

## Abstract

Castor oil has the potential to be a renewable resource for the synthesis of high-value-added chemicals. Currently, first-generation castor oil derivatives such as sulfonated castor oil, Turkish red oil, ethoxylated castor oil, and hydrogenated castor oil are produced in India. These second and third-generation derivatives have more value than the first-generation products. The technological challenges are higher temperatures for conversion, suitable catalyst development, and green production process. The work focuses on the conversion of castor oil derivatives from methyl ricinoleate to sebacic acid, 2-octanol, heptaldehyde, and methyl undecanoate by using thermal-catalytic cracking and alkali-splitting reaction.

This work focuses on the thermal cracking and catalytic cracking of methyl ricinoleate, the major component of castor oil, in a micro fixed bed reactor used to produce methyl undecanoate and heptaldehyde. Methyl undecanoate and heptaldehyde have broad applications in polymers, cosmetics, and drug industries. The effect of flow rate, sweeping gas flow rate, preheating, and reaction temperatures were examined briefly. The lanthanum supported on zeolite HZSM-5 effectively converts methyl ricinoleate to bio-oil. The synthesis of lanthanum-loaded on HZSM-5 has been further confirmed through the characterizations of the catalyst. The DFT was performed to examine the experimental results and distribution of the products involved in dissociating methyl ricinoleate. Assuming C-C bond scission followed by the cleavage of the OH bond, the reaction energy of methyl undecanoate and heptaldehyde thermal cracking is computed using DFT. Thus, DFT calculations suggested dissociating reactant methyl ricinoleate into products methyl undecanoate and heptaldehyde, which agrees with the experiment's results. This also suggested that the C11-C12 in between carbon-carbon bond dissociation is the weakest. Methyl ricinoleate was used as the raw material for alkali splitting to produce sebacic acid and 2-octanol. The reaction parameters were optimized, including the catalyst, the ratio of oleochemicals/NaOH, reaction time, and reaction temperature. Introducing Fe species into

HZSM-5 kept its thermal stability and did not affect the structure of the zeolite framework. However, as Fe concentration increased, the BET pore volume and surface area decreased. Furthermore, adding Fe species promoted the formation of more Fe oxides in the bulk and surface regions and strengthened the synergistic effect between zeolite and Fe active sites, improving the catalytic activity.

Moreover, as the Fe content increased, there was a corresponding reduction in the number of Brønsted acid sites and an increase in the number of Lewis acid sites. This modification reduced the cracking ability of Fe/HZSM-5 but improved its dehydrogenation property, thereby enhancing its selectivity towards C<sub>5+</sub> hydrocarbons and yield of aromatics. The increased formation of graphitic carbon species was caused by the excessive addition of Fe loading, which decreased the alkali-splitting reaction and its catalytic activity.

The work concludes that if the thermal and catalytic reaction is carried out on a large scale, it could be economically viable. The drawbacks generally observed in high-pressure processes are almost negligible in this case. The obtained thermal and catalytic cracking and alkali-splitting reaction products were high purity. Hence, the oleochemicals do not require further purifications and can be used directly to synthesize various industrially essential chemicals.