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 is vaporized before entering the reactor where two reactions take place:

$$C_3H_7OH \rightarrow C_3H_6 + H_2O \tag{1}$$

$$C_3H_7OH \rightarrow C_3H_6O + H_2$$
 (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 given process.
- 2. Utilize reaction stoichiometry to determine product yields at different conversions.

## **Equipment**

Put a picture of the final reactor system here.

## Questions to answer before running the experiment

1. Ultimately, we would like to be able to measure the molar percentage yields of the two reaction products propanal and propylene. How will the measurements in this set-up 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 beaker?

2.	The reactor can be set to either 300 or 350°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 may 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: Record all measurements in Table 1 below.

- 1. Set the 3-way valve at the reactor exit to the exhaust.
- 2. Set the reactor temperature to 300°C.
- 3. Turn on the evaporator heater.
- 4. Turn on the pump and open the valve to feed n-propanol to the evaporator.
- 5. Allow the system to reach steady state (1 minute).
- 6. Turn the 3-way valve so the reactor effluent flows to the condenser.
- 7. Once liquid starts collecting in the beaker, start a timer and measure the change in volume of liquid collected in the beaker.
- 8. Use the bubble flow meter and a timer to measure the volumetric flow rate of gas leaving the reactor.
- 9. Repeat the measurements of liquid and vapor flow rates to obtain average values.
- 10. Set the 3-way valve at the reactor exit to the exhaust.
- 11. Set the reactor temperature to be 330°C and allow the system to reach steady state (1 minute).
- 12. Turn the 3-way valve so the reactor effluent flows to the condenser.
- 13. Record liquid and vapor flow rates.
- 14. Repeat the measurements of liquid and vapor flow rates and calculate average values. Record these values in Table 1 and Table 2.

Table 1

Temperature	Liquid volume change (mL)	Time	Liquid volumetric flow rate (mL/s)	Vapor volume change (mL)	Time	Vapor volumetric flow rate (mL/s)
300°C						
300°C						
300°C						
300°C						
average						
330°C						
330°C						
330°C						
350°C average						

Use the data in Table 1 to compute average mass flow rates of liquid into the beaker and enter in Table 2. The liquid density is 0.8 g/mL. Use the data in Table 1 to compute average molar flow rates using the ideal gas law and enter in Table 2.

Table 2

Temperature	Liquid volumetric flow rate (mL/s)	Liquid mass flow rate (g/s)	Vapor volumetric flow rate (mL/s)	Vapor molar flow rate (mol/s)
300°C average				
330°C average				

## Data analysis:

1. 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 3.

Table 3

Temperature	Propanol feed rate	Propanol exiting molar rate	Propanol exiting mass rate (g/s)
	(mol/s)	(mol/s)	mass rate (g/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 propional dehyde and water. Use stoichiometry to determine the mass flow rates of propional dehyde 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 C<sub>3</sub>H<sub>6</sub>O and water can be determined by relating them to the fraction of propanol that reacted through a given pathway. For example:

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

where  $n^{\cdot 0}_{propanol}$  is the molar flow rate of ethanol into the reactor,  $n^{\cdot}_{propanol}$  is the molar flow rate of ethanol 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.

(4) The quantity  $\frac{x(n^{\cdot 0}_{propanol}-n^{\cdot}_{propanol})}{n^{\cdot 0}_{propanol}}$  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 aren't (or if they weren't), what would this tell you physically?

#### **Questions to answer**

- 1. How does reactor temperature affect the outlet gas flow rate? Why do you think it has the effect it does?
- 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?	