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Mathematica as an Efficient Tool to Optimize the Kinetic Study of Ethyl Acetate Hydrolysis

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ABSTRACT

Mathematica is a powerful program for computing both numeric and algebraic calculations as well as graphing two and three dimensional curves and surfaces. It is used increasingly in many fields of science now such as physics, engineering, chemistry and even biology because of the fast interaction of mathematics with almost the fields of science nowadays.

We report here, optimizing the kinetic data for the hydrolysis of ethyl acetate through caustic soda via using Mathematica.

Key words: Mathematica**,** Hydrolysis; Kinetics, Optimization.

INTRODUCTION

The kinetic study for the saponification reaction of ethyl acetate with caustic soda in order to produce ethanol and sodium acetate is considered as one of the main models for hydrolysis reactions. This reaction could be implemented using a liquid plug flow reactor. The significance of this reaction as one of the most important reactions in the field of industrial and applied chemistry is due to the fact that ethanol which is considered as a strategic material in chemical process industries. Ethanol is simply reacts with acetic acid producing ethyl acetate and sodium acetate where both can be used in several applications including soap production. [1-19]

The chemical kinetics is investigated via extensive study for reaction rate and its dependence on the reaction speed, temperature, flow rate, and concentration. [20-28] The alteration of those previously mentioned parameters will lead to optimized process and hence obtain better results.[29-37]

Factors like time and cost are considered as decisive factors that are controls adoption of process design and also to decide the applicability of certain synthetic routes or eliminate others.

However, a batch distillation is used to separate ethanol from sodium acetate in saponification reaction, ethanol can also reacts in a continuous flow reactor with acetic acid in order to produced ethanol again. [38-45]

2. EXPERIMENTAL

A mixture containing ethyl acetate and sodium hydroxide (1:1) was introduced in a flow basis while using a concentration of 0.1 M for both ethyl acetate and sodium hydroxide. The temperature was then altered within the range 20 - 60 °C. [45]

3. RESULTS AND DISCUSSION

Mathematica is used to obtain more accurate and optimized results. The arte constant is simply calculated from the obtained concentration results as shown in Figure 1 based on the calculated results from Table 1. [45]

Table 1: The Effect of Time on Reaction at 30°C

Time (min)	V (NaOH)	C	1/C
10	7.2	0.078	12.82051
15	7.3	0.077	12.98701
20	7.5	0.075	13.33333
25	7.6	0.074	13.51351
30	7.7	0.073	13.69863

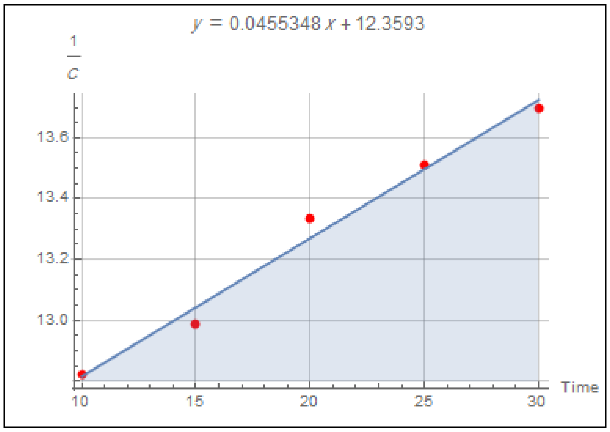

Figure 1: Relation between Concentration – Time at 30 °C.

The slope is simply calculated as follows:

K = slope = 0.0457 dm^3/mol.min = 0.000762 L/mol.s

$$\frac{1}{c} - \frac{1}{c_0} = 0.000762t$$

Similarly, Mathematica is used to obtain more accurate and optimized results. The arte constant is simply calculated from the obtained concentration results as shown in Figure 2 based on the calculated results from Table 2. [45]

Table 2: The Effect of Time on Reaction at 40°C

t (min)	V (NaOH)	C	1/C
10	7.5	0.075	13.33333333
15	7.6	0.074	13.51351351
20	7.7	0.073	13.69863014
25	7.8	0.072	13.88888889
30	8.3	0.067	14.92537313

