401 Report Outline

Commented [GC1]: Reminder: Insert table of contents and title page after finished

1.0 Introduction

· Introduce/discuss the saponification reaction

· Introduce/discuss the reactor types – Batch, CSTR, PFR (design features, pro's/con's, industrial uses)

· Introduce/discuss the usage of conductivity to measure the extent of reaction

· Introduce the specific technical objectives

2.0 Experimental Methodology

2.1 Equipment and Apparatus

· Present process flow diagrams or annotated photo's for each reactor system and highlight the reactor vessel, feed tanks, feed streams, product stream, mixers, temperature probe, conductivity probe, temperature control system, and flow control system

· Brief narrative to introduce the reactors and the key components noted above (be sure to indicate the size of the respective reactors). **Note – discussion of the sequential procedures is not necessary.**

2.2 Operating Variables

· Indicate the reactants used and feed concentrations

· Summarize the operating conditions investigated for each reactor system (temperatures, flow rates, mixing speed, batch time or residence time)

3.0 Results

(Note: Where specified, a figure is required. Tables are recommended for the remaining parameters to efficiently summarize results for the respective trials. Present results using the specified units of measure.)

3.1 Thermodynamic Analysis

· Using the thermodynamic data posted on Courseweb, estimate the heat of reaction and the standard Gibbs free energy change of the reaction (kJ/mol)

· Using the Gibbs free energy change of the reaction, estimate the equilibrium constant (K_{eq}) at room temperature, 35C, and 45C

· Using K_{eq}, estimate the equilibrium conversion for the reaction at each reaction temperature

· Estimate the adiabatic reactor temperature at the equilibrium conversion

3.2 Batch Reactor

· **Plot of conversion versus time** for each reaction temperature (combine the three reaction temp's on one plot for each lab session)

· **Plot of 1/C_{NaOH} versus time** for each session **(use the data from the first three minutes)**. Combine the three reaction temp's on one plot for each lab session.

· Reaction rate coefficient 'k' (L/mol-sec) for each reaction temperature

· Activation energy estimate (kJ/mol)

· Productivity versus reaction temperature (to achieve a conversion of 70%) – moles NaAc/time/reactor volume (mol NaAc/L-min)

3.3 Old CSTR

· **Plot of steady-state conversion (%) versus reaction temperature**. **Combine the results for each session/residence time on one plot to facilitate comparison.**

· Residence time (min) versus flow rate (mL/min)

· Reaction rate coefficient 'k' (L/mol-sec) for each reaction temperature

· Activation energy estimate (kJ/mol)

· **Plot of steady-state productivity versus reaction temperature – moles NaAc/time/reactor volume (mol NaAc/L-min). Combine the results for each session/residence time on one plot to facilitate comparison.**

3.4 New CSTR

· Steady-state conversion (%) for single CSTR, CSTR's in series (conversion in each individual reactor and overall conversion)

· Residence time (min) versus flow rate (mL/min)

· Steady-state productivity for single CSTR, overall result for CSTR's in series – moles NaAc/time/reactor volume (mol NaAc/L-min)

· **Levenspiel plots (1/R vs. X) for each session comparing the individual series reactors versus the single reactor (see example)**

3.5 PFR

· **Plot of steady-state conversion (%) versus reaction temperature**. **Combine the results for each session/residence time on one plot to facilitate comparison.**

· Residence time (min) versus flow rate (mL/min)

· Reaction rate coefficient 'k' (L/mol-sec) for each reaction temperature

· Activation energy estimate (kJ/mol)

· **Plot of steady-state productivity versus reaction temperature – moles NaAc/time/reactor volume (mol NaAc/L-min). Combine the results for each session/residence time on one plot to facilitate comparison.**

3.6 Statistical Analysis ***(Final Report only)***

· Develop 95% confidence intervals for the reaction rate coefficients (at RT, 35C, 45C) and the activation energy

· Use the Arrhenius expression derived from literature data to estimate values for the reaction rate coefficient at room temperature, 35C and 45C

· Compare the 95% CI results for activation energy and k with the literature values/estimates

4.0 Analysis & Discussion

(Use sub-sections to organize your discussion. Refer to the Technical Report Guidelines for structure and flow)

4.1 Thermodynamic Analysis (T.O. #1)

· Discuss your findings and implications for the saponification reaction

4.2 Batch Reactor (T.O. #2)

· Discuss your findings and provide some quantification of trends and comparisons

· Propose explanations for your observations based on governing principles (batch reactor design principles, temperature effect, Arrhenius, etc.)

4.3 Old CSTR (T.O. #3)

· Discuss your findings and provide some quantification of trends and comparisons

· Propose explanations for your observations based on governing principles (CSTR design principles, temperature effect, residence time effect, Arrhenius, etc.)

4.4 New CSTR (T.O. #4)

· Discuss your findings and provide some quantification of trends and comparisons

· Propose explanations for your observations based on governing principles (residence time effect, single vs. cascade design, etc.)

4.5 PFR (T.O. #5)

· Discuss your findings and provide some quantification of trends and comparisons

· Propose explanations for your observations based on governing principles (PFR design principles, temperature effect, residence time effect, Arrhenius, etc.)

4.6 Reactor Comparisons (T.O. #6)

· Compare the results across reactor types. Identify trends for conversion and productivity versus reactor type

· Identify optimum reactor-type/operating parameters for conversion and productivity

*4.7 Stat. Analysis and Literature Value Comparison **– FINAL REPORT ONLY** (T.O. #7)*

· Compare the 95% confidence intervals for activation energy and reaction rate coefficient to the literature values/estimates and discuss your findings.

5.0 Summary & Conclusions

- Follow the approach outlined in the Technical Report Guidelines
- Briefly summarize key findings for each technical objective
- Use some quantification to dimensionalize key trends (e.g., %'s for comparisons)

6.0 Future Work (Progress Report Only)

7.0 References

8.0 Appendix

(Note: Due to the length of the reports, inclusion of experimental data is not required)

8.1 Appendix – Sample Calculations

8.1.1 Thermodynamic Analysis

- Estimate of the heat of reaction and the standard Gibbs free energy change of the reaction
- Estimate of the equilibrium constant (K_{eq}) and equilibrium conversion
- Estimate the adiabatic reactor temperature at the equilibrium conversion

8.1.2 Batch

- Temperature corrected lambda values for NaOH and NaAc
- Point in time conversion from conductivity data
- Plot of versus time to determine 'k'
- Plot of ln(k) versus 1/T to determine Ea
- Productivity calculation at 70% conversion

8.1.3 Old CSTR

- Temperature corrected lambda values for NaOH and NaAc
- Steady-state conversion from conductivity data
- Residence time calculation
- Determination of 'k' from steady-state data
- Plot of ln(k) versus 1/T to determine Ea
- Productivity calculation at steady-state

8.1.4 New CSTR

- Temperature corrected lambda values for NaOH and NaAc
- Steady-state conversion from conductivity data for single CSTR and CSTR's in series

- Residence time calculation for single CSTR and CSTR's in series
- Productivity calculation at steady-state for single CSTR and CSTR's in series

8.1.5 PFR

- Temperature corrected lambda values for NaOH and NaAc
- Steady-state conversion from conductivity data
- Residence time calculation
- Determination of 'k' from steady-state data
- Plot of ln(k) versus 1/T to determine Ea
- Productivity calculation at steady-state

8.1.6 Statistical Analysis **(Final Report Only)**

- 95% confidence interval determination for the reaction rate coefficients and the activation energy
- Include an example of a reaction rate coefficient estimate using the Arrhenius expression derived from literature.

Example Levenspiel plot for New CSTR: