Worksheet: Material balances on a CSTR

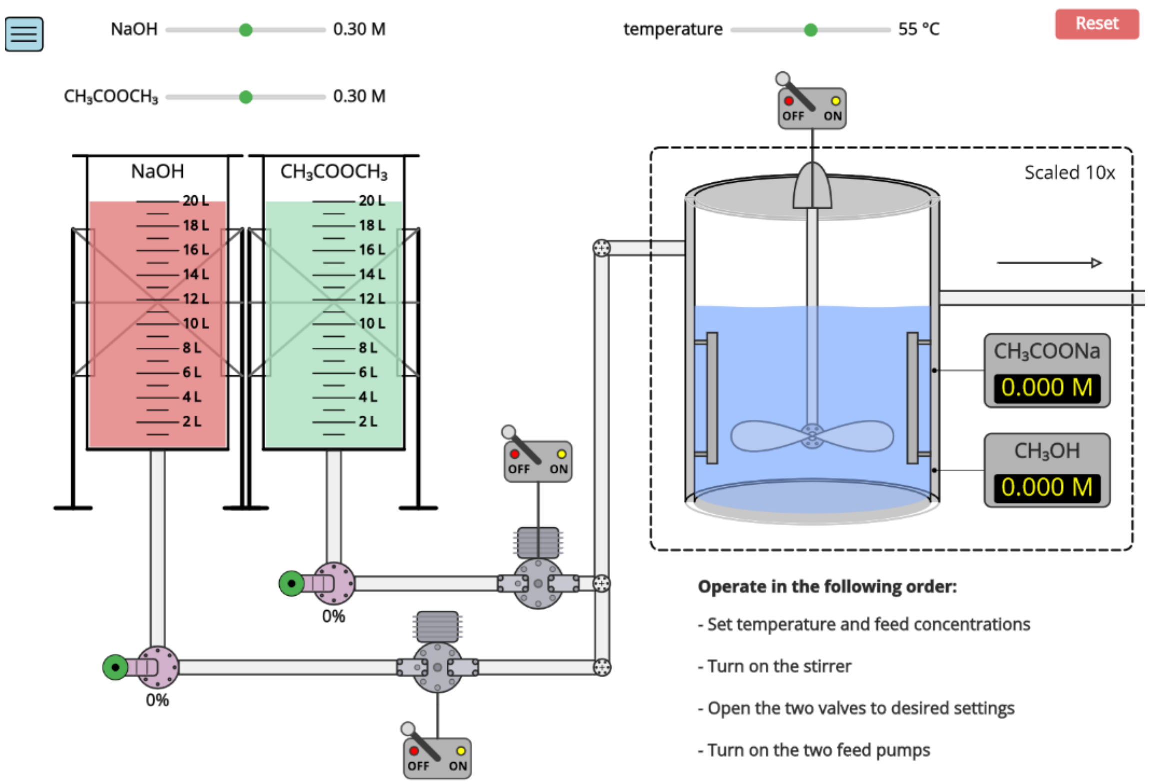
Name(s) ____

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 2.0 L, starts filled with solvent (water).

1. Turn on the motor to start the stirrer.
2. Select concentrations of the two feed tanks and record in the Table below.
3. Select valve openings for the NaOH and the methyl acetate solution feeds.
4. Turn on the pumps to start NaOH and methyl acetate flow into the reactor.
5. Allow time for the system to reach steady state. Typically, the time to reach steady state is 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. The simulation accelerates time, so it takes less time to reach steady state.
6. Use stopwatch on your phone to measure the volume change of each feed tank and record in the Table. Calculate the two volumetric flow rates and record them in the table. Calculate the feed concentrations (C_{A0}, C_{B0}) of the two reactants:

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

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

   where

   v_A = volumetric feed rate from the tank containing reactant A

   v_B = volumetric feed rate from the tank containing reactant B

   $C_{A,feed}$ = concentration of reactant A in the feed tank

   $C_{B,feed}$ = concentration of reactant B in the feed tank

Flow stream	Tank Concentration (mol/L)	Volume change (L)	Elapsed time (s)	Volumetric flow rate from tank (L/s)	Feed concentrations (mol/L)
NaOH					
CH_3COOCH_3					

Add the two flow rates together to obtain the total volumetric flow rate and record below.

v = ______________

Record the product concentrations in the reactor in the Table.

