CLB 320 Kinetics

Experiment 5 Kinetics Modelling Results

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1. Abstract

Theoretical models suggest that the reaction rate constant k at a particular temperature is, as the name implies, constant regardless if a CSTR, PFR or Batch reactor kinetics are being modelled.

The experiment results discussed in this report pertain to experiment 5, where k, m, and n values were determined from experimental data obtained from a single CSTR reactor at different flow rates. After the kinetics values were determined, the expectation was that these would be the same for the CSTRs in series, the PFR and Batch reactor.

Overall, the conversion rates predicted were lower than the experimental values in all the reactors. Each set of results for the respective reactors follow.

Keywords: Continuously Stirred Tank Reactor, Plug Flow Reactor, Batch Reactor, reaction rate, reaction kinetics, order of reaction

2. Nomenclature

No.	Symbol	Description	Units
1	r_i	Rate of reaction	$-\frac{mol_i}{V.t}$.
2	V	Volume	m^3
3	t	Time	s
4	N_i	Mole	mol_i
5	m, n	Order of reaction	
6	k	Reaction constant	
7	C_i	Concentration	$\frac{mol_i}{m^3}$
8	F_i	Rate of flow	$\frac{mol_i}{s}$
9	Q_i	Volumetric flow rate	$\frac{m^3}{s}$
10	K_i	Conductivity	mS
11	x_i	Conversion	

3. Single CSTR Reactor

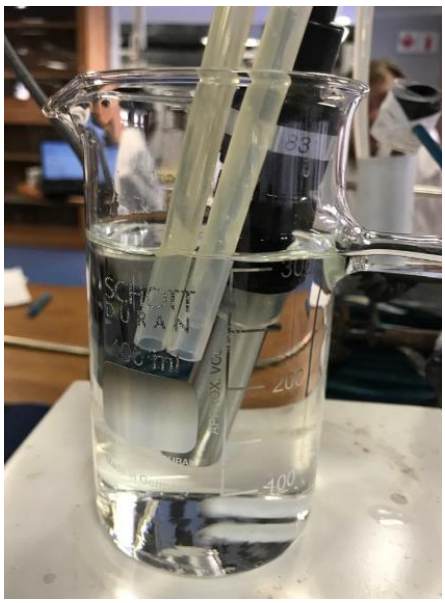

Figure 1: Single CSTR set-up

Steady state conductivities were recorded at flowrates of 24-, 30-, 50-, and 60 mL/min
The experimental conversion rates were calculated with

$$x = \frac{K_{start} - K}{K_{start} - K_{final}} \tag{1}$$

These data were plotted using python. A theoretical kinetics graph was drawn using the following equations

$$F_{i0} - F_i = r_i V \tag{2}$$

$$C_{i0} - C_i = \frac{r_i V}{Q} = r_i \tau \tag{3}$$

$$r_A = -k C_A^n C_B^m \tag{4}$$

A theoretical concentration profile was fitted onto the experimental concentration profile by changing the values of k, m, and n. The results of which are shown in Figure 2.

