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PRODUCTION OF EPOXIDIZED PALM OIL – DERIVED OLEIC ACID BY USING ACIDIC ION EXCHANGE RESIN (AIER) : EPOXIDATION METHOD AND KINETIC STUDY

Muhammad Amir Syazwan Bin Che Mamat Azman, Jumain Bin Mohd Jalil and Aliff Farhan Bin Mohd Yamin

Faculty of Chemical Engineering, Universiti Teknologi MARA, Cawangan Pulau Pinang, 13500 Permatang Pauh, Pulau Pinang Malaysia

**Corresponding author: jumain.jalil@gmail.com*

Abstract:

This research done to study the epoxidation reaction for different parameters such as type of catalyst used and agitation speed. The fatty acid content in vegetable oil will undergo epoxidation reaction to produce epoxide. The process start with the formic acid (FA) will react with hydrogen peroxide (H2O2) in order to produce performic acid (PFA) in aqueous and side product is water (H2O). Then, transfer of acid in aqueous ,PFA (aq) to the oil phase, PFA (oil). Meanwhile, the PFA (oil) will react with oleic acid (OA) to produce epoxy oleic acid (EOA) and formic acid (FA) in oil phase. Finally, the transfer of carboxylic acid to the aqueous phase. Besides, kinetic study also be carried by develop a single phase kinetic model to determine the value of kinetic rate constant, k for every reaction via MATLAB simulation. From the results of simulation data, this research highlights on the comparison between experimental and simulation data that has been obtained. In addition, effect of catalyst used and different level of agitation speed on the value of k also has been studied.

***Keywords*:**

Epoxidation, catalyst ,agitation speed, kinetic model, kinetic rate constant, MATLAB simulation

Objectives:

- To develop kinetic model for epoxidation process of palm oil by using MATLAB simulation.
- To study relation parameters for type of catalyst used and agitation speed for the epoxidation process by simulated data.

Methodology:

The process flow illustrate on the epoxidation of palm oil based on kinetic model by using MATLAB simulation and effect of related parameters to the value of kinetic rate constant, k

Objective 1 : To develop kinetic model by using MATLAB simulation

1. Develop differential equation d[C] / dt
2. Solve the equation d[C] / dt
3. Analyse the results of simulation data
4. Plot graph OOC concentration versus time
5. Comparison between experimental and simulation data

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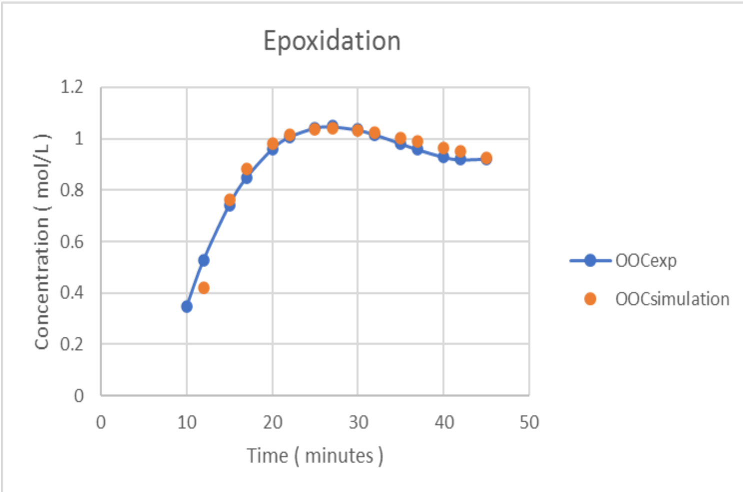
Objective 2 : To study relation parameters for type of catalyst used and agitation speed for epoxidation by simulated data