Use stoichiometry to calculate the reactant concentrations in the reactor.

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	Concentration in reactor (mol/L)	Conversion of NaOH
CH_3COONa		---------------------
CH_3OH		---------------------
NaOH		
CH_3COOCH_3		---------------------

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

Repeat these measurements by clicking the "Reset" button and then changing the reactant feed concentrations and/or their flow rates and use these measurements at several conditions to determine the order of the reaction with respect to CH_3COOCH_3. Assume the reaction is first order in NaOH.

Flow stream	Tank Concentration (mol/L)	Volume change (L)	Elapsed time (s)	Volumetric flow rate from tank (L/s)	Feed concentrations (mol/L)
NaOH					
CH_3COOCH_3					

Reactant	Concentration in reactor (mol/L)	Conversion of NaOH
CH_3COONa		
CH_3OH		
NaOH		
CH_3COOCH_3		

Flow stream	Tank Concentration (mol/L)	Volume change (L)	Elapsed time (s)	Volumetric flow rate from tank (L/s)	Feed concentrations (mol/L)
NaOH					
CH_3COOCH_3					

Reactant	Concentration in reactor (mol/L)	Conversion of NaOH
CH_3COONa		
CH_3OH		
NaOH		
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Flow stream	Tank Concentration (mol/L)	Volume change (L)	Elapsed time (s)	Volumetric flow rate from tank (L/s)	Feed concentrations (mol/L)
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CH_3COOCH_3					

Reactant	Concentration in reactor (mol/L)	Conversion of NaOH
CH_3COONa		
CH_3OH		
NaOH		
CH_3COOCH_3		

Flow stream	Tank Concentration (mol/L)	Volume change (L)	Elapsed time (s)	Volumetric flow rate from tank (L/s)	Feed concentrations (mol/L)
NaOH					
CH_3COOCH_3					

Reactant	Concentration in reactor (mol/L)	Conversion of NaOH
CH_3COONa		
CH_3OH		
NaOH		
CH_3COOCH_3		

Flow stream	Tank Concentration (mol/L)	Volume change (L)	Elapsed time (s)	Volumetric flow rate from tank (L/s)	Feed concentrations (mol/L)
NaOH					
CH_3COOCH_3					

Reactant	Concentration in reactor (mol/L)	Conversion of NaOH
CH_3COONa		
CH_3OH		
NaOH		
CH_3COOCH_3		

Flow stream	Tank Concentration (mol/L)	Volume change (L)	Elapsed time (s)	Volumetric flow rate from tank (L/s)	Feed concentrations (mol/L)
NaOH					
CH_3COOCH_3					

Reactant	Concentration in reactor (mol/L)	Conversion of NaOH
CH_3COONa		
CH_3OH		
NaOH		
CH_3COOCH_3		

Data Analysis

Use the data to obtain the rate constant at each condition using one of these mass balances.

A mass balance on a CSTR for reactant A for a first-order reaction is:

$$0 = v * C_{A0} - v * C_A - k_1 * C_A V$$

A mass balance on a CSTR for reactant A for a second-order reaction is:

$$0 = v * C_{A0} - v * C_A - k_2 * C_A C_B V$$

where

v = volumetric flow rate (L/s)

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

C_{B0} = concentration of reactant B (CH_3COOCH_3) in the feed stream (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 (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:

$0 = v * C_{A0} - v * C_A - k * C_A(C_{B0} - C_{A0} + C_A)V$

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

Plot conversion of reactant A versus residence time (V/v) for the same feed concentrations.

Questions to answer

1. 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?

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