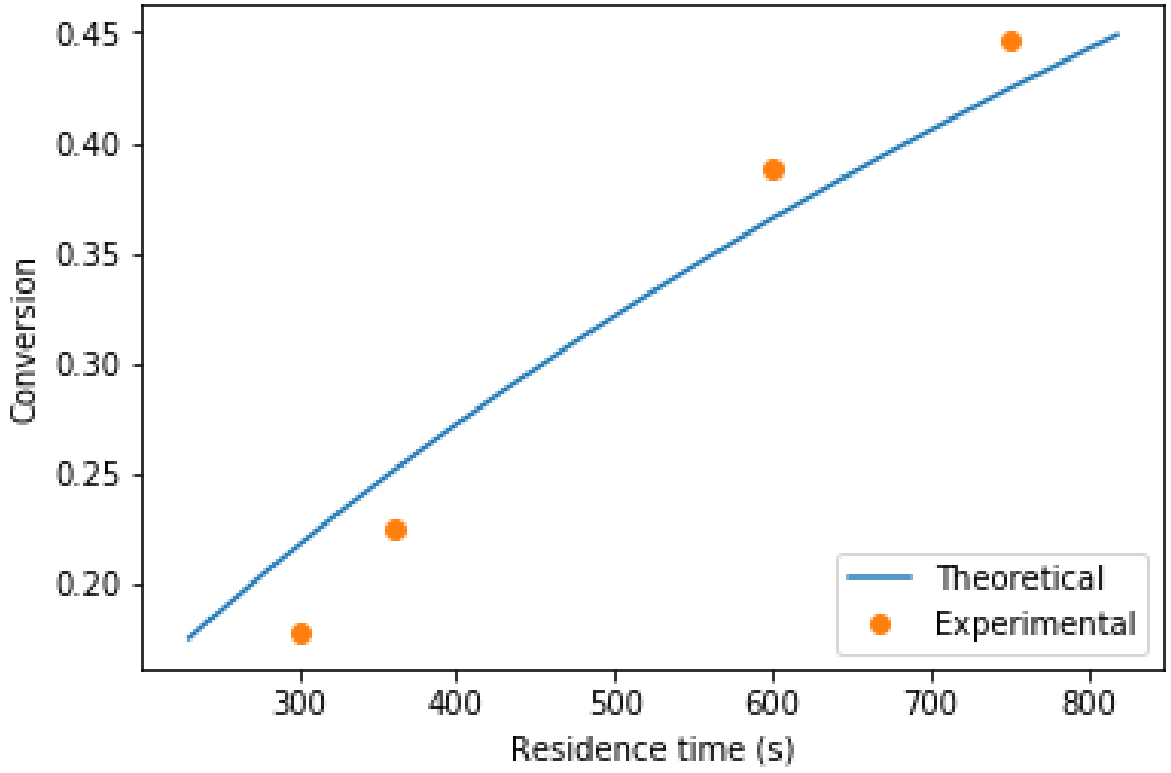

Figure 2: Conversion vs time for a single CSTR

Theory would predict that conversion should be higher for longer residence times (slower flow rates). The line of best fit shows that the conversion is predicted to be higher than what the experimental results show at longer residence times and lower conversions are predicted than the experimental results at shorter residence times.

The results of the fitted curve are tabulated in Table 1.

Table 1: Single CSTR curve fit results

Symbol	Value	Units
$\boldsymbol{k}$	0.0114	$\frac{L}{mol.s}$
$\boldsymbol{m}$	2	
$\boldsymbol{n}$	0	
$\boldsymbol{V}$	300	mL
$\boldsymbol{C_A}$	0.08	$\frac{mol}{m^3}$
$\boldsymbol{C_B}$	0.04	$\frac{mol}{m^3}$
$\boldsymbol{Error}$	$1.32 * 10^{-6}$	