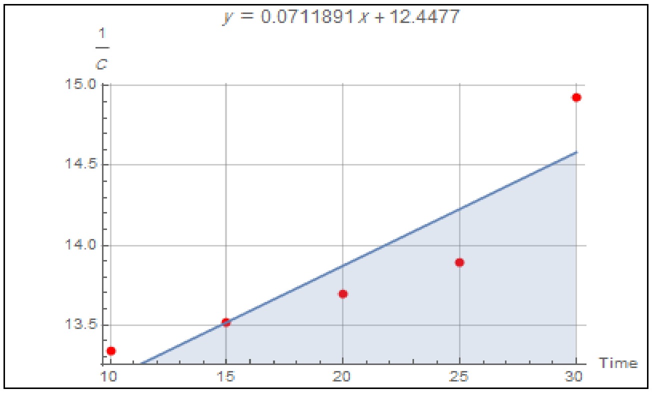

Figure 2: Relation between Concentration – Time at 40 °C.

From the equation of the line in figure 2, the slope could be calculated as follows:

K = slope = 0.0712 dm^3/mol.min = 0.001187 L/mol.s

$$\frac{1}{c} - \frac{1}{c_0} = 0.0001187t$$

Similarly, Mathematica is used to obtain more accurate and optimized results. The arte constant is simply calculated from the obtained concentration results as shown in Figure 3 based on the calculated results from Table 3. [45]

Table 3: The Effect of Time on Reaction at 50°C

t (min)	V (NaOH)	C	1/C
10	8	0.07	14.28571
15	8.4	0.066	15.15152
20	8.5	0.065	15.38462
25	8.7	0.063	15.87302
30	9	0.06	16.66667

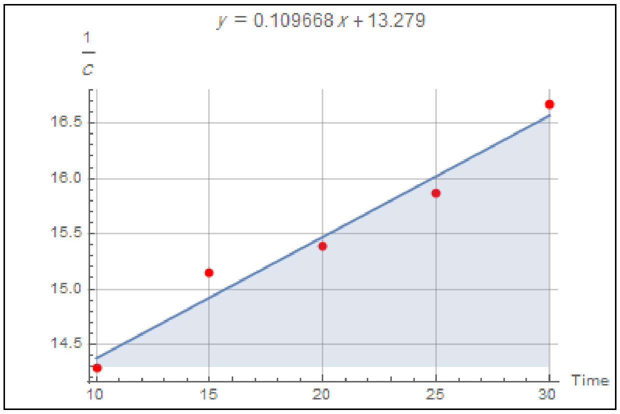

Figure 3: Relation between Concentration – Time at 50 °C.

From the equation of the line in figure 3, the slope could be calculated as follows:

K = slope = 0.0712 dm^3/mol.min = 0.0022 L/mol.s

$$\frac{1}{c} - \frac{1}{c_0} = 0.0022t$$

Similarly, Mathematica is used to obtain more accurate and optimized results. The arte constant is simply calculated from the obtained concentration results as shown in Figure 4 based on the calculated results from Table 4. [45]

Table 4: The Effect of Time on Reaction at 55°C

t (min)	V (NaOH)	C	1/C
10	8.2	0.068	14.70588
15	8.5	0.065	15.38462
20	8.7	0.063	15.87302
25	8.9	0.061	16.39344
30	9.3	0.057	17.54386

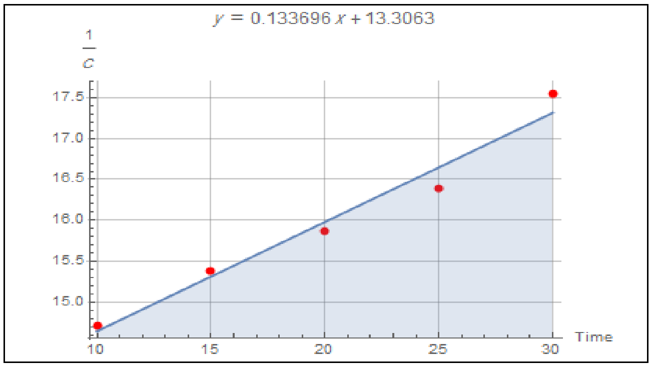

Figure 4: Relation between Concentration – Time at 55 °C.

