Report on

Residence Time Distribution

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The purpose of this experiment was to design and test reactor variables to determine two different conditions, the minimum reactor volume and the maximum throughput, for the saponification of ethyl acetate that will achieve 85% conversion. This report outlines the findings of reaction conversion given three different reactor configurations. Reactor conditions of flowrate, stir rate and number of reactors were varied to determine the ideal conditions for the saponification reaction. It was predicted that variables that increased residence time, such as high reactor volume and low flowrate, would lead to increased average conversions. Furthermore, an increase in the stir rate would produce a higher average conversion due to the formation of a more-ideal reactor (i.e. perfect mixing). The pulse-input experiment model and the segregation model were used to analyze the results later proving the hypotheses correct. It was then concluded that a minimum of two CSTRs with a flowrate of 10 rpm achieved 85%. As predicted, as the number of CSTRs decreases, a lower flowrate is needed. Conversely, with an increasing flowrate, a larger number of CSTRs are needed. Thus, to reach 85% conversion, four CSTRs at a 30 rpm flowrate were needed. However, for maximum conversion, a large volume and small flowrate are needed.

Executive Summary

The purpose of this experiment was to research components of reactor configuration and design to achieve process specifications. This report outlines the design of various reactor configurations to achieve an 85% conversion for an irreversible second-order reaction in a continuous process; specifically, for the saponification of ethyl acetate. Two different optimizations were determined while achieving the desired conversion: utilizing the minimum number of reactors, and utilizing the maximum reactor throughput. The attached report communicates findings of optimized reactor design to achieve these specifications. Reaction conversion was calculated using kinetic data for the saponification of ethyl acetate as researched by Kuheli Das, Sahoo, Sai Baba, Murali and Swaminathan in the Journal of Chemical Kinetics.

Another contributing factor to the mean conversion is the Residence Time Distribution (RTD) function, which is a qualitative measurement of the amount of time different fluid elements have spent in the reactor [1]. Several different reactor configurations were explored and are described in the attached report that affect the RTD. Components of flowrate, reactor volume, and stir rate in a CSTR system were varied to optimize the process RTD, leading to optimized reaction conversion with maximum throughput and minimum volume.

It was predicted that increasing residence time by using high reactor volume and low flowrate would increase average conversions. Furthermore, an increase in the stir rate would produce a higher average conversion due to the formation of a more-ideal reactor (i.e. perfect mixing). The pulse-input experiment model and the segregation model were used to analyze the results later proving the hypotheses correct.

The pulse input experiment was implemented to calculate the residence-time distribution function. Bromophenol blue was injected into a given configuration and measured with a spectrophotometer to generate values of absorbance over time. In combination with kinetic data, the absorbance data and segregation model were used to calculate mean conversions for the saponification of ethyl acetate.

It was determined that a minimum number of two CSTRs with a flowrate of 10 rpm achieved 85% conversion, fulfilling the first condition. Low reactor volumes (using fewer CSTRs) required lower flowrates to achieve the same specifications, and conversely, as flowrate increased, a larger number of CSTRs was required to reach the desired conversion. Therefore, to fulfill the second condition of maximum throughput and still reach 85% conversion, four CSTRs at a 30 rpm flowrate were required. It was concluded that a fully optimized process will use a combination of large volume and small flowrate to maximize the residence time distribution.

In future work, it is recommended that a comparison study be conducted to determine if the stiff plastic tubes used in the reactors ensured the flow of the dye reached the bottom of the reactors. Additional studies could be conducted to explore the reaction kinetics associated with saponification of ethyl acetate by varying temperature and determine the effects on the kinetics and conversion.

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Introduction

The purpose of this experiment was to design and test reactor variables to determine two different conditions, the minimum reactor volume and the maximum throughput, for the saponification of ethyl acetate that will achieve 85% conversion. Ethyl acetate itself is used as a solvent in the food industry [1]. The saponification reaction of ethyl acetate is one of the most well-known reactions in chemistry, often used as a model example of second-order reaction kinetics [2]. Rate laws are determined by experimental observation, with second-order reactions depending on the product of concentrations of the individual reacting species according to the power law model. This is further discussed in the Theory section of this report [3].

The optimization of chemical reactions is crucial for developing chemical processes that are both economically and environmentally efficient. Understanding how to account for non-ideal conditions in a given reactor design helps to further optimize chemical processes. Reactor design balances factors such as reactor volume, residence time distribution, and reaction kinetics to obtain desired reaction conversions. Reactor configuration contributes to overall design, with variables such as parallel or in-series reactors, flowrate, and stir rate affecting the effectiveness of a reaction.