4. Two CSTR's in Series

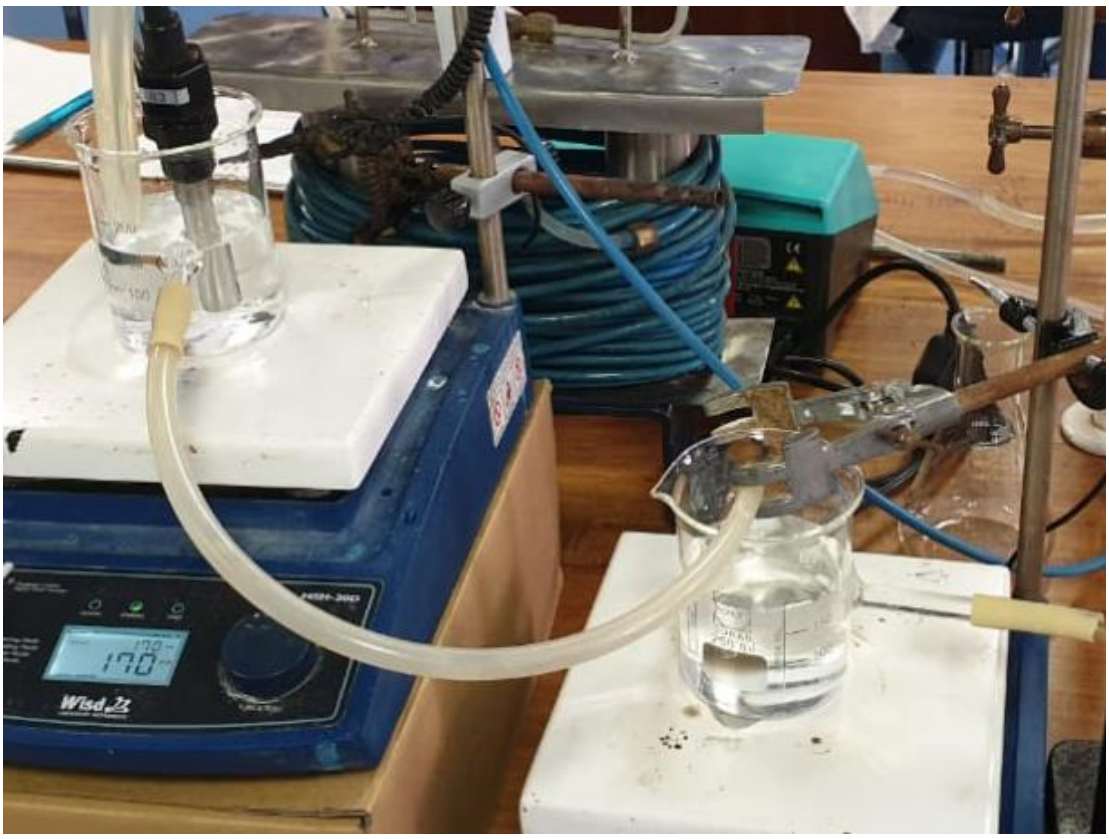

Figure 3: Two CSTR's in Series

The k, m and n values obtained from the single CSTR kinetics analysis was used to graph the predicted conversion profile against the overall experimental data as seen in Figure 4 below.

When observing the results over both CSTR's, the theoretically predicted conversion is much lower than that of the experimental data. When looking at the individual CSTR's, it was noted that CSTR1 had a higher conversion rate than what was predicted and CSTR2 had a lower conversion rate than predicted. The reaction rate is much greater in CSTR1 than CSTR2. The deviation from what was predicted could possibly be from an observed oscillation in the volume of CSTR1. This would mean that the residence time is higher in CSTR1 which would lead to a higher conversion than predicted, and also a lower conversion than predicted in CSTR2. Overall, the residence time is higher because of the oscillating holdup which may account for the higher conversion rates.

For a repeat of the experiment, it is considered that the spouts on the beakers should be in line with the bottom and the outlet pipes should be below the fluid level in each respective CSTR. This may reduce the oscillation of flow.

