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Master Thesis Defense

NOVEL INVESTIGATION OF CATALYTIC HYDROGENATION AND OXIDATION OF 1,3-BUTADIENE

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Abstract

The hydrogenation of 1,3 Butadiene (BD) is an important industrial process that is generally used to generate butene, which is a key feedstock to produce a variety of chemicals such as polymers, plastic, and synthetic rubber. This process involves reacting BD with hydrogen using different metallic Ni-based catalysts. In this study, Ni/Al_2O_3 and Ni/Nb_2O_5 catalysts were used and investigated to perform the hydrogenation reaction because of their high hydrogenation activity and high surface area and porosity.

The catalytic reactions were conducted using a quartz tube reactor between a temperature range of 50 and 400 °C at regular intervals of 50 °C under operating pressures of 1 atm. A comprehensive analysis of the products from the reaction was done using gas-chromatography with mass spectrometry (GC-MS) detector, where we noticed both mono-substituted aromatics, and gases products such as butenes. We noticed that a 100% conversion of BD occurred at 200 °C and collaborated our GC-MS results with infrared spectroscopy in order to develop a reaction mechanism and confirm the presence of certain products. In this way, we show the low-temperature conversion of BD represents an economically efficient method to add value to less-useful, more-reactive hydrocarbons with conjugative double bonds into high-value petrochemicals such as BTX.

The oxidation of butadiene is an efficient method of converting harmful compounds like butadiene to more useful syngas and oxygenates such as CO, CO_2. For this purpose, we investigate the use of Ni and Cu based catalysts such as 5% Ni/Al_2O_3, 5% Ni/Nb_2O_5 and 5-10% $Cu\text{-}CeO_2/Nb_2O_5$ to analyze the different products possible, their chemical nature, selectivity/ relative yields, and through (GC-MS), gas chromatography-thermal conductivity detector (GC-TCD) and infrared spectroscopy (FTIR) techniques. Furthermore, in order to investigate the catalysts' properties, their structure and its effect on the hydrogenation and oxidation reactions more deeply, we employed comprehensive characterization methods such as X-ray diffraction (XRD), FTIR, scanning electron microscopy with energy-dispersive spectra (SEM-EDS), Brunauer Emmett-Teller (BET), Thermogravimetric analysis (TGA) and hydrogen-temperature programmed reduction (H_2-TPR). An important side product obtained in our reactions was acetaldehyde, which was a result of carbonylation of the double bonds in BD. The results show the role of ceria and niobium supports to enhance the catalyst performance and activity by changing the oxygen vacancies and their capability to store oxygen. With their role in both metallic based catalysts, Ce and Nb activated copper oxide surface catalyst to deliver the desired products and results. The prepared 10 wt.% copper catalyst with 10 wt.% of ceria and 80% niobium has the utmost catalytic performance with 100% conversion of butadiene, and highest selectivity towards CO_2 of 98% at the temperature range of 300-500 °C. The findings of this study provide a practical environmental application in the catalytic enhancing of unstable hydrocarbon compounds.

Keywords: 1,3-Butadiene, Heterogeneous catalysts, Hydrogenation, Oxidation, Ni-based catalysts, Cu-based catalysts, Conversion, Selectivity, Percentage Yield, Aliphatic and Aromatics, Characterization