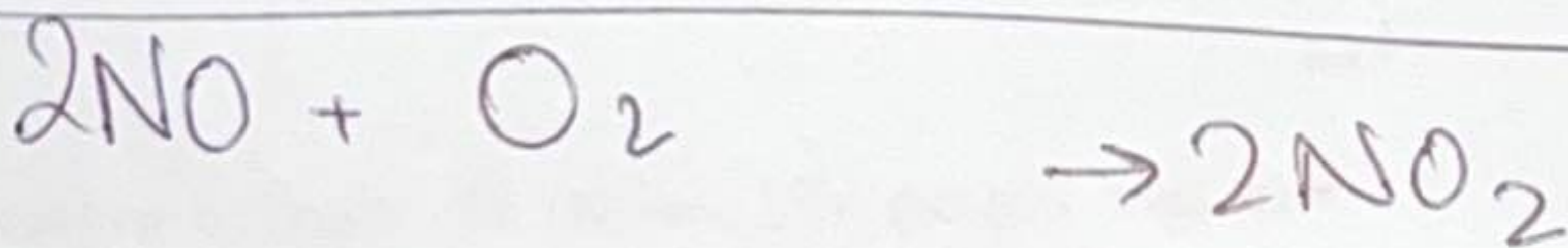
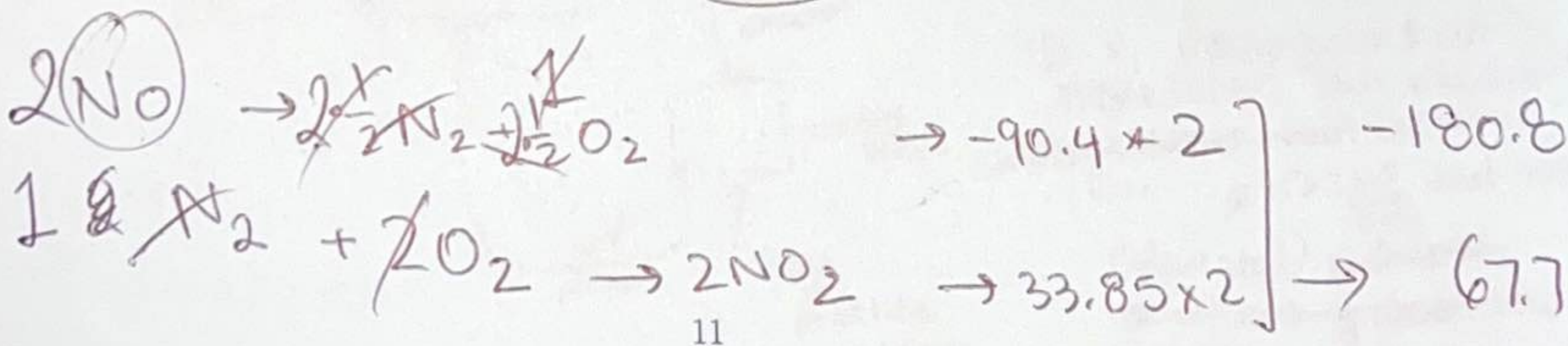
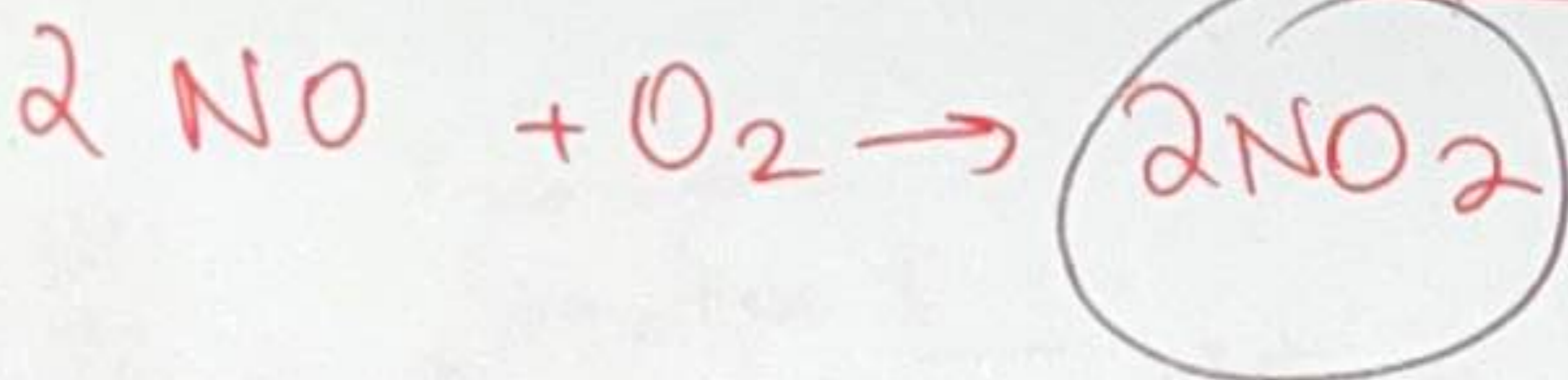
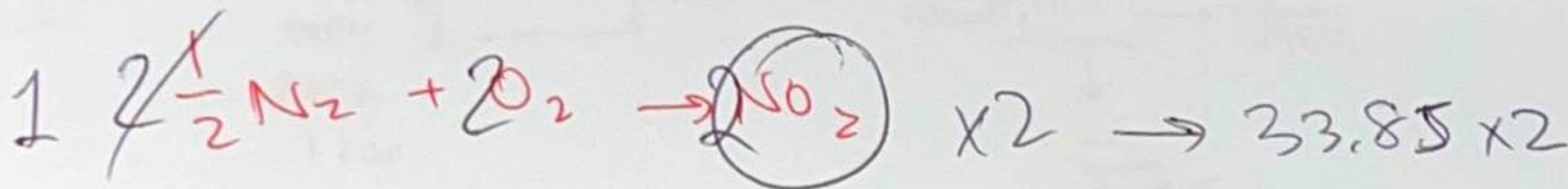
