

A Novel Corncob-Based Catalytic Biodiesel production Process: Kinetic Modeling and Simulation

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Abstract

In the current work, a sulfonic group-functionalized porous carbonaceous catalyst based on corncob ($I_{R=1}^{t=5} - C_{T=723}^{t=8} - S_{T=393}^{t=15}$) was used for esterification of oleic acid. Langmuir-Hinshelwood–Hougen-Watson (LHHW) kinetic model was used to correlate the experimental data. The correlation coefficient (R^2) obtained for all the kinetic parameters was close to 1, suggesting a very good statistical consistency of the experimental data fitting. The adsorption equilibrium constant for oleic acid (K_O) was found in the range of 25.850 to 3.250 for a temperature range from 328 to 338 K. This value was much higher than other adsorption equilibrium constants for methanol (K_M), methyl oleate (K_F) and water (K_W), indicating a strong affinity of oleic acid to the catalyst surface. Moreover, the adsorption affinity of oleic acid on the catalyst surface was approximately 325 times higher than that of methanol. The calculated activation energies and frequency factors were found to be 61.989 kJ/mol and $2.934E+8 \text{ m}^3/\text{mol.kg}_{\text{cat}}.\text{sec}$, respectively for the forward reaction and 71.899 kJ/mol and $9.183E+8 \text{ m}^3/\text{mol.kg}_{\text{cat}}.\text{sec}$, respectively, for the backward reaction. The obtained kinetic parameters were incorporated in the Aspen Plus simulator (ver. 8.6) to simulate the continuous biodiesel production process. The simulation result showed 99.09% oleic acid conversion which was close to the experimentally observed conversion (99%).

Keywords: Corncob; Oleophilic Acid Catalyst; Esterification; LHHW kinetics; Aspen Plus.