This report outlines various reactor configurations attempting to yield 85% conversion with two conditions: minimum reactor volume and maximum throughput. Components contributing to the residence time distribution were varied to derive conclusions about optimizing the saponification of ethyl acetate. It was hypothesized that variables which increase residence time, such as high reactor volume and low flowrate, will lead to increased average reaction conversions. Additionally, variables that establish a more-ideal reactor, such as high stir rate in a CSTRs to establish ‘perfect’ mixing, will produce a higher average reaction conversion.

Theory

Consider a Continuous Stirred Tank Reactor (a CSTR), where some of the atoms entering the reactor leave the reactor almost immediately, and others stay for a long time. The residence time is how long an atom or molecule remains in the system of reactors. The reaction conversion also depends on how long the atoms or molecules remain in the system of reactors, and so the residence time can significantly affect reaction conversion. However, the residence time is dependent on many things. A function, called the *residence time distribution* (RTD), is used to find the average residence time of an atom in the system of reactors. The RTD of a reactor is a characteristic of the mixing that occurs in the chemical reactor [3].

There are many methods to determine the RTD, but most involve a non-reactive chemical, called a tracer, added into the system of reactors. Tracers are generally a type of dye, but always have a physical or chemical quality which can be recorded as it moves through the system. As the tracer moves through the reactor system, it can be assumed that it is representative of the residence time for an average molecule in the system. There are two well-known experiments used to determine the RTD of a reactor: The Pulse Input Experiment and the Step Tracer Experiment.

The Pulse Input Experiment

In the Pulse Input Experiment (used in this experiment), a small amount of tracer is quickly injected into the reactor and the concentration of the tracer is graphed with-respect-to time. Consider two points of time, t and Δt, such that the amount of tracer leaving the system is essentially the same. To find the amount of tracer leaving the reactor, there must be an understanding that the number of moles in a system is directly proportional to the molar flowrate and the time difference. This is shown is Equation 1 below [3].

$$\Delta N = F(t) * \Delta t \tag{1}$$

Where: ΔN is the amount of tracer accumulated over time Δt
F(t) is the molar flowrate
Δt is the time difference over which number moles are calculated

The molar flowrate is generally difficult to determine, and therefore, it is further divided into two finite quantities: the concentration and the volumetric flowrate. The molar flowrate is directly proportional to the concentration and the volumetric flowrate as shown is Equation 2.

$$F(t) = C(t) * v \tag{2}$$

Where: C(t) is the concentration as a function of time
v is the volumetric flowrate

Therefore, to get the amount of tracer leaving the reactor between time t and Δt is a product of the concentration, the volumetric flowrate, and the time difference, as shown in Equation 3 [1]

$$\Delta N = C(t) * v * \Delta t \tag{3}$$

If the amount of tracer leaving the reactor at any given time is divided by the total amount to tracer injected, and the fraction of the material that has a residence time in the reactor between times t and t + Δt is found. This is shown in Equation 4 below.

$$\frac{\Delta N}{N_o} = \frac{v * C(t)}{N_o} \Delta t \tag{4}$$

Where: N_o is the total amount to tracer injected

In the above reaction, the residence time distribution is defined as the molar flowrate divided by the total amount of tracer injected into the reactor, as shown in Equation 5.

$$E(t) = \frac{v * C(t)}{N_o} \tag{5}$$

Where: E(t) is the residence time distribution function

The practical method to find the residence time distribution from the Pulse Input Experiment is using the concentration versus time data.

The differential form of Equation 4 is given in Equation 6 below. This is the numerator for the residence time distribution function seen in Equation 5.

$$dN = v * C(t)dt \tag{6}$$

The total amount of tracer,N_o, is the product of the total concentration over time and the volumetric flowrate as shown in Equation 7 below. This is the denominator for the residence time distribution [1].

$$N_o = \int_0^\infty v * C(t)dt \tag{7}$$

The residence time distribution now is calculated as ratio of Equation 6 and 7. As the volumetric flowrate is a constant, it is not seen in Equation 8 below.

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt} \tag{8}$$

Figure 1, below, shows the pulse response to the concentration versus time curve [3].

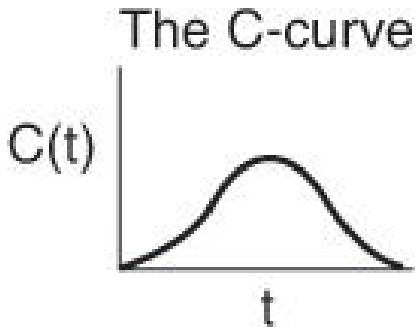

Figure 1: Concentration versus time graph for a Pulse Response

The concentration versus time curve is used to find the area under the curve, or the denominator to the residence time distribution function. It is shown in Equation 9.

$$Area = \int_0^\infty C(t)dt \tag{9}$$

As all of the tracer has been removed within time t = 0 and t = ∞, the fraction of the material leaving within that time is 1. This is shown in Equation 10 below [1].

$$\int_0^\infty E(t)dt = 1 \tag{10}$$

With Equation 9 and a function depicting concentration versus time, the RTD can be found.

Step Tracer Experiment

The step tracer experiment is another way to determine the residence time distribution of a reactor. In this experiment, at time t = 0, a constant volumetric flowrate of tracer is added to the reactor. It is continuously added until the concentration of the tracer in the reactor stabilizes. Using the data, the step tracer experiment gives, the cumulative distribution function is derived from a step input. The cumulative distribution function, $D(t)$, gives the fraction of material that has been in the reactor at time t or less, and can be differentiated to obtain the RTD function. The cumulative distribution function is dependent on the outlet concentration of the tracer and the initial concentration. This initial concentration is a constant, and the outlet concentration depends on the time. This is seen in Equation 11 below.

$$E(t) = \frac{dD(t)}{dt} = \frac{d}{dt}\left[\frac{C_{out}(t)}{C_0}\right]_{step} \tag{11}$$

Where: E(t) is the residence time distribution
D(t) is the cumulative distribution function
$C_{out}(t)$ is the outlet concentration
C_0 is the initial concertation

The Step Tracer Experiment may be easier to carry out experimentally than the pulse experiment, however it can be difficult to maintain a constant tracer concentration in the feed. It also relies on differentiation, rather than integration, of data, which can lead to errors, and requires a large volume of tracer, which can lead to high experimental costs. Therefore, was not used in this experiment. However, either method will provide a residence time distribution that can be used to predict conversion.

Predicting Conversion from Residence Time Distribution

Predicting conversion in a non-ideal reactor uses a combination of the information from the residence time distribution function, kinetic data, and one of the many mathematical models. The mathematical model chosen is dependent on the number of adjustable parameters. One of the most common models used is the segregation model.

Segregation Model

The segregation model visualizes a chemical reaction taking place as a series of droplets running through the reactor in a continuous stream. A single droplet does not react with other droplets in the reactor, hence they stay segregated. Because the droplets do not interchange with any of the molecules, each droplet can be treated as a small batch reactor. Applying the segregation model to small batch reactors, the mean conversion of the system can be calculated by the principles described in Equation 12 [1].

$$\begin{bmatrix} Mean\ conversion \\ of\ droplet\ over \\ time\ spent \\ in\ the\ reactor \end{bmatrix} = \begin{bmatrix} Conversion \\ achieved\ in\ a\ droplet \\ after\ spending\ a\ time, t, \\ in\ the\ reactor \end{bmatrix} * \begin{bmatrix} Fraction \\ of\ droplets\ that \\ spend\ between \\ t\ and\ t + dt \\ in\ the\ reactor \end{bmatrix} \tag{12}$$

This word equation can be transformed into a variable form as shown in Equation 13. This equation shows that the mean conversion is a product of the conversion after spending time in the reactor and the residence time distribution.

$$d\bar{X} = X(t) * E(t)dt \tag{13}$$

Where: $d\bar{X}$ is the mean conversion
X(t) is the conversion after spending time t in the reactor
E(t) which is the residence time distribution

Rearranging Equation 13, Equation 14 is found. This equation describes the mean conversion as a derivative of time.

$$\frac{d\bar{X}}{dt} = X(t)E(t) \tag{14}$$

Then summing over all of the droplets, the mean conversion for the system can be achieved as seen in Equation 15.

$$\bar{X} = \int_0^\infty X(t)E(t)dt \tag{15}$$

The overall conversion of the system can be found through rate law principles and stoichiometric calculations. The rate law for a second order reaction is described in Equation 16.

$$-r_A = kC_A^2 \tag{16}$$

Where: r_A is the reaction rate
k is the reaction rate constant
C_A is the concentration

From stoichiometric calculations the concentration can be described as a function of number of moles and reactor volume or a function of initial concentration and conversion. This can be seen in Equation 17.

$$C_A = \frac{N_A}{V_0} = C_{A0}(1 - X(t)) \tag{17}$$

Where: N_A is the moles of the tracer
V_0 is the reactor volume
C_{A0} is the initial tracer concentration
X(t) is the conversion as a function of time

Equation 16 and Equation 17 are combined and rearranged to for Equation 18. Equation 18 calculates the overall conversion as a function of time.

$$X(t) = \frac{kC_{A0}t}{1 + kC_{A0}t} \tag{18}$$

Where: X(t) is the conversion as a function of time
k is the reaction rate constant
C_{A0} is the initial tracer concentration
t is time

