



Kinetic modelling of the alumina catalyzed epoxidation of fatty acid esters in a batch reactor

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1. Introduction

The use of vegetable oil as industrial feedstock could be a promising substitute to petroleum-derived sources. For instance, production of biodiesel from transesterification of vegetable oils is a well-developed process at the industrial level. Vegetable oils are used in industry because they are renewable, biodegradable, non-toxic and abundant.

One of the first step is the epoxidation of vegetable oils. Epoxidized vegetable oils can be seen as platform molecules because they can be transformed into different chemicals [1] such as polyols, carbonated vegetable oils [2] and polyurethanes [3-4].

Conventionally, production of epoxidized vegetable oils is done by the Prileschajew method. It is a liquid-liquid reaction system, with several consecutive and parallel exothermic reactions [5]. The first step is the production of percarboxylic acid in the aqueous phase. Then, the percarboxylic acid diffuses into the organic phase to epoxidize the unsaturated groups. Due to the presence of several exothermic reactions, the risk of thermal runaway exists [6-7].

The Prileschajew method presents some issues such as: production of organic waste during the process, acidity increase of the reaction mixture which favors the side reaction of ring opening, separation step and waste treatment are more demanding, and use of corrosive acids.

Hence, direct epoxidation of vegetable oil by oxygen and hydrogen peroxide is seen as a better option concerning thermal safety, waste treatment and selectivity [10].

To the best of our knowledge, there is not kinetic model for the direct epoxidation of vegetable oil by hydrogen peroxide in the literature. Therefore, a kinetic model for the alumina-catalyzed epoxidation of methyl oleate is proposed with the aim of investigating the most suitable reaction mechanism and gather kinetic data able to describe the system.

2. Methods

The kinetic study of the direct epoxidation of methyl oleate was conducted in an isothermal and isobaric reactor. Hydrogen peroxide was added step-wise with a peristaltic pump. The influence of flow rate, temperature, reactant molar ratio and catalyst concentration was investigated.

Independent experiments were ran by isolating certain side reactions that takes place in the system such as the hydrogen peroxide decomposition reactions . This approach eases the estimation of kinetic constants during the modelling stage.

3. Results and discussion

The utilization of a semi batch reactor mode was found to increase the yield of epoxide over a 20% compared to the classical batch mode used in previous studies of this reaction [8-9].

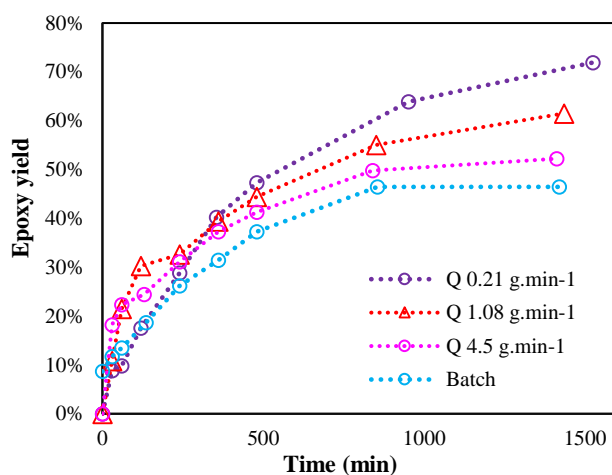


Figure 1. Influence of mass flowrate at 75 °C

External and mass transfer resistance were evaluated by old fashion methods and were found to be negligible due to efficient mixing and small catalyst particle size.

4. Conclusions

A kinetic model for the heterogeneous catalysed epoxidation of methyl oleate was developed. Some kinetics were estimated independently in order to minimize errors. A non-linear regression method was used to estimate the kinetic constants by using the experimental concentrations of epoxide, double and hydrogen peroxide as observable. The model fits quite well with the experimental concentrations.

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