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Worksheet: Material balances on a CSTR

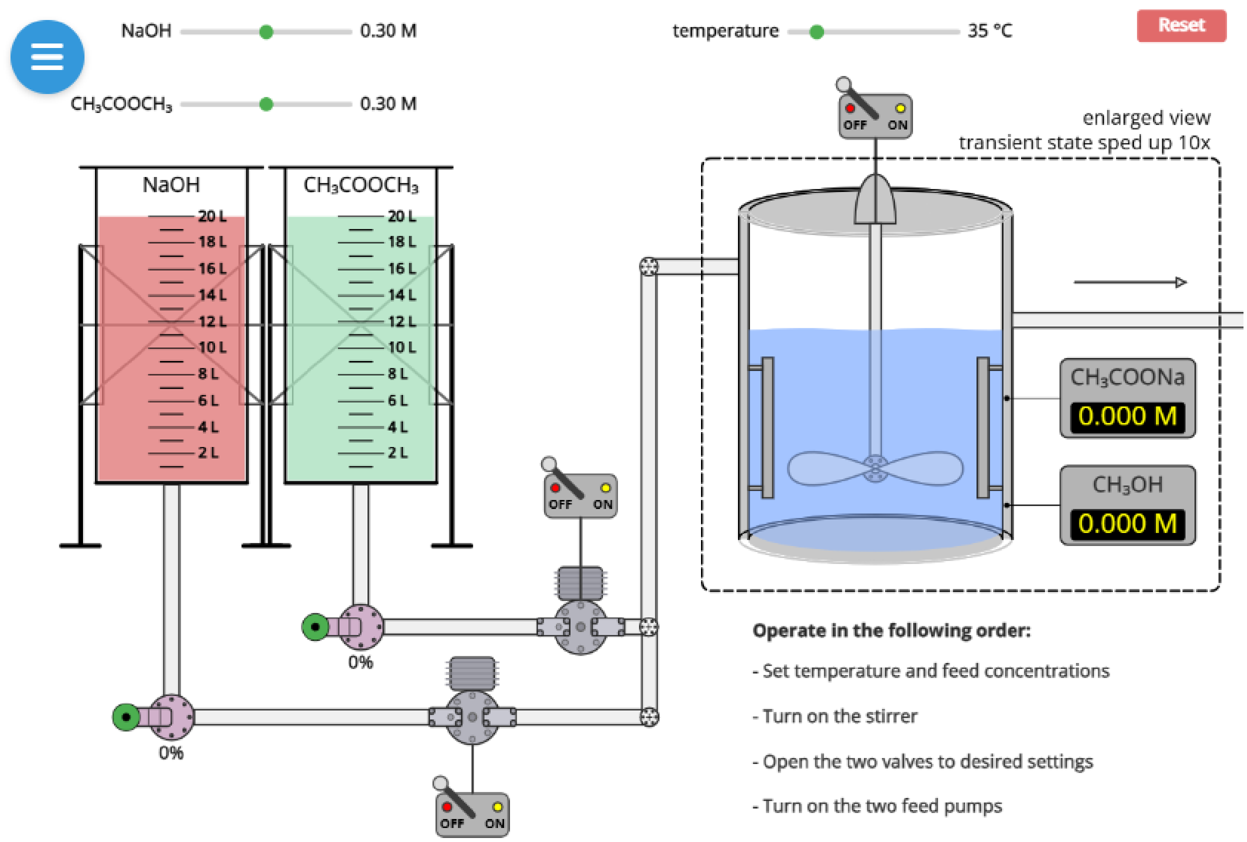
Name(s) ____

In this experiment, two liquid reactants in aqueous solutions flow into a steady-state, continuous stirred tank reactor (CSTR). The objective is to determine the rate constant and the reaction order with respect to one of the reactants.

Student learning objectives

1. Be able to apply mass balances to a chemical reactor.
2. Be able to explain how changing the flow rate to a CSTR changes the rate of reaction and the conversion.

Experimental Diagram



Assumptions

The reactor is well mixed, so the concentrations of reactants and products in the reactor are identical to those concentrations leaving the reactor.