After solving Equation 18, the results can be fed back into Equation 15 to calculate the mean conversion. Another important aspect to consider is that concentration is generally hard to calculate directly. Beer-Lambert law is a relationship between absorbance and concentration- and absorbance can be calculated quite easily. Beer-Lambert law is shown below as Equation 19 [3].

$$A = \varepsilon * l * c \tag{19}$$

Where : A is the absorbance
ε is the absorptivity coefficient
l is the length of path
c is the concentration

If Equation 19 is rearranged in terms of concentration, Equation 20 is found and is shown below.

$$c = \frac{A}{\varepsilon * l} \tag{20}$$

As both the absorptivity coefficient and the path length are constants, both will divide out in the equation to find the residence time distribution.

Materials and Methods

This experiment analyzed the residence time distribution of a second order reaction. This was done by performing a pulse input experiment in a series of CSTR reactors.

Apparatus

The apparatus used in this experiment was an array of different appliances used to pump liquid to and from the reactors and to measure the absorbance of the dye. The spectrophotometer is a machine which was used to measure the absorbance of the tracer. A spectrometer flow cell was placed in the spectrophotometer to collect samples of the tracer. Two peristaltic pumps were used to establish a constant flowrate during experimentation and to take samples to the spectrophotometer. The tracer used was Bromophenol Blue. A six-place stir plate was used to facilitate agitation for CSTRs during experimentation. Four 125ml vacuum flasks were used to hold fluid during the experiment and act as the CSTRs. Four stir bars were placed in flasks, and paired with the multi-place stir plate; these stir bars were used to agitate the solution during experimentation. Series of tygon tubing were used to facilitate the transfer of fluid through the various configurations (an example is shown in Figure 2 below). Four rubber stoppers were placed on the vacuum flasks; they facilitated the entry of fluid into the CSTR and the exit of fluid to the next stage in the process. Firm tubing of 10 cm in length were inserted into the rubber stoppers and inside the flasks to allow the fluid entry into the CSTR to descend to the bottom of the tank, and be instantaneously agitated. A stop-cock was used to administer the dye to the reactor. Four doughnut-weights were used to keep the CSTRs from moving.

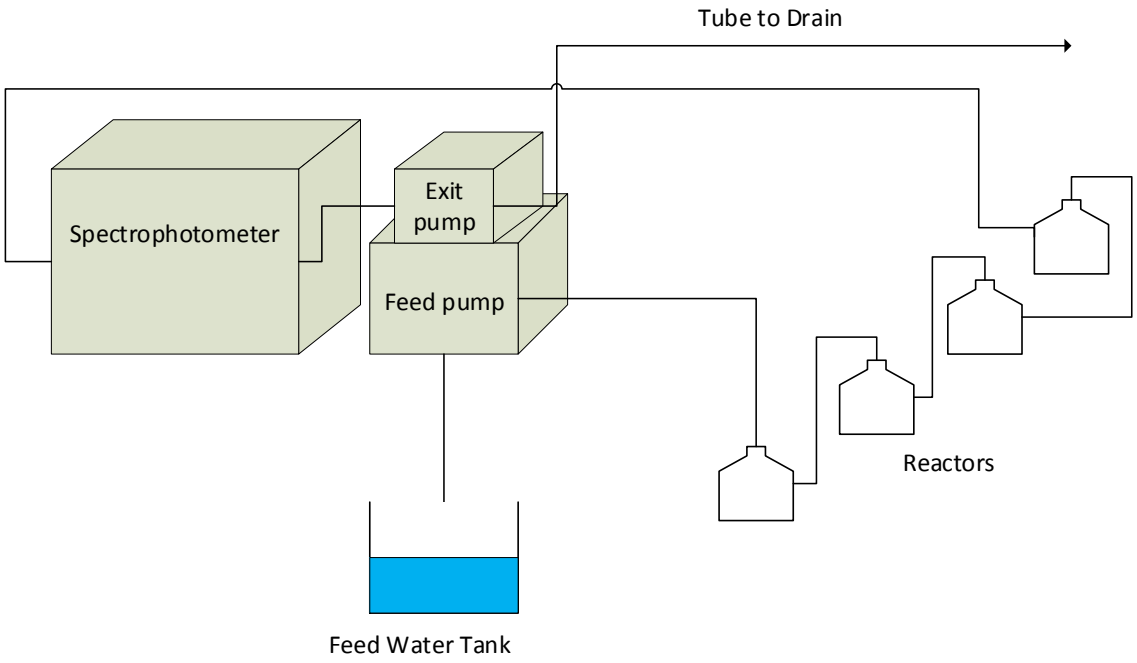

Figure 2: The set-up of the four CSTRs in series.

