Fuel Processing Technology 285 (2026) 108429

Contents lists available at ScienceDirect

Fuel Processing Technology

journal homepage: www.elsevier.com/locate/fuproc

Remarkably high stability of relatively small iron amount exchanged into HZSM-5 catalysts toward ethanol conversion into ethylene: Experimental and computational studies

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ARTICLE INFO

Keywords:
Bioethanol conversion
Catalytic dehydration
Green ethylene
DFT simulation
Fe–O–Si active site

ABSTRACT

The sustainable production of green ethylene from bioethanol provides a realistic pathway to lowering the carbon footprint of conventional petrochemical routes. In this study, Fe exchanged H-ZSM-5 catalysts with a Si/Al ratio of 26 and different iron contents were synthesized and characterised using Powdered X ray Diffraction (PXRD), Fourier Transform Infrared Spectroscopy (FT-IR), Pyridine Infrared Spectroscopy (Py-IR), Ammonia Temperature Programmed Desorption (NH_3-TPD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Absorption Spectroscopy (AAS), and Thermogravimetric Analysis (TGA). Catalytic tests were performed in a fixed bed reactor by varying temperature between 200 and 300 °C and weight hourly space velocity (WHSV) from 2 to 19 h^{-1}. The 3Fe ZSM-5 catalyst containing 2.3 wt% Fe achieved 98% bioethanol conversion and more than 95% ethylene selectivity at 280 °C and WHSV of 9 h^{-1}, while remaining stable for 56 h on stream. Acidity characterization revealed that Fe incorporation weakens strong Brønsted sites and generates Lewis acid sites, limiting secondary reactions and coke formation. Consistently, TGA showed around 11% less coke compared to the parent zeolite. Density Functional Theory (DFT) calculations using DMol3 identified Fe-O-Si motifs with Fe-O distances of 1.99 to 2.02 Å.

1. Introduction

The quest to generate renewable green ethylene from bioethanol, a non-fossil and eco-friendly feedstock, has been a significant focus of study for many years. The fossil fuel-based ethylene production process is highly energy-intensive and accounts for the most crucial volume of ethylene produced globally [1]. The current global market size for ethylene accounts for 127 MMT and is by far the most prominent commercial petrochemical produced by volume [2]. Ethylene is a versatile raw material that produces approximately 75% of petrochemical products. Its monomer synthesises polyethylene, vinyl chloride, styrene, and polymer products [3]. Fossil fuel-based ethylene can be controlled by the dehydration of bioethanol produced from renewable sources [4].

The fermentation of agricultural feedstocks, such as corn and sugarcane, as well as other cellulosic biomass, generally produces bioethanol. The produced bioethanol is catalytically converted to ethylene following two dehydration routes: the intramolecular and intermolecular dehydration of ethanol. However, both catalytic dehydration processes may occur in parallel.

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https://doi.org/10.1016/j.fuproc.2026.108429
Received 9 December 2025; Received in revised form 14 February 2026; Accepted 23 February 2026
Available online 10 March 2026