Because the reactor is well mixed, the temperature is the same everywhere in the reactor.

The density of the liquid feeds is the same as the density of the effluent from the reactor.

Questions to answer before beginning the experiment

If the volumetric flow rate to an isothermal CSTR increases, does the reactant concentration in the reactor increase or decrease for a first- or second-order reaction? Why?

If the volumetric flow rate increases to an isothermal CSTR, is more product produced per hour or is less product produced per hour? Explain.

Run the experiment

The reactor, which has a volume of 1.0 L, starts filled with solvent (water). Note that the size of the reactor is enlarged relative to the size of the feed tanks.

1. Select a temperature ___________
2. Move the stirrer switch to ON.
3. Select concentrations of the two feed tanks and record in the Table below.
4. Move the valve openings to a percentage greater than zero for the NaOH and the CH_3COOCH_3 solution feeds.
5. Move both pump switches to ON to start NaOH and methyl acetate flow into the reactor. Note that the pump switches cannot be moved to ON unless the stirrer is ON.
6. Allow time for the system to reach steady state; this time is typically about four times the reactor residence time, which is V/v, where V is the reactor volume and v is the total volumetric feed rate to the reactor. In the simulation, the time to reach steady state is 1/10th of the time for a physical reactor.
7. Use the stopwatch on your phone to measure the volume changes of the two feed tanks and record in the table. Calculate the volumetric flow rates leaving the two feed tanks and the total volumetric flow rate v into the reactor and record in the table. Because mixing the two feed streams dilutes the concentrations of the two reactants, calculate their concentrations entering the reactor (C_{A0}, C_{B0}):

   $$C_{A0} = \frac{v_A C_{A,feed}}{v_A C_{A,feed} + v_B C_{B,feed}}$$

   $$C_{B0} = \frac{v_B C_{B,feed}}{v_A C_{A,feed} + v_B C_{B,feed}}$$

   where

   v_A = volumetric feed rate from the tank containing reactant A (L/s)

   v_B = volumetric feed rate from the tank containing reactant B (L/s)

   $v = v_A + v_B$ = total volumetric flow rate into reactor (L/s)

   $C_{A,feed}$ = concentration of reactant A in the feed tank (mol/L)

$C_{B,feed}$ = concentration of reactant B in the feed tank (mol/L)

Flow stream	Feed tank concentration (mol/L)	Feed tank volume change (L)	Elapsed time (s)	Volumetric flow rate (L/s)	Feed concentration (C_{A0}, C_{B0}) (mol/L)
NaOH					
CH_3COOCH_3					
Total (v)					

8. Record the product concentrations in the reactor in the table below and use stoichiometry to calculate the reactant concentrations in the reactor.
9. Calculate the conversion of NaOH. Conversion of A (X_A) for a constant-density system is:

$$X_A = \frac{C_{A0} - C_A}{C_{A0}}$$

Species	Reactor concentration (mol/L)	NaOH conversion
CH_3COONa		
CH_3OH		
NaOH		
CH_3COOCH_3		

The density of the fluid does not change so the volumetric flow rate is the same at the reactor inlet and outlet.

For measurements using the same feed tank concentrations but different valve openings, change the valve openings, repeat steps 6 - 9, and record values in the tables below. For measurements at different feed tank concentrations, click the "Reset" button, change the feed tank concentrations, repeat steps 2- 9, and record values in the tables below. Make measurements at different conditions to determine the order of the reaction with respect to CH_3COOCH_3. Assume the reaction is first order in NaOH.