From the equation of the line in figure 4, the slope could be calculated as follows:

K = slope = 0.0712 dm^3/mol.min = 0.001187 L/mol.s

Table 5: Calculated Results at Different Reaction Temperatures.

T	K	1/T	ln K
303	0.000762	0.0033	-7.17956
313	0.001187	0.003195	-6.73633
323	0.0018	0.003096	-6.31997
328	0.002	0.003049	-6.21461

The data in Table 6 are linearly interpolated with *Mathematica 10* to get a relation between the slopes k of the reactions with the temperature, and the data with the corresponding line are plotted in figure 5.

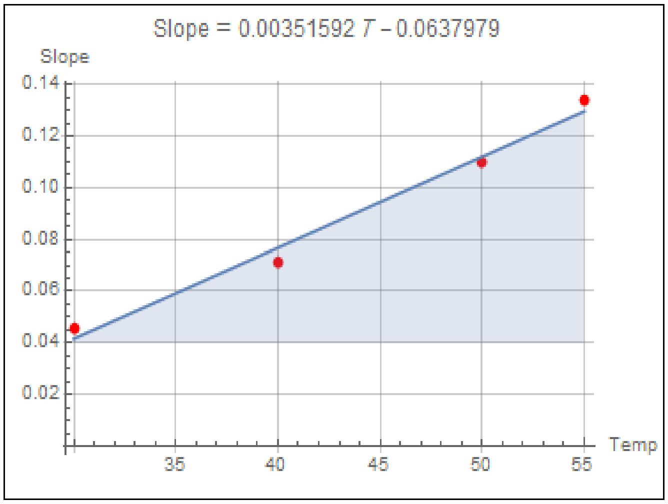

Figure 5: Representation of Slope – Temperature data

Plot between ln K vs. 1/T to ensure that the reaction is second order reaction.

In table 5, the values of the calculated slopes k are given with the temperature at each reaction

$$\frac{1}{c} - \frac{1}{c_0} = 0.001187t$$

The activation energy of the reaction was investigated using Arrhenius equation. The proposed kinetic model was found to be second order kinetic model based on the experimental data that were processed in order to find a relation between ln(k) and (1/T) as shown in Figure 6.

Table 6: values of the calculated slopes k are given with the temperature at each reaction

T (℃)	30	40	50	55
K (dm^3/mol . min.)	0.0455348	0.0711891	0.109668	0.133696

From the equation in figure 5, we find that the slopes increase with the temperature with a rate of change 0.0035192

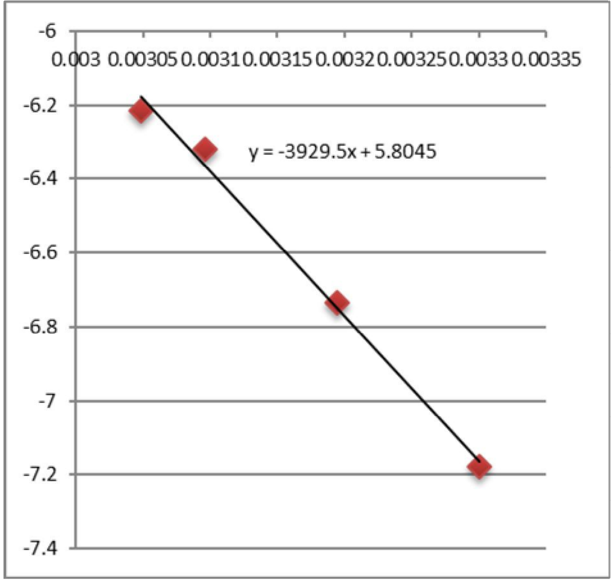

Figure 6: Activation Energy Based on Second Order Kinetic Model.

Since the plotted data gives a straight line between ln k vs. 1/T, then the experiments follow Arrhenius correlation and the Slope = - E/R = - (-3929.5), So, E = (8.314) (3929.5) = 32669.86 kJ/mol

4. CONCLUSION

In conclusion, Mathematica was used as a powerful program for computing both numeric and algebraic calculations in many fields of science now such as physics, engineering, chemistry and even biology.

We report here, optimizing the kinetic data for the hydrolysis of ethyl acetate through caustic soda via using Mathematica.

It was determined that the order of the reaction is a second-order reaction.

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