SIIC096

KINETIC MODELLING OF DIHYDROXYSTEARIC ACID (DHSA) PRODUCTION FROM PALM KERNEL OIL-BASED OLEIC ACID

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Dihydroxystearic Acid (DHSA) is a chemical compound that belongs in the hydroxy fatty acid group which is mainly used in cosmetic industries. DHSA usually produced by the process of *in-situ* epoxidation of oleic acid, followed by the hydrolysis of the epoxidized oleic acid. This study focuses on the kinetic modelling of the production of DHSA. The purpose of this study is to establish a kinetic model of one-pot synthesis of DHSA via continuous *in-situ* epoxidation and hydrolysis process and to fit the kinetic model with the experimental data to obtain the reaction rate constants (*k*) and activation energy (*Ea*). Assumptions was made which then applied to the reaction scheme in order to develop a new reaction scheme for the kinetic model. MATLAB was the software used for developing the model where ODE45 function in MATLAB were used to solve the ordinary differential equation (ODE) by applying fourth-order Runge-Kutta method. From the model, reaction rate constants (*k*) were determined. The reaction rate constants (*k*) determined were then used to obtain the activation energy (E_a) of the reaction by constructing the Arrhenius plot for the reaction at temperature 55°C and 75°C.

***Keywords*:** Dihydroxystearic Acid (DHSA), epoxidation, kinetic modelling, reaction kinetics, activation energy .

Methodology: Basically, in developing kinetic model assumptions on the reaction process first needs to be made as the assumptions will be applied into the reaction scheme to developed a new reaction scheme. Ordinary differential equations (ODE) are then developed based on the new reaction scheme and by applying the rate law equation along with fourth-order Runge Kutta method. The kinetic model for DHSA production are then developed in MATLAB once the ODE have been developed. The ODE are solved by using the ODE45 function in MATLAB. Once the kinetic model generated, the kinetic model need to be fit with the experimental data. Fitting is perform in order to determine the reaction rate constants (k). Method used for fitting is non-linear least square regression method. The activation energy (Ea) was determined by plotting the Arrhenius plot in Microsoft Excel. The Arrhenius plot was plotted by plotting ln k vs 1/Temperature.

Results:

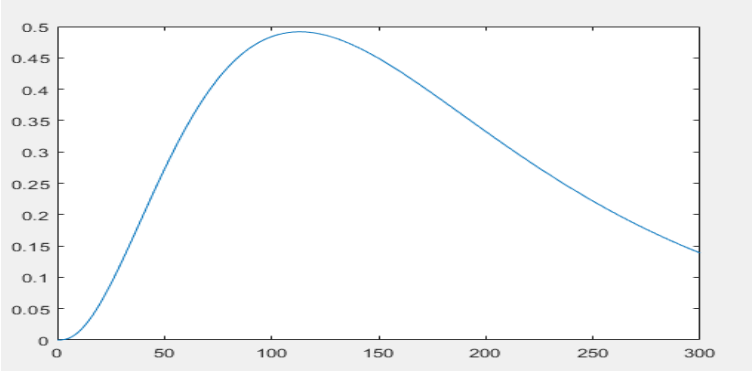

Figure 3.2.1 Curve generated from the model

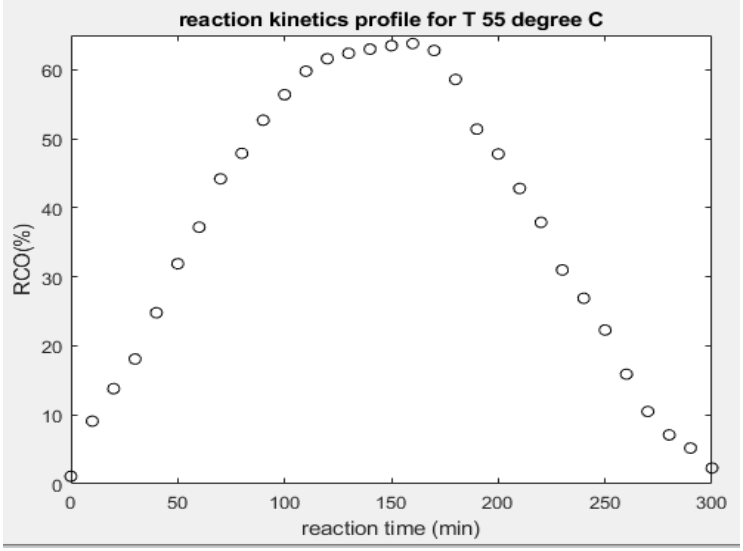

Figure 3.2.2 Curve plotted from experimental data

Table 3.3.1 Reaction rates constants (*k*) [22]

REACTION RATES	**T 65°C**	**T 75°C**
*k*1 (min^{-1})	7×10^{-4}	7.3×10^{-3}
*k*2 (min^{-1})	3.9×10^{-3}	8.60×10^{-3}
*k*3 (min^{-1})	1.48×10^{-1}	5.11×10^{-1}
*k*4 (min^{-1})	1.03×10^{-2}	2.17×10^{-2}
*k*5 ($M^{-1}.min^{-1}$)	2×10^{-4}	6.0×10^{-4}
*k*6 ($M^{-1}.min^{-1}$)	1.65×10^{-2}	2.83×10^{-2}
*k*7 (min^{-1})	3.95×10^{-2}	4.93×10^{-2}
*k*8 (min^{-1})	8.45×10^{-2}	8.63×10^{-2}

Table 3.3.2 Activation energy (*Ea*) for each reaction

REACTION NAMES	REACTION	ACTIVATION ENERGY (J/mol)
Performic acid formation (Forward reaction)	1	229283
Performic acid formation (Reverse reaction)	2	77332.7
Epoxidation	3	121177
Hydrolytic cleavage of the epoxy ring (DHSA formation)	4	72872.2
Cleavage of the epoxy ring (Degradation by formic acid)	5	107434
Cleavage of the epoxy ring (Degradation by performic acid)	6	52759
Thermal decomposition of formic acid (Forward reaction)	7	21672.9
Thermal decomposition of formic acid (Reverse reaction)	8	2061.29

Conclusion: DHSA is produced by the continuous epoxidation and hydrolysis of PKO and performic acid with the presence of hydrogen peroxide as oxidizing agent. DHSA can be applied in various types of industries but mostly can be found in cosmetic and polyurethane industries. Kinetic model for DHSA production is important in order to determine the reaction kinetics where the reaction kinetics is one of the important parameters used in reactor modelling. In this study the kinetic model for the production of DHSA was developed in MATLAB software where the ODE45 function in MATLAB were used to solved the ODE by applying the fourth-order Runge Kutta method. In this study the kinetic model managed to be generated however due to processor error in fitting the reaction rates constants (k) cannot be generated. The reaction rates constant (k) in this study were obtained from the previous study and then applied in Arrhenius plot to determine the activation energy (Ea). From the activation energy (Ea) determined, it can be concluded that the production of DHSA is a slow reaction process. This is due to the high number of activation energy (Ea) which makes the reaction under kinetic limited regime and free from mass transfer coefficient. As for recommendation, fitting needs to be performed with different methods or software to reduce the time taken to generate the reaction rate constants (k).