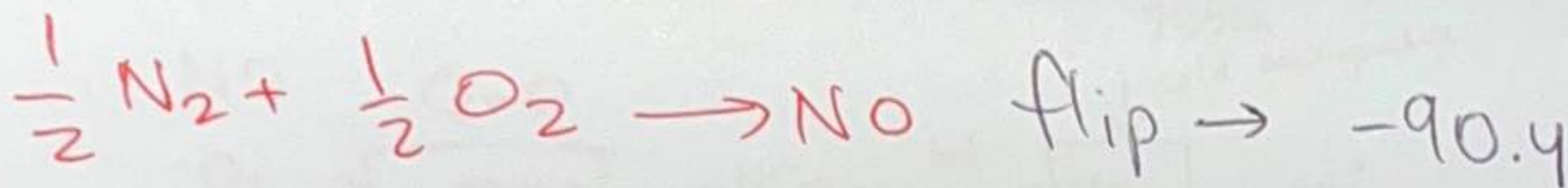
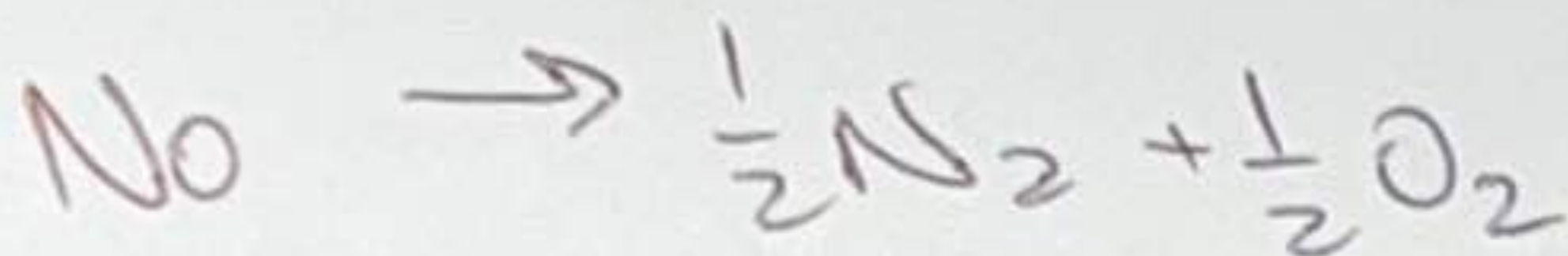
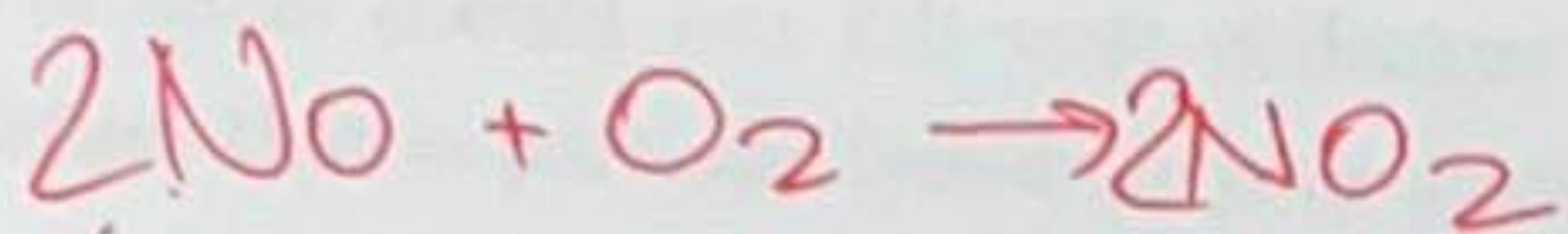
Consider the following formation reactions:



4/4

4 pts.

(a) Compute the standard heat of reaction for the reaction which produces NO_2 from NO and O_2 .



-113.1 kJ/mol

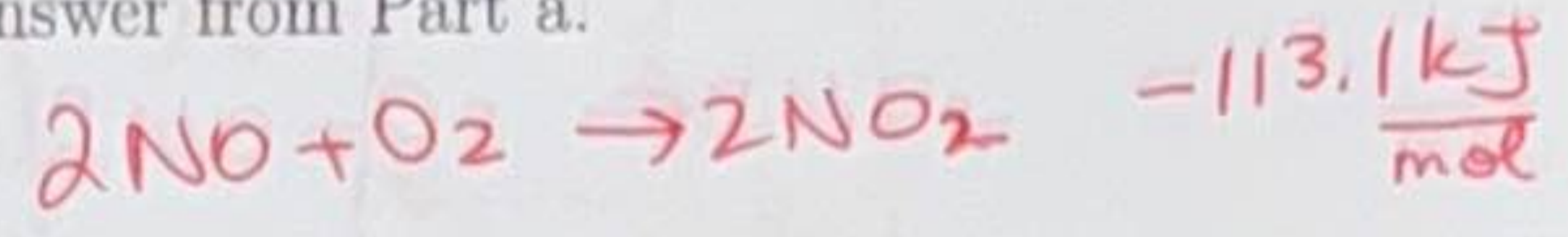
6 pts.