Methods

First, the system was primed to ensure that all of the reactors used were filled with water. During each round of trials, different number of reactors were used. In the first round of trials only one reactor was used; in the second round, two reactors were used; and finally, four reactors were used in the third round of trials. During the trials, flowrate and stir rate were varied. Three different flowrates- 10, 20, 30 rpm- and three different stir rates – 5, 10, and 20 revolutions per minute -were explored. Once the system was filled with water, the dye was injected. Using a syringe and a stopcock, 6 mL of dye was injected into the system. The syringe was then filled with water twice to ensure that all of the dye was pushed into the system. The mixture of water and dye slowly flowed through the system and into the spectrophotometer where the absorbance was measured and recorded using LabView technology. After the dye was fully out of the system, the next trial was started using the same operating procedures. This process was repeated for all trials performed. After trials were completed the system was pumped free of water and disassembled.

Results

Three variables were adjusted within this experiment to determine their effect on overall reaction conversion: the flowrate, the stir speed, and number of CSTRs. Effects of each change will be discussed in detail below.

Flowrate

As shown in Table 1 below, when the flowrate increased, with everything else kept constant, there is a decrease in overall conversion. Table 1 also shows that the residence time decreases as flowrate increases. This is in line with the hypothesis- as residence time decreases, so does the reaction conversion. The fluid is being pushed into and out of the reactor faster at a higher flowrate. Then each droplet of fluid stays in the reactor for a smaller amount of time. This causes the residence time of the droplet in the fluid to decrease, and that in turn decreases conversion.

Table 1 - Effect of flowrate on the conversion and residence time.

Trial Number	Number of CSTR	Stir rate (rpm)	Flowrate (rpm)	Residence Time (s)	High Concentration Conversion
10	2	5	10	218.630	0.866
11	2	5	20	114.965	0.794
12	2	5	30	81.985	0.761

Stir Speed

The stir rates were also varied and a change in conversion was seen as shown in Table 2. The stir rate does not affect the residence time because the segregation model is being used to explain the mixing. The reason the residence time is varying in Table 2 is that the flowrates were also being changed from trial to trial. Now focusing in on the stir rate, the conversion increases slightly as conversion increases. Also with increasing stir rate, the CSTRs that are in use act more closely to ideal CSTRs which have perfect mixing.

Table 2 - Effect of stir rate on conversion and residence time

Trial Number	Number of CSTR	Stir rate (rpm)	Flowrate (rpm)	Residence Time (s)	High Concentration Conversion
1	1	5	10	55.537	0.698
2	1	5	20	55.537	0.660
3	1	5	30	55.537	0.698
4	1	10	10	100.968	0.780
5	1	10	20	47.674	0.674
6	1	10	30	42.751	0.660
7	1	20	10	92.514	0.764
8	1	20	20	56.459	0.702
9	1	20	30	38.931	0.638

Number of Reactors

It is seen from Table 3 below that as there is an increase in the number of reactors, there is an increase in the reaction conversion. Reaction conversion is directly proportional to the residence time within a

reactor, and if a chemical needs to go through many reactors a single droplet will have more time to react. This in turn increases the reaction conversion. As the number of reactors increase, the fluid in the reactors spend more time in the reactors because they have more volume to travel through. This in turn increases the residence time.

Table 3: Effect of number of CSTRs on reaction conversion

Trial Number	Number of CSTR	Stir rate (rpm)	Flowrate (rpm)	Residence Time (s)	High Concentration Conversion
1	1	5	10	55.537	0.698
10	2	5	10	218.630	0.866
19	4	5	10	650.405	0.965

The goal of this experiment was to explore two design specifications, either maximum throughput or minimum reactor volume, that achieved 85% conversion. Table 4 displays all of the trials that achieved 85% conversion.

Table 4: All Trials which achieved 85 % Conversion

Trial Number	Number of CSTR	Stir rate (rpm)	Flowrate (rpm)	Residence Time (s)	High Concentration Conversion
16	2	20	10	192.324	0.858
24	4	10	30	191.416	0.864
21	4	5	30	243.781	0.865
10	2	5	10	218.630	0.866
26	4	20	20	280.601	0.907
23	4	10	20	287.285	0.908
20	4	5	20	281.063	0.908
27	4	20	30	366.943	0.917
25	4	20	10	669.448	0.947
22	4	10	10	722.471	0.950
19	4	5	10	650.404	0.964

Table 4 shows that with a fewer number of CSTRs, a lower flowrate is need to achieve 85% conversion. With increasing flowrate, a larger number of CSTRs is needed to achieve 85% conversion. Maximum throughput is described as a high flowrate. In order to achieve 85% conversion at a high flowrate four CSTRs are needed. The minimum reactor volume need to achieve 85% conversion is two CSTRs, however the flowrates has to be low in order to achieve 85% conversion.

