MODELLING AND OPTIMIZATION OF CITRONELLYL LAURATE ESTERIFICATION IN BATCH REACTOR

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AUTHOR'S DECLARATION

I declare that the work in the thesis was carried out in accordance with the regulation of Universiti Teknologi MARA. It is original and is the results of my own, unless otherwise indicated or acknowledge as reference work.

I, hereby acknowledge that I have been supplied with the Academic Rules and Regulations, Universiti Teknologi MARA, regulating the conduct of my study and research.

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SUPERVISOR'S CERTIFICATION

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ABSTRACT

Batch esterification reactors are frequently used in the food and pharmaceutical industries. In general, batch esterification is a complex process since the system involves a nonlinear dynamic behaviour due to its kinetic characteristics and unsteady state process. Due to these reasons, the modelling and optimization of the batch esterification reactor is difficult and the application of dynamic optimization is often more desired to control the dynamic nature of the batch process. Among all the advanced optimization strategies, model-based optimization techniques have been largely extended and have gained prominence during the past decades. In this work, an orthogonal collocation method was developed by using dynopt code package strategy as its optimization parameter structure. The batch esterification process was represented by the first principle model which involved kinetic, mass and energy balance equations. The results obtained from the kinetic studies indicated that the citronellyl laurate esterification process follows an ordered bi-bi mechanism with R^2 value of 0.982. Then, the first principle model equations are solved using the 4^{th} order Runge-Kutta method which is available in the MATLAB and has been validated with experimental data with an average R^2 value of 0.9793. The validated first principle model was used to study the dynamic behaviour of the esterification process and it was found that the ester conversion increased with increasing reactor temperature and reaction time. Three different objective functions were employed to be simulated in this optimization which are maximum conversion rate of citronellyl laurate, minimum reaction time to achieve highest conversion rate, and maximum process profits in form of minimum reactant cost. The maximum conversion rate of citronellyl laurate that can be achieved in the simulation was 89.81% for around 49.059 minute in optimum temperature of 312.0058 K. Citronellol was identified as the limiting reactant by which the degree of dilution of citronellol and lauric acid are 90% and 11.25% respectively from its initial concentration. In order to study the minimum time required to reach specified conversion, the maximum rate of conversion that was proposed to be 97%. It was observed that the reaction must be carried out for 76.28 minutes for the simulation to reach the targeted conversion which are 97%. Finally, as the relative cost for β-citronellol in the industry was RM 3.2463/M, minimum reactant cost that could be obtained from the optimized process was RM 0.0019/M. As a conclusion, the dynamic optimization was able to fully condone the intrinsic nature of batch process and suitable to be implemented in future online optimization.