Worksheet: Mass and mole balances on a reactor

Name(s):_____

Fill in all sections - These are today's notes.

In this experiment n-propanol liquid is fed to a steady-state reactor system. The n-propanol vaporizes before entering the reactor where two reactions take place:

$$C_3H_7OH \rightarrow C_3H_6 + H_2O$$
 (1)

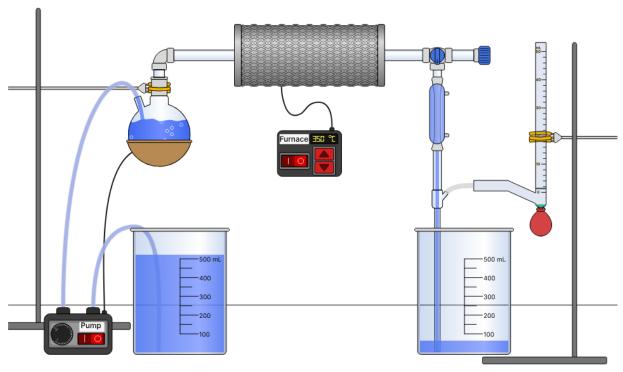
$$C_3H_7OH \rightarrow C_3H_6O + H_2$$
 (2)

Some n-propanol reacts to produce propylene and water (reaction 1), and some reacts to produce propanal and hydrogen (reaction 2). The remaining n-propanol leaves the reactor without reacting.

Student Learning Objectives

- 1. Write material balances around different control volumes in a process.
- 2. Utilize reaction stoichiometry to determine product yields at different conversions.

Equipment



Questions to answer before running the experiment

1. We would like to measure the molar percentage yields of the reaction products propanal and propylene. How will the measurements in this experiment enable you to determine those yields? If reaction produces more propylene than propanal, how will this affect the rate at which liquid accumulates in the product beaker?

2. Set the reactor temperature to either 300 or 330°C. How might the rates of liquid and gas exiting the reactor change as a function of temperature? If one goes up, must the other go down?

3. To analyze the results, we will assume the reaction is operating at steady state. However, there may be an undesired side reaction that continuously produces solid species that accumulate inside the reactor. How would one use the measurements to detect whether this might be a major issue?

Running the experiment

- 1. Set the 3-way valve at the reactor exit to the exhaust.
- 2. Turn on the reactor furnace (I is on) and set the reactor temperature to 300°C.
- 3. Turn on the pump (I is on), which also turns on the evaporator heater, and turn the pump dial to select a feed flow rate of n-propanol to the evaporator.
- 4. Allow the system to reach steady state.
- 5. Turn the 3-way valve so the reactor effluent flows to the condenser.
- 6. Start a timer to measure the change in volume of the feed beaker and record measurements in Table 1.
- 7. You may need to "reset beakers" to complete measurements of the liquid and vapor flow rates out of the reactor
- 8. Once liquid starts collecting in the beaker, start a timer and measure the change in volume of liquid collected in the beaker and record measurements in Table 1.

- 9. Click and hold on the red bulb of the bubble flow meter until a "bubble" move ups the meter. Use a timer to measure the volumetric flow rate of gas leaving the reactor and record measurements in Table 1.
- 10. Repeat the measurements of liquid and vapor flow rates to obtain average values.
- 11. Set the 3-way valve at the reactor exit to the exhaust.
- 12. Click "reset beakers".
- 13. Set the reactor temperature to 330°C.
- 14. Repeat steps 4 12 at 330°C.

Table 1

Temperature	Feed liquid volume change (mL)	Time	Feed liquid volumetric flow rate (mL/s)
300°C			
300°C			
300°C			
300°C average			
330°C			
330°C			
330°C			
330°C average			

Table 2

Temperature	Product liquid volume change (mL)	Time	Product liquid volumetric flow rate (mL/s)	Vapor volume change (mL)	Time	Gas volumetric flow rate (mL/s)
300°C						
300°C						
300°C						
300°C average						
330°C						
330°C						
330°C						
330°C average						

Use the data in Tables 1 and 2 to compute average mass flow rates of liquid out of the feed beaker

and into the product beaker and enter the values in Table 3. The liquid density is 0.8 g/mL. Use the data in Table 2 to compute average gas molar flow rates using the ideal gas law and enter the values in Table 3.

Table 3

Temperature	Feed liquid volumetric flow		Product liquid	Product liquid mass flow rate		Gas molar flow rate
	rate (mL/s)	rate (g/s)	rate (mL/s)	(g/s)	(mL/s)	(mol/s)
300°C average						
330°C average						

Data analysis:

 Solve for the <u>molar</u> flow rate of propanol entering and exiting the reactor from the known mass flow rates in the system at each temperature. This can be done based on the stoichiometry of the gas products: each time one mole of propanol reacts, one mole of gas (either hydrogen or propylene) exits the reactor.

Determine the mass flow rate of propanol exiting the reactor using its molecular weight. Record these values in Table 4.

Table 4

Temperature	Propanol exiting molar rate (mol/s)	
300°C		
330°C		

2. Determine the <u>composition of the liquid stream</u> exiting the condenser at each temperature. The remaining mass accumulating in the beaker (after subtracting the propanol mass flow rate exiting the reactor) is due to propanol and water.

Use stoichiometry to determine the mass flow rates of propanol and water: each time a mole of propanol reacts, it produces a mole of water (which weighs 18 grams) or a mole of propanal (which weighs 58 grams). The outlet mass flow rate of the liquid phase m_{out} is:

$$\dot{m}_{out} = \dot{m}_{propanol} + \dot{m}_{C3H6O} + \dot{m}_{water}$$
 [1]

where $\dot{m}_{propanol}$ has already been determined. The mass flow rates of C₃H₆O and water can be determined by relating them to the fraction of propanol that reacted through a given pathway. For example:

$$\dot{m}_{C3H6O} = x(\dot{n}_{propanol}^0 - \dot{n}_{propanol})MW_{C3H6O}$$
 [2]

where $\dot{n}_{propanol}^{0}$ is the molar flow rate of propanol into the reactor, $\dot{n}_{propanol}$ is the molar flow rate of propanol out of the reactor, and x is the fraction of reacted propanol that produced propanal. Thus, the quantity (1-x) is the fraction of reacted propanol that produces water.

A related expression can be written for the mass flow rate of water. Thus, equation [1] can be expressed in terms of a single unknown x, which can be solved for to determine the liquid composition.

3. The quantity $\frac{x(\dot{n}_{propanol}^{0} - \dot{n}_{propanol})}{\dot{n}_{propanol}^{0}}$ is one measure of the fractional molar yield of propanal,

i.e., what fraction of the fed reactant ends up being directed toward the propanal-producing reaction. Determine the fractional molar yields of propanal and propylene as a function of temperature.

4.	Compute a total mass balance on the entire system. In other words, determine the mass flow rate into the reactor, and then sum up the mass flow rates of all compounds exiting the reactor. (This requires determining the mass flow rate of the vapor stream!) Are the inlet and outlet mass flow rates equal? If they are not (or if they were not), what would this tell you physically?
Qu	estions to answer
1. I	How does reactor temperature affect the outlet gas flow rate? Why do you think it has the effect oes?
2. \	What are sources of error in the measurements? What could cause mass balances to be in error?
3. \	What safety measures would you employ if making this measurement in the laboratory?