1. Plot graph value of k versus type of catalyst used
2. Plot graph value of k versus agitation speed

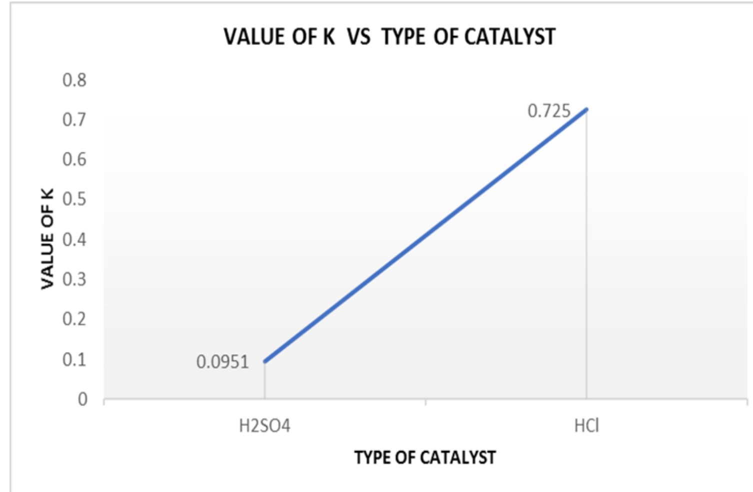
Results:

Table 1 : Results of simulation data

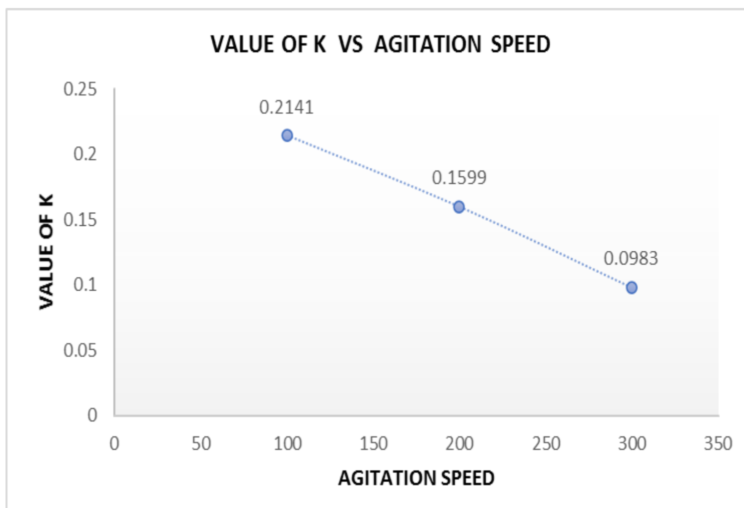
Exp	Initial Concentration			k_{11}	k_{12}	k_{21}	k_{31}	Error Min	Concentration of Epoxy
	H_2O_2	FA	OA						
1	1.4714	1.4714	2.9484	0.3089	0	0.2141	0	0.1350	0.6086
2	1.4714	1.4714	2.9484	0.2664	0	0.1599	0	0.1098	0.5554
3	1.4714	1.4714	2.9484	14.9454	0.1787	0.0983	0.0479	0.1093	0.7041
4	1.4714	2.9484	2.9484	8.9078	3.2367	0.0951	0.2407	0.1520	0.5399
5	1.4714	2.9484	2.9484	3.4512	5.4238	0.7250	0.0533	0.2501	0.7692
6	1.4714	2.9484	2.9484	14.3052	7.8131	0.2318	0.0010	0.2152	0.6227
7	1.4714	4.4226	2.9484	10.0314	13.1145	0.2685	0.0052	0.1616	0.6181
8	1.4714	4.4226	2.9484	15.0000	0.2208	0.0750	0.5547	0.1008	0.8181
9	1.4714	4.4226	2.9484	4.8041	1.0138	0.2393	0.0029	0.2474	0.6348
10	2.9484	1.4714	2.9484	5.1452	1.1228	0.1584	0.1958	0.1548	0.8159
11	2.9484	1.4714	2.9484	15.0000	0.3457	0.4218	2.4105	0.2720	0.6861
12	2.9484	1.4714	2.9484	14.9916	0.0670	0.1715	0	0.2300	0.6754
13	2.9484	2.9484	2.9484	14.1367	0.2656	0.2851	0	1.8325	1.4702



Graph 1 : Comparison between experimental and simulation data



Graph 2 : Effect of type of catalyst to the value of k



Graph 3 : Effect of agitation speed to the value of k

Conclusion:

There were 13 experiments that being run in the MATLAB simulation to ensure the result with the optimum value. The experimental data that obtained from the previous experiments being used as a raw data for running the simulation . The initial concentration of hydrogen peroxide, formic acid and oleic acid were used the value from the previous experiment as a reference to find value of kinetic rate constant, k . From all the experiments that being run ,experiment 8 was chosen as the best one based on optimized epoxidation result obtained where it recorded the lowest error compared to other experiments which only 0.1008 . The kinetic rate constant for this experiment 8 were k_{11} = 15.0000 mol/ L. min, k_{12} = 0.2208 mol/ L. min, k_{21} = 0.0750 mol/ L. min, k_{31} = 0.5547 mol/ L. min . The concentration of epoxy that obtained from this simulation was 0.8181 mol/L.