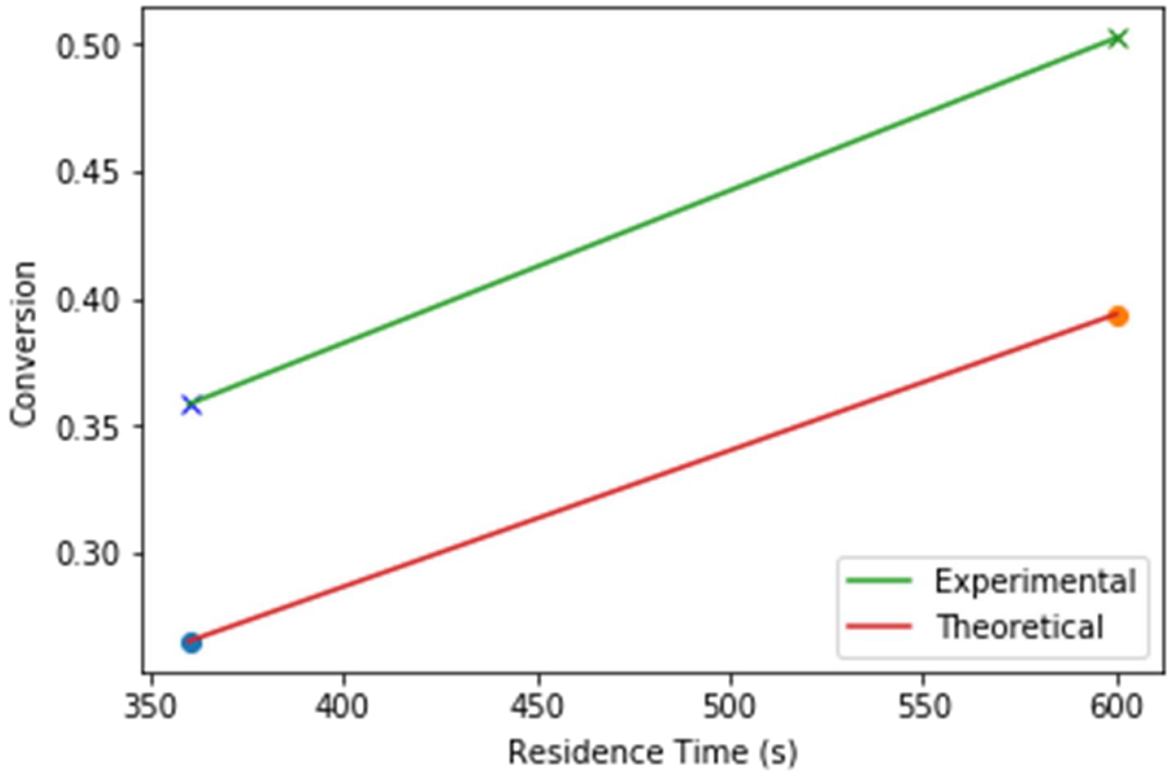

Figure 4: Conversion vs Time for 2 CSTR's in series

5. Batch Reactor

Figure 5: Batch Reactor

The following equations was used for the batch reactor

$$\frac{1}{V}\frac{dN_B}{dt} = r_B = -k\, C_A^m C_B^n \qquad (5)$$

The reaction for the batch experiment was run for more than an hour. The theoretical prediction for conversion was again lower than the data showed. The experimental conversion was 93% where the theoretical prediction based on the CSTR k, m, and n values was 79%. The conversion profile is shown in Figure 6 below.