6/6

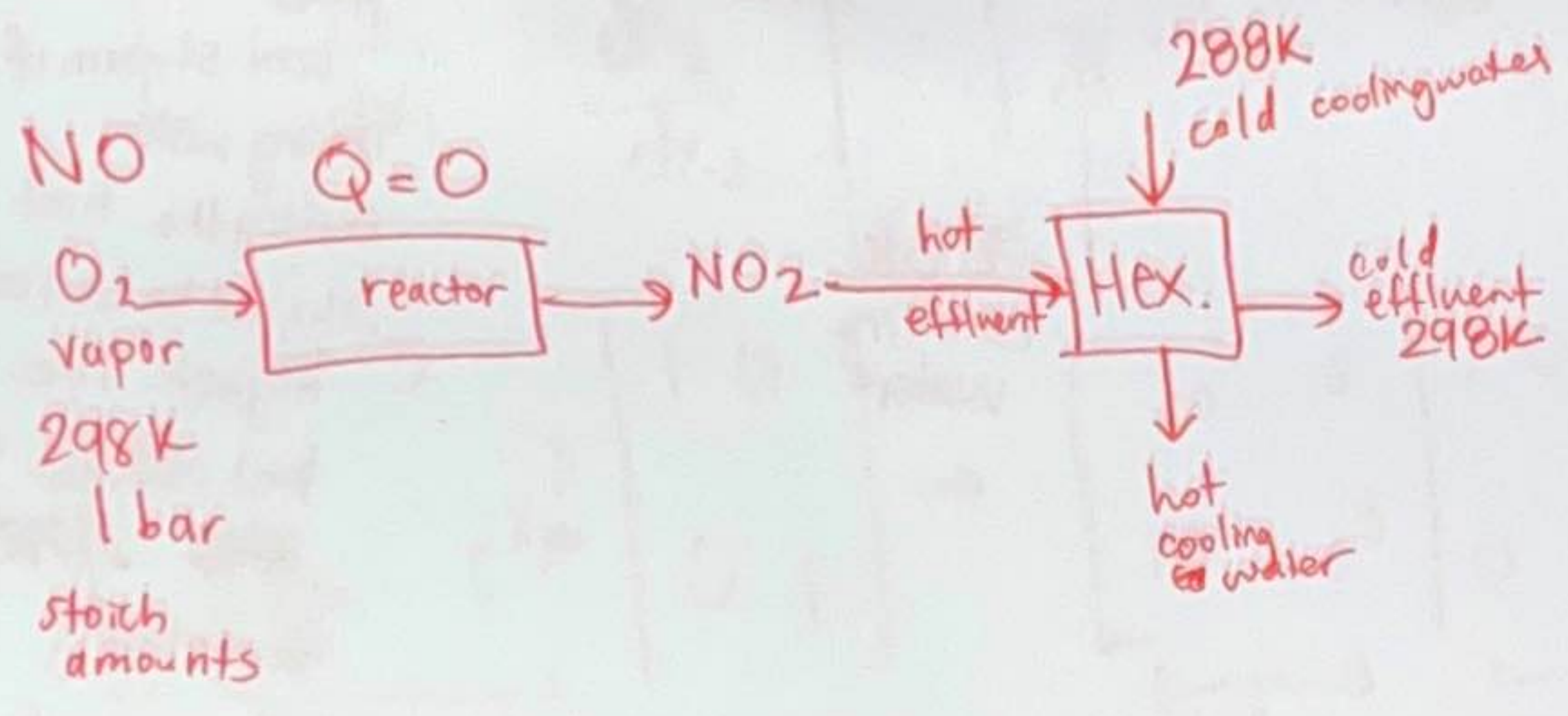
(b) Your colleague is designing a process in which NO and O₂ are fed in stoichiometric amounts in the vapor phase at standard conditions (298 K and 1 bar) to a reactor to produce NO₂ according to the reaction in Part a. This colleague has developed two design alternatives for obtaining a stream at ~~100 F~~ ^{298K} after the reaction occurs, but is having difficulty deciding which makes sense. The two alternatives are as follows:

- i. Operate the reactor adiabatically and add a heat exchanger supplied by cooling water at 288 K after the reactor so that the temperature of the reactor effluent stream at the heat exchanger outlet is at 298 K.
- ii. Operate the reactor such that some of the reactor contents are drawn off, passed through a heat exchanger where the fluid on the other side of the exchanger is high pressure steam, and returned to the reactor such that the reactor effluent stream is at 298 K.

Which of these should you tell your colleague to use? Provide a thorough justification that is partially based on your answer from Part a.

