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# Abstract

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This Thesis is focused on several aspects of enzymatic esterification of fatty acids and alcohol using a commercial immobilized lipase (Novozyme 435) as catalyst. The main goals of this study are to analyse the influence of several operating variables on the reaction performance, to obtain a kinetic model of the system and to analyse the influence of the external mass transfer phenomena.

Based on the stated objectives, the present Thesis is organized as follows:

In Chapter 1- introductory - the importance of the fatty acid esters as well as their main uses and applications are presented. In addition, it is highlighted the relevance of the catalysis by immobilized enzymes, acquired during the last years. Different alternative ways of obtaining fatty acid esters and different media where the reaction takes place are described. Some aspects related to the structure, function and reaction mechanism of the immobilized lipase used are also presented.

In Chapter 2 the experiments carried out are described in detail. Firstly, the raw materials and catalyst features are analysed. Secondly the experimental equipment as well as the methodology utilized on carrying out all the experiments are presented. Finally, the analytical methods used for evaluating the course of the reaction are described.

The influence of operating variables such as temperature, initial molar ratio, enzyme concentration, and initial water content on the equilibrium conversion and the initial reaction rates is analysed in Chapter 3. Although a detailed study on the reuses of the enzyme was not carried out, it could be

reused and the results are shown in this chapter. At the end of the chapter, a theoretical study on the external mass transfer effects is presented.

In Chapter 4, a kinetic model describing the set of experimental data is proposed. The different reaction mechanisms by which the esterification reaction could take place are analysed for several kinetic models. For the proposed model the kinetic parameters are obtained fitting them to the experimental data from Chapter 3.

The importance of solving, from a rigorous point of view, the chemical equilibrium and the phase equilibrium simultaneously in a two-phase liquid system, is presented in Chapter 5.

Finally, the most important conclusions as well as the possible future directions extracted from the studies concerning to the present Thesis are summarized in Chapter 6.