Discussion

The hypothesis for this experiment was supported by the results. As the residence time increases the conversion increases. The three variables that were changed in this experiment each affect the system to a different extent. Changing the number of CSTRs affects the residence time and the conversion the most, followed by the changes in the flowrates, and finally the change in the stir rates.

The number of reactors play the largest role in determining conversion as the residence time is affected most through this method. The residence time is the average amount of time a reactor spends in the reactor before a final product is produced. The reason the residence time is such an important variable in conversion is it gives information on how much the reaction has gone to completion. If a molecule has a small residence time, it can be assumed that not much of the reaction has been completed. This in turn affects the conversion. When the number of reactors are increased, a molecule has more volume to react in, and therefore more time to react. This affects conversion greatly. This implies that in an industrial process it may be best if the number of reactors can be increased to increase conversion.

Changing the flowrate was the second most important variable in increasing conversion as, once again, changing flowrate will change the residence time. An increasing flowrate decreases the conversion. If a droplet of reactant is pushed into and out of a reactor at a fast speed, the droplet will have a small residence time and may not have time to convert into the product. In summary, if we have a high flowrate, the residence time decreases, and this deceases the conversion. This also applies to the real world, if more reactors cannot be added, it may be beneficial to decrease the flowrate of the reactant into the reactor.

According to Table 1 and Table 2 in the Results section, the affect that the stir rate has on the system is low compared to that of flowrate. This result was expected in this experiment because the system was not an ideal setup for perfect mixing. Another reason that the stir speed affects the conversion the least is that it does not affect the residence time. However, a higher stir speed does increase the conversion slightly. A higher stir speed makes a CSTR more like an ideal CSTR, where the reactant reaches the concentration of substance in the reactor immediately. This means that in the industrial application, if neither number of CSTRs or flowrate can be changed, increasing stir speed would increase conversion.

It was determined that in order to achieve 85% conversion at maximum throughput there needed to be four CSTRs. This is supported by the varying conversion values and residence times in Table 1 and Table 3. The higher the flowrate, the lower the residence time, however there needs to be enough time for the reaction to take place to achieve 85% conversion. To ensure this there has to be a higher number of reactors. It was also determined that in order to achieve 85% conversion with the minimum reactor volume two CSTR reactors are needed at a low flowrate. This result is supported by the varying conversion values and residence times in Table 1 and Table 3. The lower the flowrate, the higher the residence time therefore with a low number of CSTRs and a low flowrate 85% conversion can be achieved. However, if the flowrate is increased, the 85% conversion threshold is not achieved.

The system that was used to model this reaction was accurate enough to gain results, however there could be improvements made to the set up. The reactors were not well mixed by the stir bars and stir plate that were used, they were mixed enough but it could be improved upon. In order to gain absorbance readings, the absorbance fuel cell inlet tube was inserted into the outlet tube of the last reactor. There was sometimes air in the line or the computer failed to give a reading of the absorbance. The trend of the data was obvious enough to fill these gaps, however this set up could be improved upon by having a more reliable way to pump the outlet stream into the spectrophotometer.

During the experiment, stiff plastic tubes were inserted into the reactors to ensure that the flow of the dye reached the bottom of the reactors rather than just floating on top. In the future, a comparison study could

be performed without the stiff tubing to see if this addition to the setup is helpful in experimentation. In addition, the use of a more permanent equipment set-up would be ideal. This would minimize the leaking at the connections as well as the air that leached into the system. The focus of this experiment was on the residence time distribution but lacked depth on the other elements of reactor design. Another avenue of reactor design that could be explored is the reaction kinetics. One example of how this could be explored is by varying temperature to see how it affects the reaction kinetics and conversion.

Conclusions

This experiment explored the effects of flowrate, stir speed, and the number of reactors on the residence time distribution. It was predicted that variables that increased residence time, such as high reactor volume and low flowrate, would lead to increased average conversions. Furthermore, an increase in the stir rate would produce a higher average conversion due to the formation of a more-ideal reactor (i.e. perfect mixing).

Using the pulse-input experiment model and the segregation model to analyze the results, the following conclusions were made regarding the hypothesis: a low flowrate, increased conversion; an increase in stir speed did not significantly increase the conversion; and an increase in the number of reactors, increased conversion. The stir speed did not affect the average reaction conversion as significantly as anticipated due to the non-ideal set-up of the apparatus.