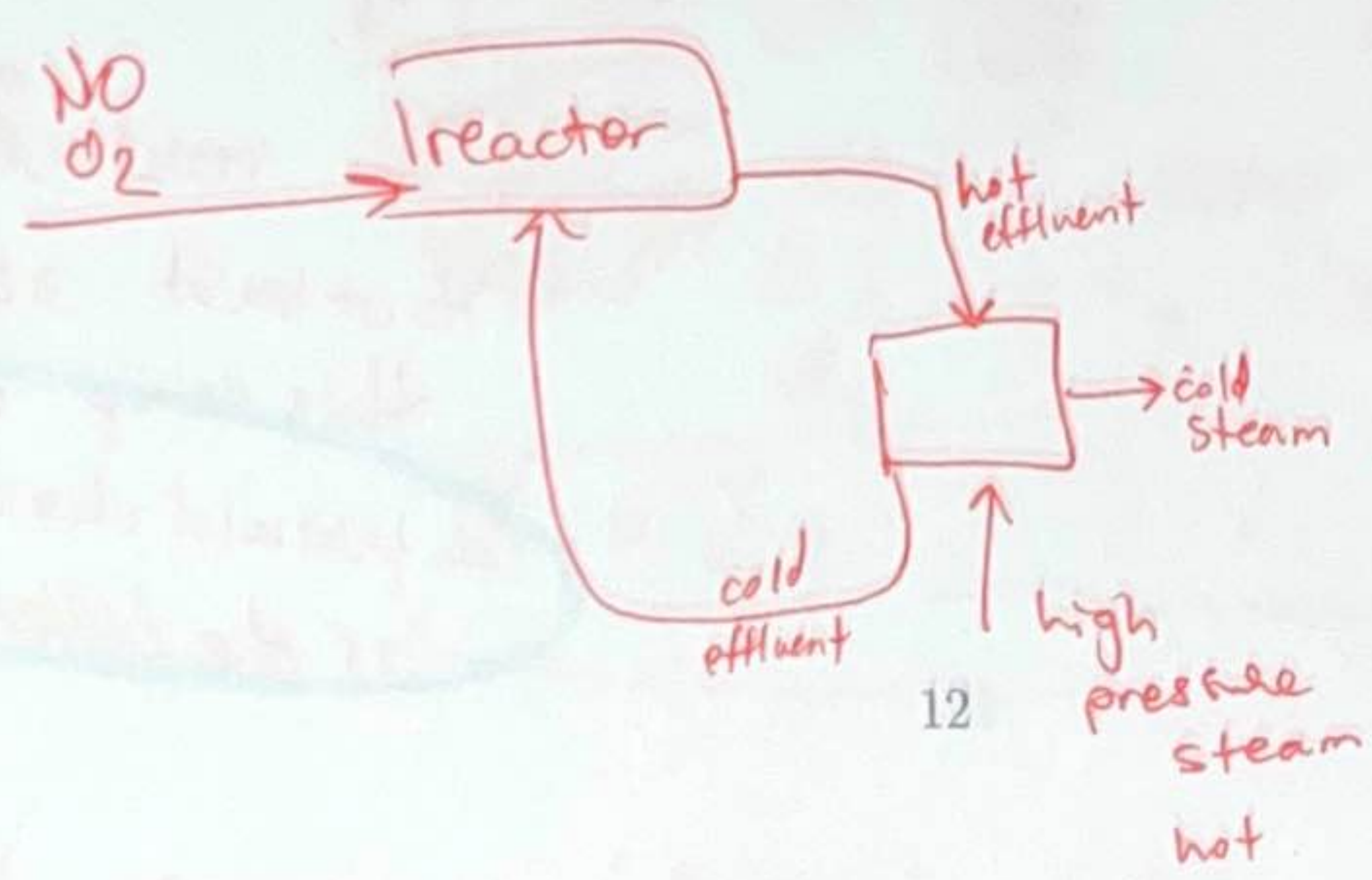


①



OR

②



→ is exothermic

This design would not make sense. This reaction ~~absorbs~~ ~~releases~~ heat (as seen from $\rightarrow 113.1 \frac{\text{kJ}}{\text{mol}}$ that was calculated) and so the reactor ~~will~~ ~~of~~ absorb heat. Since the reaction is exothermic, so ~~the~~ in order to cool down the reactor effluent, see heuristics for an exothermic reaction.