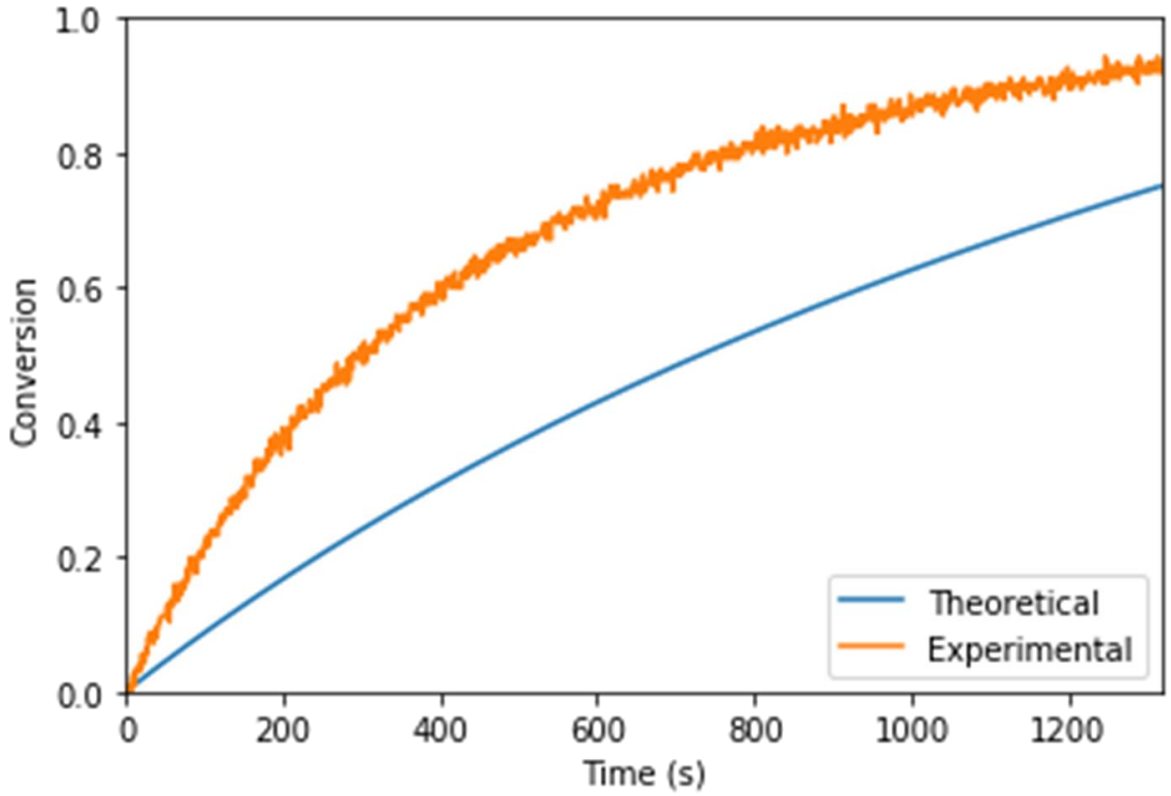

Figure 6: Conversion vs time profile for the Batch Reactor

Since the batch reactor is the simplest of all the reactors analysed, it could easily be presumed that less can go wrong, therefore, it is easier to control which would lead to more reliable predictions of k, m, and n values. A repeat experiment to develop a kinetics model should begin with a batch experiment for this reason.

6. The PFR reactor

The analysis of the PFR reactor made use of the following equation

$$\frac{dC_B}{dV} = \frac{r_B}{Q} = -\frac{k * C_A^n C_B^m}{Q} \tag{6}$$

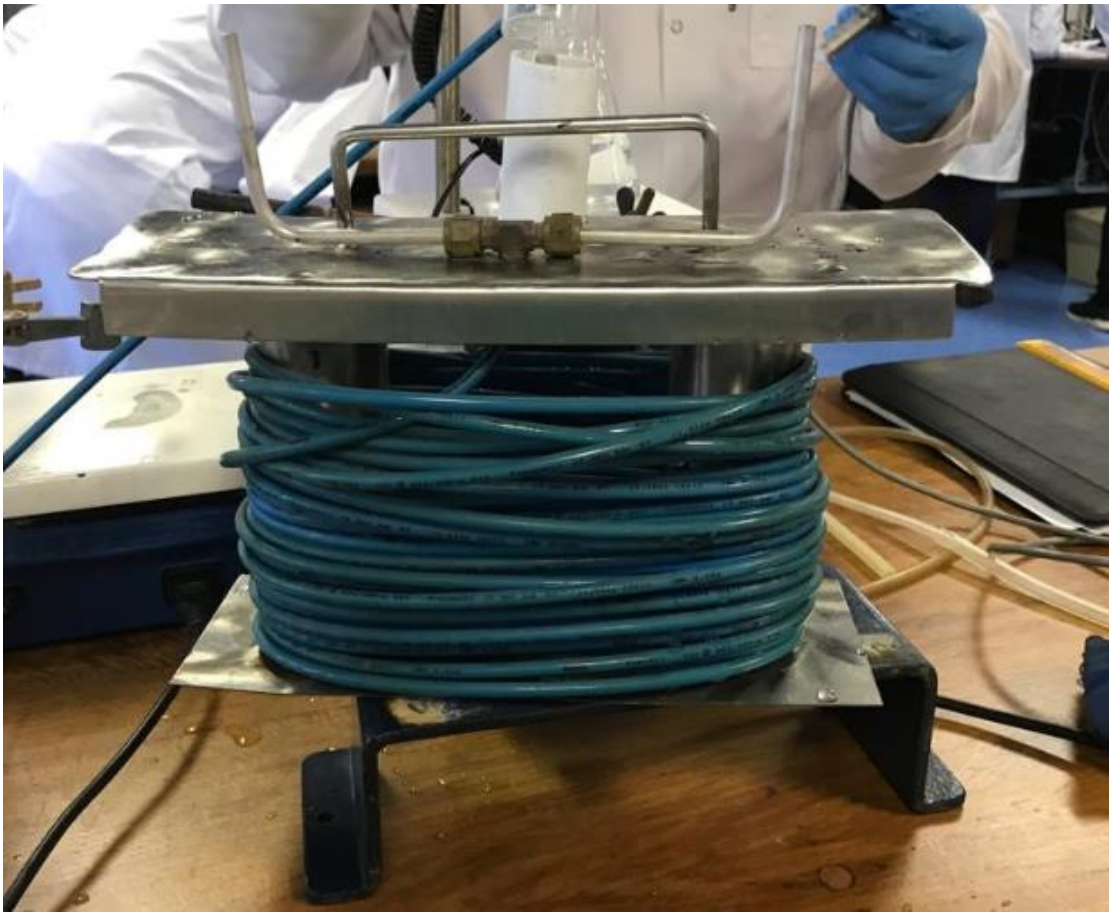

Figure 7: PFR reactor

The volume of the PFR was determined both by calculating the internal volume with a length of 20m and an internal diameter of 4mm. The total volume would be 251mL. The PFR was also filled then the emptied contents where measured to be approximately 261mL.