It was concluded from this information what the minimum number of reactors (reactor volume) and maximum throughput (flowrate) would produce a conversion of at least 85%. A minimum of two CSTRs with a flowrate of 10 rpm achieved 85%. With a decreasing number of CSTRs, a lower flowrate is needed. Conversely, with an increasing flowrate, a larger number of CSTRs are needed. Thus, to reach 85% conversion, a volume of four CSTRs at a 30 rpm flowrate was needed. However, for maximum conversion, a large volume and small flowrate are needed. From the conclusions drawn from the data, the saponification of ethyl acetate can be optimized based on the needs of the company designing the process.

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Appendix

This appendix details the calculations and code used to determine the results of the experiment. All the data collected is shown at the end.

Sample Calculations

Calculating mean conversion:

1. Using the data of bromophenol blue absorbance versus time, fit the experimental data to the Gaussian Model and apply the Beer-Lambert Law to obtain $C(t)$ shown in Figure 3.

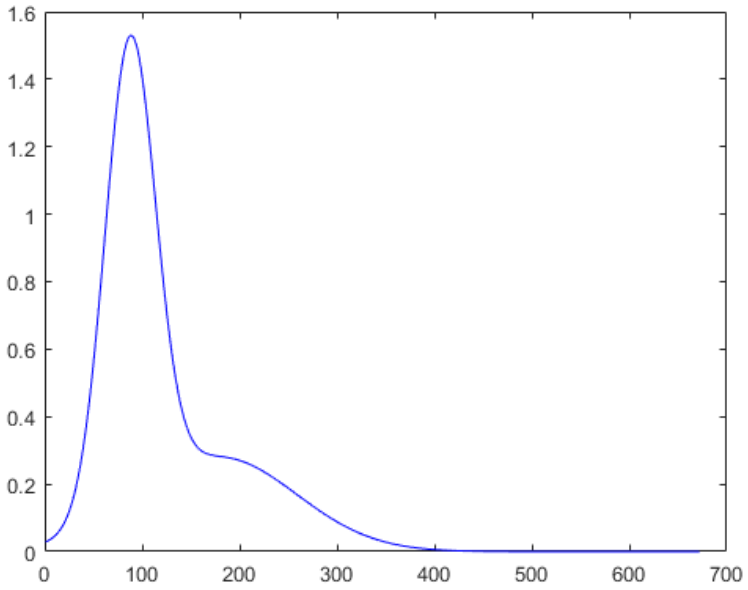

Figure 3: Concentration of bromophenol blue during a given trial

2. Using $C(t)$ and the equation below (Equation 8 from the Theory section), the Residence Time Distribution function is calculated, shown in Figure 4.

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt}$$

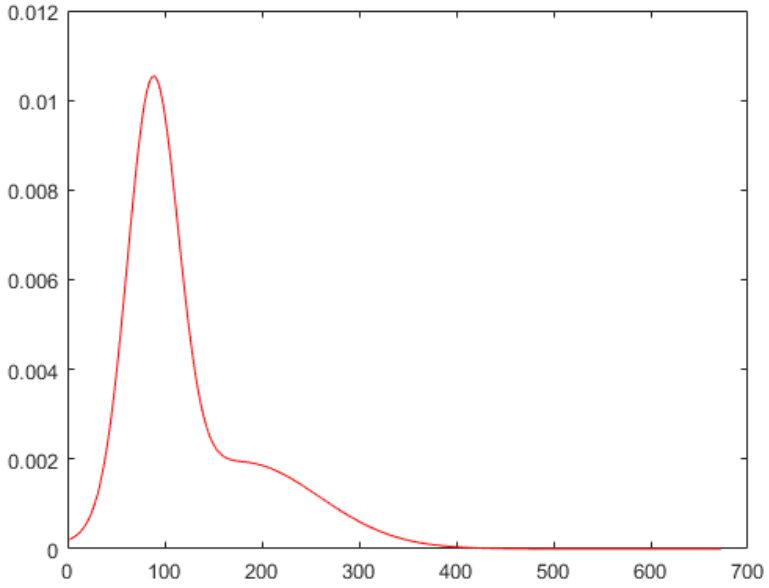

Figure 4: Residence Time Distribution function for a given trial

3. A function of reaction conversion in terms of time is shown below in Figure 5. Values of the concentration of bromophenol blue C_{A0} and rate constant k are used.