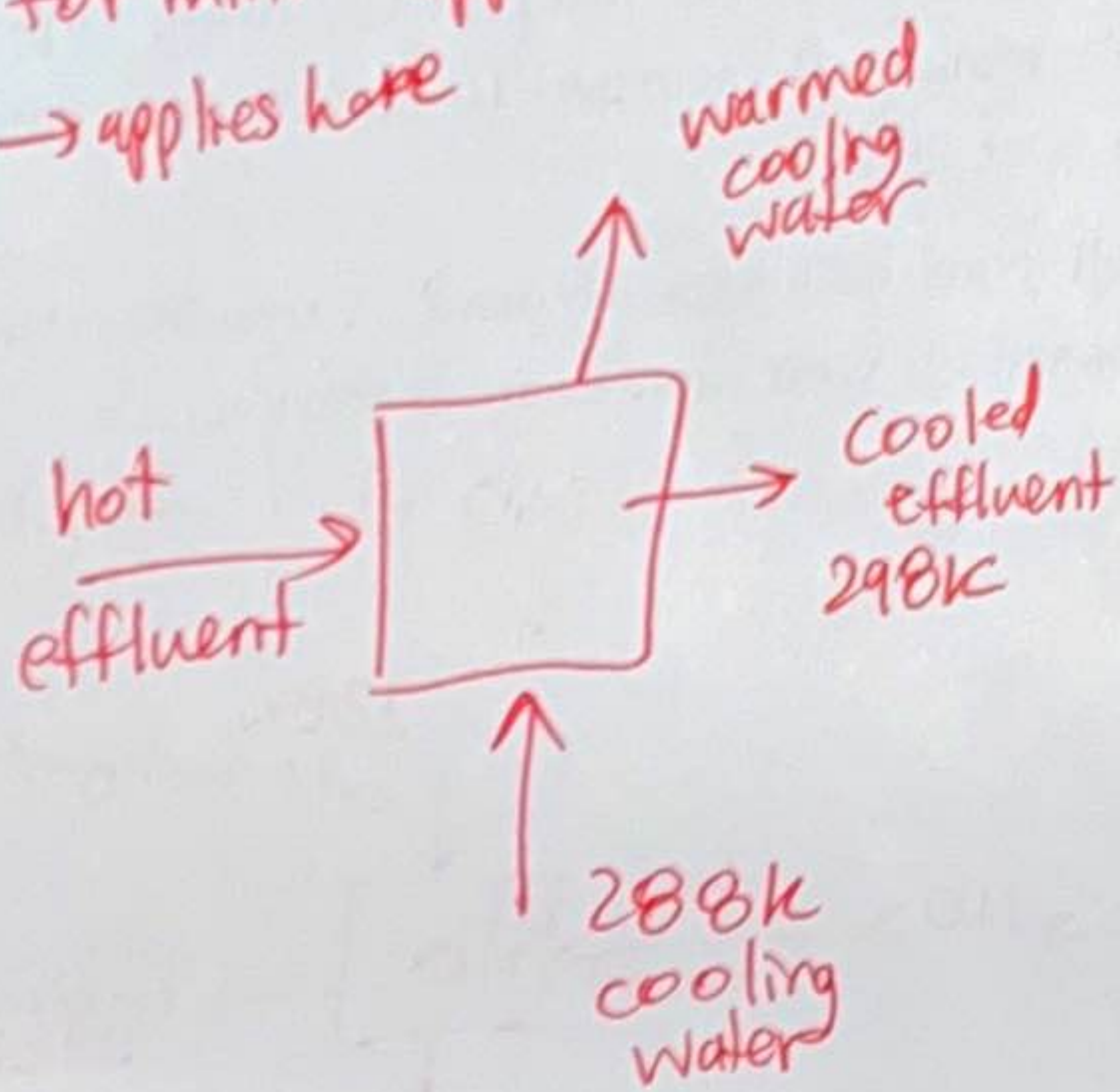
For highly exothermic heats of reaction: use excess reactant, inert diluent, cold shots.

For less exothermic heats of reaction: circulate reactor fluid to an external cooler or use a jacketed vessel or cooling coils.

For this design, the heuristic of sending reactor fluid to an external cooler applies.

However, high pressure steam is a heating utility, so it would not cool down the reactor effluent because in order to heat exchange, it must be colder than the effluent, and usually steam is a heating utility.

Heuristics for min. approach T : 20°F for T at or above ambient \rightarrow applies here



The min. approach T is 20°F which means the ~~warmed~~ hot stream of cooling water exiting the heat exchanger should be at least 318K if not higher. The inlet hot effluent must be ~~248~~ ~~278~~ or ~~lower~~ higher ~~to satisfy~~ 308K to satisfy the min. approach T .

If the reactor ~~inlet~~ ^{outlet} stream is at least 308K , then this setup would work. I would choose (A) as the better design.

