11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Theoretical and experimental analysis of Jatropha oil transesterification by Heterogeneous Basic Catalysts

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Abstract – In this paper, the alkali-catalyzed transesterification of jatropha oil to biodiesel using heterogeneous base catalysts was studied, by experimental design and quantum calculations. The experimental study demonstrates that Calcined Mg–Al hydrotalcite at 400ºC was found the most effective catalyst for the transesterification of jatropha oil, obtaining conversion of jatropha oil of 94%. The theoretical kinetic study demonstrated than the reaction of ethanol is more slowly than methanol due to the low rate of formation of anion ethoxide.

Conventional homogeneous catalysts are expected to be replaced in the near future by heterogeneous catalysts mainly because of environmental constraints and simplifications in the existing processes. The kinetic of the heterogeneous transesterification reactions have been studied for many vegetable oils. Although biodiesel of Jatropha oil have been produced in commercial scale in India, there are no published kinetics reports with this raw material. In this paper the reaction of alkali-catalyzed transesterification of jatropha oil using Mg–Al hidrotalcites as heterogeneous catalyst were studies using computational chemistry methodologies relating with the experimental kinetic results.

The kinetic modeling was carried out with Origin and Statistica softwares, to determinate the mechanism and determining step of the reaction. Uncalcined and calcined hydrotalcites at 200ºC, 400ºC and 600ºC were used as heterogeneous catalysis. The reactions were studied with quantum method rb3lyp/lanl2dz, using Titan and Gaussian packages. In the experimental results, the good correlation between kinetic constant and the reaction yield demonstrate that Langmuir-Hinshelwood Hougen-Watson mechanism occur (Figure 1) and the theoretical calculations confirm this result (Figure 2), due to the decrease of the energy difference between the HOMO of alcohol and LUMO of glyceride when the reaction occurs on the catalyst surface. The transesterification using hidrotalcite without calcinate illustrate lows reaction yield. Calcined Mg–Al hydrotalcite at 400ºC was found the most effective catalyst for the transesterification of jatropha oil, obtaining conversion of jatropha oil of 96%. Theoretical calculations and experimental procedures demonstrated that the reactions of transesterification of jatropha oil using catalyst of hydrotalcite are not affected with use of ethanol or with presence of water in the reaction. In both case were obtain excellent conversion.

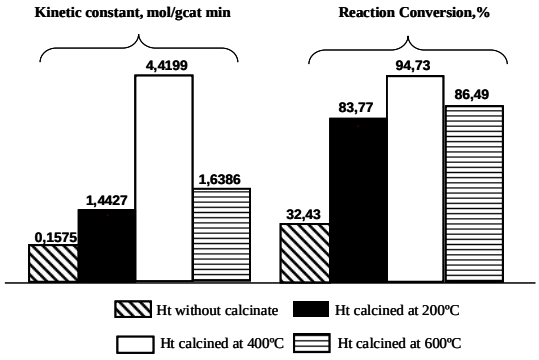

Figure 1: Kinetic and empirical results of Heterogeneous transesterification of Jatropha oil, supposed LHHW.

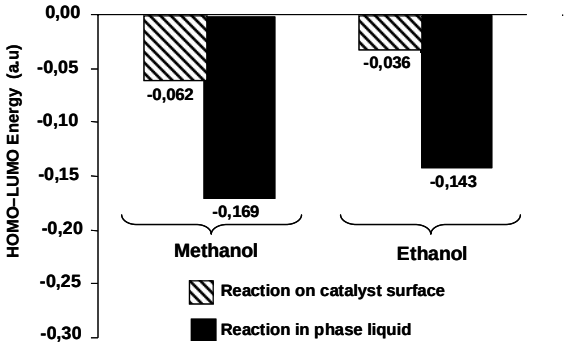

Figure 2: Difference of energy between HOMO of alcohol and LUMO of glyceride in reaction with hydrotalcite calcined at 400ºC.

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