$$X(t) = \frac{kC_{A0}t}{1 + kC_{A0}t}$$

Where: $k = 0.16$
$C_{A0} = 0.003$

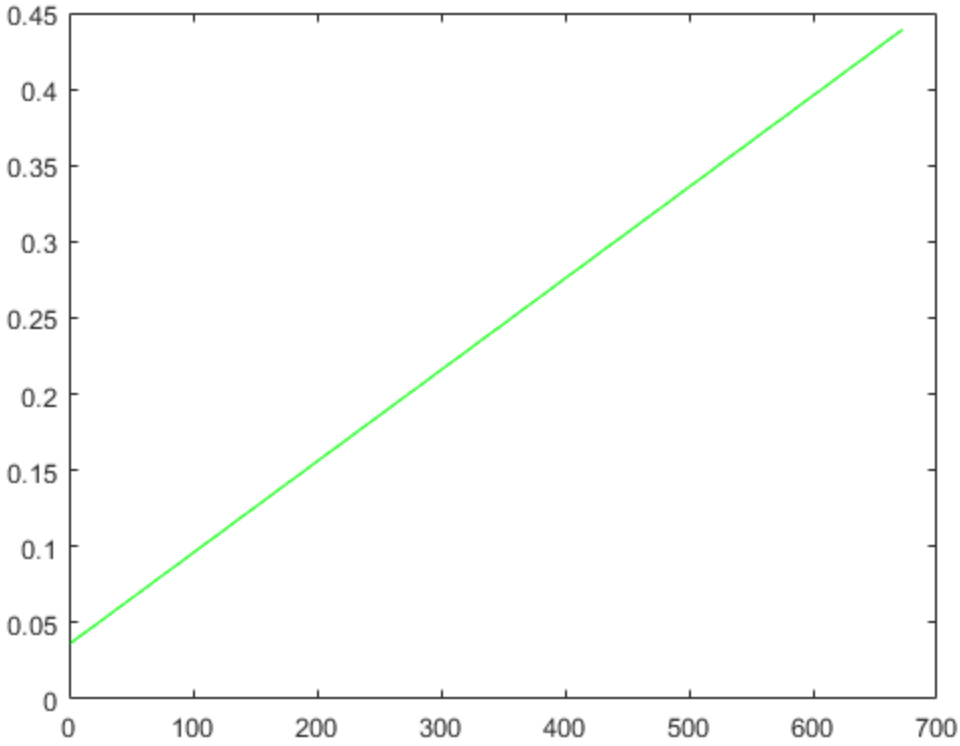

Figure 5: Reaction conversion in terms of time

4. Using conversion $X(t)$ and the Residence Time Distribution function $E(t)$ the mean conversion of the trial is calculated using the equation below.

$$\bar{X} = \int_0^\infty X(t)E(t)dt$$
$$\bar{X} = 0.10983$$

Matlab Code

Below is the code used in Matlab to compute results from the data.

```
%importing data from excel file
filename = 'T21.xlsx';
timeColumn = 'A:A';
absorbanceColumn = 'B:B';
time = xlsread(filename, timeColumn);
absorbance = xlsread(filename, absorbanceColumn);
```

```
%fitting data to gaussian model
C = fit(time,absorbance,'gauss2');
integralC = trapz(C(time));
E = C(time)./integralC; %E(t) = RTD function
tao = trapz(time .* E(logical(time))); %tao=tm=tr is mean residence time
disp("tao: " + tao);

%solving for X at mean residence time
LowConcConversion = @(t) 0.0003*t + 0.0367;
meanConversionactual = trapz(LowConcConversion(tao) .* E(logical(time))); %mean conversion at low
conc
HighConcConversion = @(t) 0.0974*log(t) + 0.3305;
meanConversionideal = trapz(HighConcConversion(tao) .* E(logical(time))); %mean conversion at high
conc
disp("low conc conversion: " + meanConversionactual);
disp("high conc conversion: " + meanConversionideal);
```

Matlab Results

```
>> T21
tao: 243.7819
low conc conversion: 0.10983
high conc conversion: 0.86584
```

Complete Data Table

Table 5: Complete data table for each trial

Trial Number	Residence Time (s)	Low Concentration Conversion	High Concentration Conversion
1	55.536	0.025	0.698
2	55.536	0.025	0.659
3	55.536	0.025	0.698
4	100.96	0.049	0.779
5	47.674	0.021	0.673
6	42.750	0.018	0.659
7	92.513	0.048	0.764
8	56.459	0.027	0.701
9	38.930	0.018	0.637
10	218.630	0.082	0.866
11	114.965	0.056	0.794
12	81.984	0.035	0.760
13	191.981	0.035	0.760
14	113.857	0.049	0.808
15	75.105	0.031	0.753
16	192.324	0.089	0.858
17	129.324	0.057	0.821
18	84.231	0.036	0.769
19	650.404	0.229	0.964
20	281.063	0.125	0.908
21	243.781	0.109	0.865
22	722.471	0.260	0.950
23	287.285	0.128	0.908
24	191.416	0.086	0.864
25	669.448	0.242	0.947
26	280.601	0.123	0.907
27	366.943	0.136	0.917