1) 2
2) 3
3) 2
4) 3

10/10

10 pts. 4. For the following system of nonlinear algebraic equations, write the equations which show what the guess for the next iteration of Newton's Method will be if the initial guess is $x_1 = 5$ and $x_2 = 3$. You can leave your solution in terms of an inverse Jacobian. Please show the form of all matrices and vectors specific to this problem.

$$5x_2 + 3e^{x_1} = 0$$

$$e^{x_2} + x_1^2 = 0$$

$$f(x_0) = \begin{bmatrix} f_1(x_{10}, x_{20}) \\ f_2(x_{10}, x_{20}) \end{bmatrix} = \begin{bmatrix} f_1(5, 3) \\ f_2(5, 3) \end{bmatrix} = \begin{bmatrix} 5(3) + 3(e^5) \\ e^3 + 5^2 \end{bmatrix}$$

$$f(x_0) = \begin{bmatrix} 15 + 3e^5 \\ e^3 + 25 \end{bmatrix}$$

Jacobian:
$$\begin{bmatrix} \frac{df_1}{dx_1} & \frac{df_1}{dx_2} \\ \frac{df_2}{dx_1} & \frac{df_2}{dx_2} \end{bmatrix}_{x=x_0} = \begin{bmatrix} 3e^{x_{10}} & 5 \\ 2x_{10} & e^{x_{20}} \end{bmatrix}$$

$J^{-1} \rightarrow \left[\begin{array}{cc|cc} 3e^{x_{10}} & 5 & 1 & 0 \\ 2x_{10} & e^{x_{20}} & 0 & 1 \end{array} \right] \rightarrow \left[\begin{array}{cc|cc} 3e^5 & 5 & 1 & 0 \\ 10 & e^3 & 0 & 1 \end{array} \right]$ } J^{-1} can be found through this

This will give the inverse matrix here by plugging in guesses \rightarrow This will give the inverse there
 Find identity matrix here \rightarrow This will then give inverse

$$J \Delta X = -f(x_0)$$

$$\Delta X = J^{-1} * -f(x_0)$$

$$X_1 = X_0 - J^{-1} f(x_0)$$

$X_0 = \text{your guess} = \begin{bmatrix} x_{10} \\ x_{20} \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \end{bmatrix}$

$$X_1 = \begin{bmatrix} 5 \\ 3 \end{bmatrix} - J^{-1} \begin{bmatrix} 15 + 3e^5 \\ e^3 + 25 \end{bmatrix}$$