Once again, the theoretical conversion predictions was much lower for the two respective residence times measure, as shown in Figure 8 below.

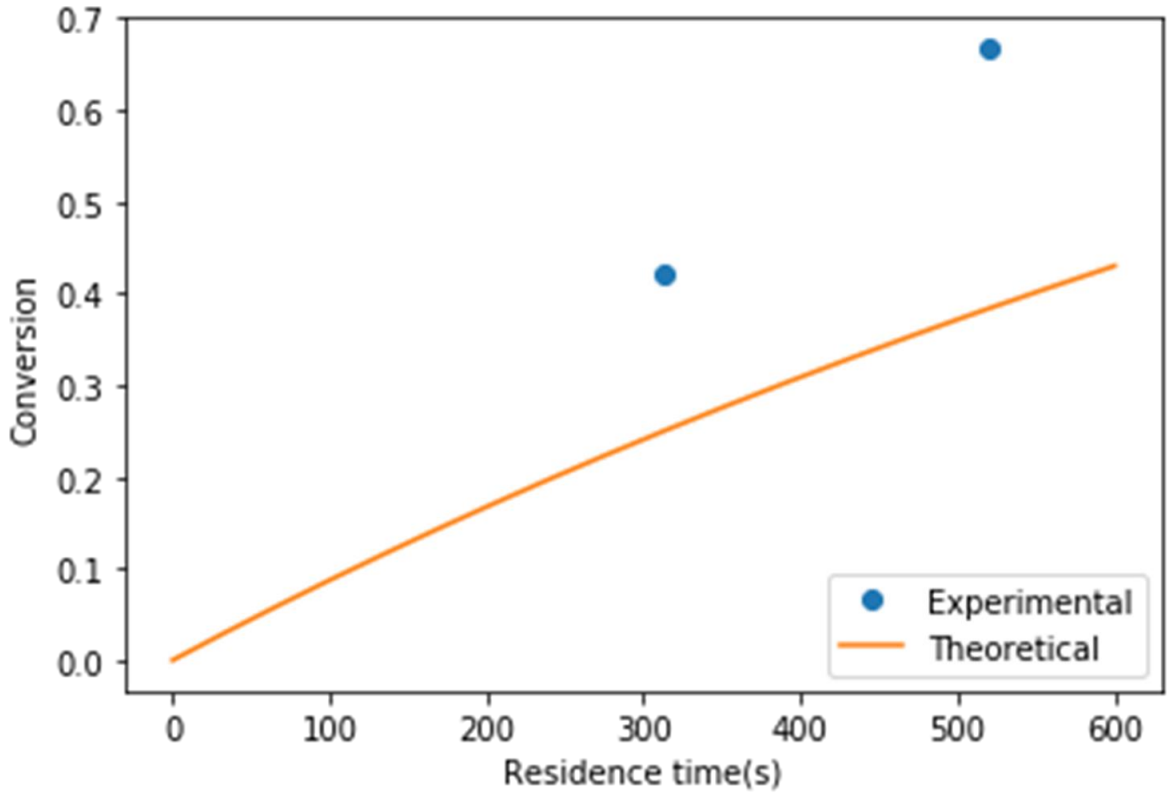

Figure 8: Conversion vs Time for the PFR reactor

7. Final discussion and possible recommendations

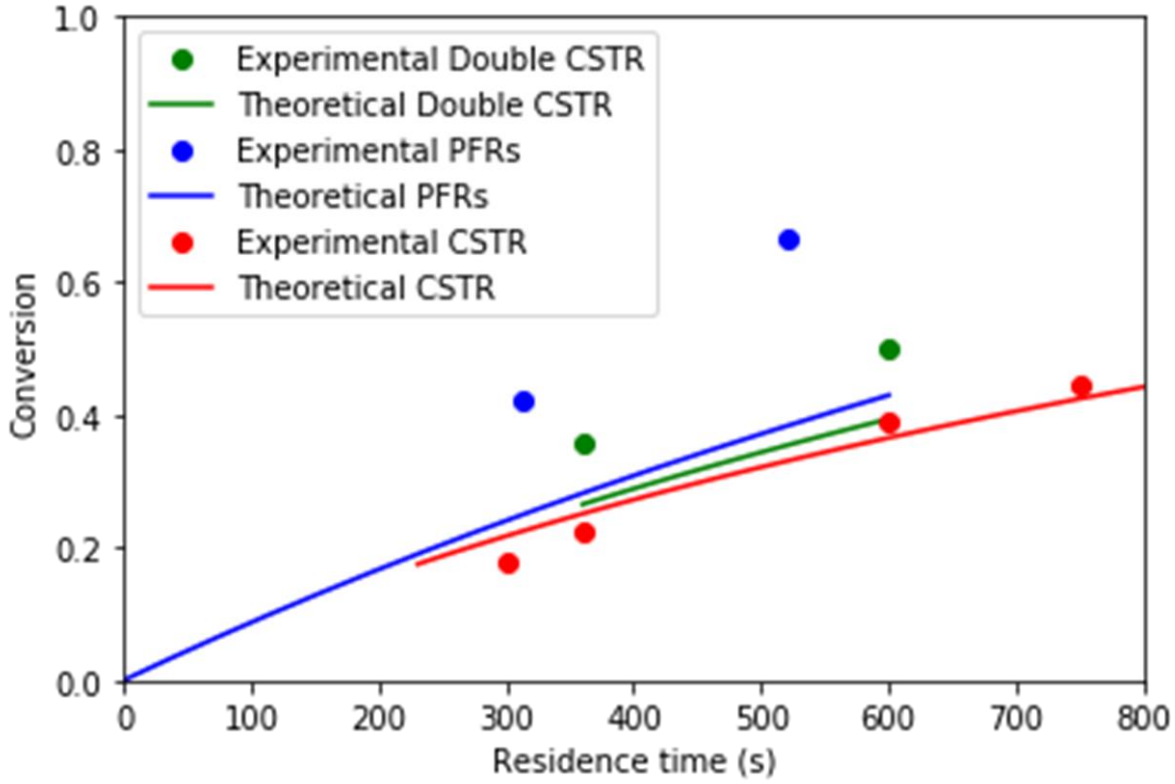

Figure 9: Combined Results for the PFR, CSTR and Batch reactors

Starting the kinetics modelling with the single CSTR already shows the theoretical best fit is less than ideal. From this point alone, one could expect that using the resulting kinetics model may not predict the kinetics across the other reactor set-ups.

As expected, the overall conversions predicted are much lower than what the data from the series CSTR and PFR showed. Additional physical problems with the set-ups are likely to have exacerbated the deviation from what the model predicted.

The peristaltic pump used for the PFR experiment was assumed to pump both inlets at the same rate. The physical calibration allowed only for one inlet or total inlet to be measured and related to the rpms of the pump. Measuring the amount of feed and product to perform a mass balance around the pump should be done to ensure that the calibration is correct.

The possible issues with the CSTR's in series were discussed in the results above. The peristaltic pump used here will also affect the results if the calibration is unreliable. In addition, the oscillation of the flow needs to be eliminated to ensure the volumes on both CSTR's, and therefore the residence times, remain constant which would allow more accurate predictions of conversion.

Besides ensuring that the pump is correctly calibrated to ensure the correct flow of both species is ensured, the actual concentration of the feeds need to be verified. If the feed

concentrations provided are not accurate, there is no way a reliable kinetics model can be developed.

In addition, it may be desirable to develop the kinetics model on the batch reactor as the set-up is the simplest and it does not rely on the peristaltic pump. By lowering the number of factors that affect the experiment, it would be reasonable to assume the kinetics model that can be developed would approximate the physical results more closely than the experiments performed above.

The conductivity probes used by two different groups performing the same experiments showed different conductivity readings for sodium hydroxide of the same concentration. As there is no way to know which one is correct, new probes that have been calibrated correctly can be recommended before repeating these experiments.

Last, but not least, human error is always a possibility, therefore, more repetitions of the experiment would be required.

8. References

Fogler, HS (2006), *Elements of Chemical Reaction Engineering*, 4th edition, Prentice Hall, USA.