Flow stream	Feed tank concentration (mol/L)	Feed tank volume change (L)	Elapsed time (s)	Volumetric flow rate (L/s)	Feed concentration (C_{A0}, C_{B0}) (mol/L)
NaOH					
CH_3COOCH_3					
Total (v)					

Species	Reactor concentration (mol/L)	NaOH conversion
CH_3COONa		
CH_3OH		
NaOH		
CH_3COOCH_3		

Flow stream	Feed tank concentration (mol/L)	Feed tank volume change (L)	Elapsed time (s)	Volumetric flow rate (L/s)	Feed concentration (C_{A0}, C_{B0}) (mol/L)
NaOH					
CH_3COOCH_3					
Total (v)					

Species	Reactor concentration (mol/L)	NaOH conversion
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NaOH		
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Flow stream	Feed tank concentration (mol/L)	Feed tank volume change (L)	Elapsed time (s)	Volumetric flow rate (L/s)	Feed concentration (C_{A0}, C_{B0}) (mol/L)
NaOH					
CH_3COOCH_3					
Total (v)					

Species	Reactor concentration (mol/L)	NaOH conversion
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CH_3OH		
NaOH		
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Flow stream	Feed tank concentration (mol/L)	Feed tank volume change (L)	Elapsed time (s)	Volumetric flow rate (L/s)	Feed concentration (C_{A0}, C_{B0}) (mol/L)
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CH_3COOCH_3					
Total (v)					

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NaOH					
CH_3COOCH_3					
Total (v)					

Species	Reactor concentration (mol/L)	NaOH conversion
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CH_3OH		
NaOH		
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Flow stream	Feed tank concentration (mol/L)	Feed tank volume change (L)	Elapsed time (s)	Volumetric flow rate (L/s)	Feed concentration (C_{A0}, C_{B0}) (mol/L)
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NaOH					
CH_3COOCH_3					
Total (v)					

Species	Reactor concentration (mol/L)	NaOH conversion
CH_3COONa		
CH_3OH		
NaOH		
CH_3COOCH_3		

Data Analysis

After the order of reaction is determined with respect to CH_3COOCH_3, use the data in the tables to obtain the rate constant at each condition using one of these CSTR mass balances:

mass balance for reactant A (NaOH) for reaction that is first-order reaction in NaOH and zero order with respect to CH_3COOCH_3 is:

$$0 = vC_{A0} - vC_A - k_1 C_A V$$

mass balance for reactant A for a reaction that is first order in NaOH and first order in CH_3COOCH_3 (second-order overall) is:

$$0 = vC_{A0} - vC_A - k_2 C_A C_B V$$

where

v = volumetric flow rate entering the CSTR (L/s)

C_{A0} = concentration of reactant A (NaOH) in the feed stream entering the reactor (mol/L)

C_{B0} = concentration of reactant B (CH_3COOCH_3) in the feed stream entering the reactor (mol/L)

C_A = concentration of reactant A in the reactor (mol/L)

C_B = concentration of reactant B in the reactor (mol/L)

k_1 = first-order rate constant (s^{-1})

k_2 = second-order rate constant (L $mol^{-1}s^{-1}$)

V = reactor volume (1.0 L)

Since the reaction is A + B → C + D, stoichiometry requires that the amount of A that reacts must equal the amount of B that reacts: $C_{A0} - C_A = C_{B0} - C_B$

Thus, the mass balance in terms of C_A for a second-order reaction is:

$$0 = vC_{A0} - vC_A - k_2 C_A (C_{B0} - C_{A0} + C_A) V$$

Experiment	Rate constant
1	
2	
3	
4	
5	
6	
7	
8	
Average	

Using a temperature pf 30ºC, select reactant feed concentrations. Make measurements for four flow rates (the same valve opening for each feed valve) that cover a wide range of residence times. Record the values in the Tables below. Plot NaOH conversion versus residence time (V/v).

Flow stream	Feed tank concentration (mol/L)	Feed tank volume change (L)	Elapsed time (s)	Volumetric flow rate (L/s)	Feed concentration (C_{A0}, C_{B0}) (mol/L)
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CH_3COOCH_3					
Total (v)					

Species	Reactor concentration (mol/L)	NaOH conversion
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CH_3COOCH_3					
Total (v)					

Species	Reactor concentration (mol/L)	NaOH conversion
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CH_3OH		
NaOH		
CH_3COOCH_3		

Questions to answer

1. Explain the reason for the trend observed in the NaOH conversion versus residence time plot.

2. If this experiment were conducted in the laboratory, what might cause the conversion in the reactor to differ from that expected based on the known value of the rate constant?

3. What safety measures would you employ if making this measurement in the laboratory?