leaving this in exact form instead of simplifying

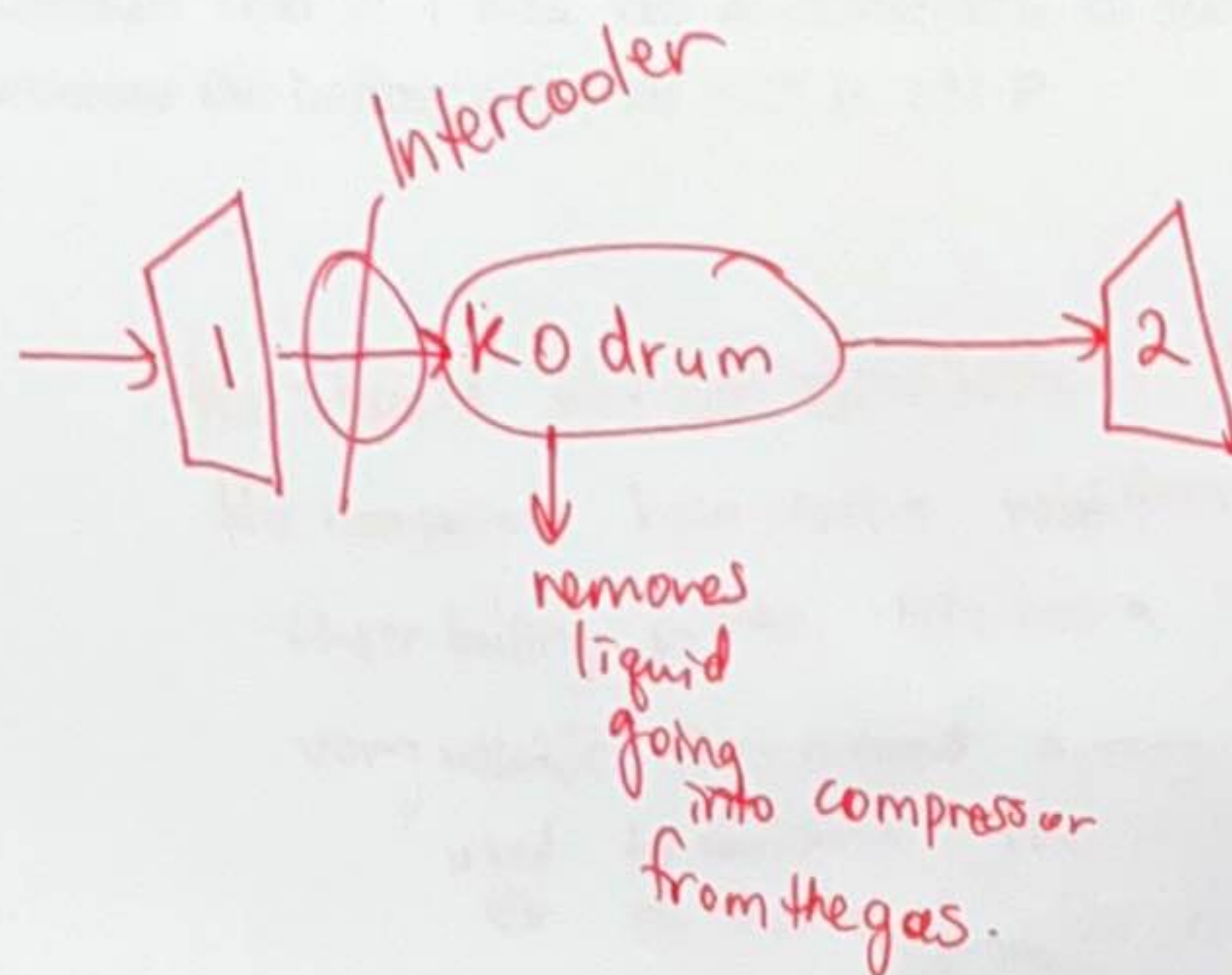
5 pts.

5. What is one of the reasons that it is often good to avoid storing hazardous and toxic chemicals? Provide a thorough and precise description.

- If storing a hazardous or toxic chemical, it can corrode the storage drum if it is also corrosive
- If there is a leak, it could be toxic to people/environment
- If it comes into contact w/ another chemical, this hazardous chemical could react with it and cause an explosion

5/5

- 5 pts ✓ 6. Consider a multistage compression system where a compressor is followed by a knock-out drum, and then the stream out of the knock-out drum is fed to another compressor. There is a missing unit in the system just described. Describe the missing unit and its purpose.



There should be an intercooler after the first compressor to be able to lower the temperature of the stream out of the compressor (usually to 100°F) because the point of multistage compression is to get the desired P increase without the T increasing above a certain point, usually 375°F.

5/5

5 pts. Consider that you would like to remove HCl , present at very low concentrations, from a stream containing large quantities of hydrocarbons. Would it likely be preferable to use distillation to remove the HCl from this mixture, or to use absorption with water? Support your answer with two reasons that are thoroughly and accurately explained.

Consider that at 1 atm, the hydrocarbons all have boiling points above 100 F, whereas the boiling point for HCl is -121 F.

You should not use distillation because assuming that the compounds have relative volatilities that are proportionate to their boiling points, HCl has a very low boiling point and is very volatile. This means a very cold refrigerant would have to be used to condense the HCl ~~to go back as reflux in the~~ at the top of the column, in the condenser. Refrigerants work at very low T's, but are very costly and not desired if there is a better option.

Absorption with water would be a better option because with absorption, a liquid solvent feed is fed into an absorber, and ~~part~~ part of the vapor phase compounds ~~are~~ mix in with the liquid ~~feed~~ solvent, so the liquid stream leaving the absorber has the desired product in it.

At a low concentration of HCl , ~~hydrocarbon~~ ~~also~~ water can be used as a solvent and the HCl can ~~be removed by~~ be removed by being dissolved in H_2O .

3.5 / 5

Please do not write below this line.

1. 34

2. 25

3. 10

4. 10

5. 5

6. 5

7. 3.5

Total: 92.5