Based on the graph 1, illustrated the comparison between the epoxy concentration from the lab experiments and simulation based on the kinetics value that were obtained in table 1 . This graph shown the best fit and less error between experiment and simulation data based on experiment 8. The graph also shown the data between experiment and simulation in the formation of epoxidation occurred at the range of 20 minutes to 40 minutes ,there was no significant difference and lower deviation of the predicted simulation data from the experimental data. There were a few ideal assumption made for comparing the simulation data and environmental data by using numerical simulation . The operation in MATLAB simulation did not considered the heat transfer and heat loss during the reaction occur. Since the reaction was rely on overall chemical equation, the reaction of each particles were react at the same time. Meanwhile, in the experimental work, any vaporize gas cannot be determined. The duration for the epoxidation reaction and oxirane ring cleavage may take some time for each reaction to be converged. Furthermore, at 25 minutes the epoxide reaction began to form due to it was the highest peak. But at 30 minutes the reaction began to degrade where the simulation cannot be fitted to the experiment data. Due to the different in fundamental between the experiment and simulation where experimental work provided new empirical data while simulation cannot. The graph gradually increases alongside the reaction until the formation of epoxide. It was due to the concentration of formic acid causes the reaction rapidly increase and the epoxy yield also increase.

In epoxidation process, the effect of catalyst used lead to the different result on reaction rate as shown in graph 2. The strong concentration of catalyst used gives impact to the reaction rate where the higher concentration of catalyst will lead to the increasing value of reaction rate. With the higher concentration of catalyst lead to increase of the total surface area and total active sites in the reaction mixture, then increased the rate of the epoxy ring cleavage. Since the kinetic rate of epoxidation is proportional to the number of active sites, the value of k also increase. Based on the graph 2 ,hydrochloric acid (HCl) recorded the highest value of k by 0.725 while sulfuric acid (H_2SO_4) recorded the lowest value by 0.0951 . The number of oxirane content was higher by using HCl acid because H^+ ion of HCl could move freely so that it influenced the reaction to operate at optimum condition. The molecules of the reaction could collide with each other and enhance the kinetic rate of epoxidation reaction. Hydrochloric acid was classified as the most strong catalyst used in this epoxidation reaction. Besides, it was observed that with the increasing of catalyst concentration lead to the formation of oxirane oxygen, increase the double bond conversion and higher epoxy yield. Hence, HCl was the best homogeneous catalyst for acidic ion exchange resin with high selectivity to the reaction formation of epoxides .

To determine the effect of agitation speed on oxirane oxygen content (OOC) value of epoxide, there were three different level of agitation speed which were at 100 rpm, 200 rpm, 300 rpm as shown in the graph 3. In general, the degree of agitation speed increased the turbulence and surface area allows to the higher interfacial areas and mass transfer that occur between two different phases of the reaction. Thus, value of k also increase. For agitation speed, the relative conversion to oxirane (RCO) increase until reached the maximum limit with the increasing of the level of agitation speed. The highest value of reaction rate, k was at 100 rpm with the value of k at 0.2141. The lower value of k due to the slow agitation speed that cause a lower turbulence or due to the degradation of epoxide start to occur. The decreasing of reaction rate at 200 rpm with the value of k, 0.1599 and at 300 rpm with the value of k, 0.0983 may due to degradation of oxirane oxygen content. It was assumed that the reaction was free from mass transfer resistance under the given circumstance. Since the agitation speed was good and the reaction was under isothermally condition, the diffusional resistance between the different phase of aqueous phase and oil phase of performic acid reacted with oleic acid to form epoxidized oleic acid can be ignored.