New Catalytic Materials to Biodiesel Production

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1 Introduction

An experimental design to produce biodiesel from the vegetable oil transesterification and esterification of linoleic, lauric, palmitic, stearic and oleic fatty acids with methanol on heterogeneous catalyst was studied. It was investigated the influence of reaction variables such as methanol/fatty acid molar ratio, catalyst amount and temperature. It was verified the influence of the independent variables and was calculated the parameters of the models based on the principles of Langmuir-Hinshelwood and Eley-Rideal. Reactivity was established experimentally by the comparison of measured and theoretical conversions for the calculations of the energy of the reactant frontier orbitals for molecular modeling with semi-empiric AM1 method by using TITAN software. These processes can produce cleaner biodiesel and glycerol. This glycerol could even be used as food or feed in Brazil

2 Materials/Methods

Theoretical study: The semi-empirical AM1 quantum chemistry method was used to simulate the reaction using Titan and Gaussian packages. Model molecules were used, considering the main fatty acids predominant in vegetable oils.

Experimental study: The kinetic modeling was carried out with Origin and Statistica softwares. A factorial design involving 3 variables (temperature of reaction, molar ratio and catalysts) was conducted in an autoclave stainless steel batch reactor.

3 Results

Kinetic study of heterogeneous catalysis using Langmuir-Hinshelwood and Eley-Rideal models did not show good correlations. However, a homogeneous second order for the fatty acid model can also be used in a simplified way. Reactivity was influenced by difference in the molecular structure of the fatty acids. Reaction rates were faster for fatty acids with more unsaturation and smaller carbon chains. Reactivity order decreased in the sequence: linoleic> oleic> lauric> palmitic> stearic. It was also found that the orbital in which the reaction occurred was through LUMO orbital of the fatty acid with HOMO of the methanol because of greater symmetry and smaller difference of energy. Thus, no steric hindrance by fatty acids in relation to pore the catalyst was observed.

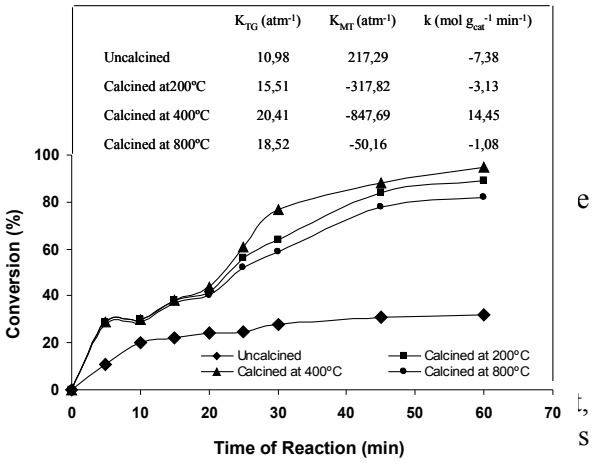

Figure 1: Transesterification kinetics with Mg-Al catalysts and its Langmuir-Hinshelwood Hougen-Watson parameters

4. Conclusions

Biodiesel can be obtained in a cleaner way using heterogeneous catalysts. Complete conversions can be obtained after about 60 min of reaction. Catalysts can be reused mainly in the case of hydroesterification, where even crude vegetable oils (non-refined) can be used producing also food grade glycerol . Biodiesel samples obtained in these processes comply with the EN 14214 standards.