

## Insights on bioethanol to hydrocarbons conversion over ZSM-5 zeolite by a transient technique

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Bioethanol plays a prominent role in the day-to-day market as an essential alternative. Majority of it is used as a source of fuel besides the increasing usage in value added chemicals [1]. ZSM-5 zeolite is found to be a well-known acidic catalyst in ethanol conversion to hydrocarbons [2]. Its shape selectivity and hydrothermal stability were an added advantage to this reaction. Researchers around the world explored the insights of the reaction in various ways to explain the mechanism. Three most debatable mechanisms that surround this reaction were hydrocarbon pool, acid-catalyzed and radical assisted paths. Yet, there was no clear evidence to support any of these mechanisms. For the first time, Temporal analysis of Products [3] was used to gain the insights of this mechanism.

A reaction pathway is proposed for the conversion of  $C_2H_5OH$  to hydrocarbons consisting of two consecutive stages as illustrated in Figure 1. The first step involves the dehydration of ethanol to ethene which can take place either via a monomolecular or bimolecular pathway with di-ethyl ether as intermediate product. In the second step, three routes for the production of light olefins can be distinguished which are mediated by different types of surface intermediates: butene formation via alkylation of adsorbed ethene ( $C_2H_4^*$ ) with gas phase  $C_2H_4$  (see Route I),  $C_3H_6$  and  $C_4H_8$  formation via different types of surface species. These surface species can either desorb or be involved in consecutive reactions and are typically called the hydrocarbon pool in the methanol-to-olefins process. The surface species do not only consist of aromatics, i.e.,  $C_{aro}^*$ , which allow enhanced production of light olefins (route III) via paring and side-chain reaction mechanisms but also of shorter lived aliphatic species, i.e.,  $C_{ali}^*$ , which can undergo  $\beta$ -scission, isomerization and alkylation (Route II). A competition exists between the routes mediated by these two types of intermediates to propene and/or butenes which depends on the reaction conditions.

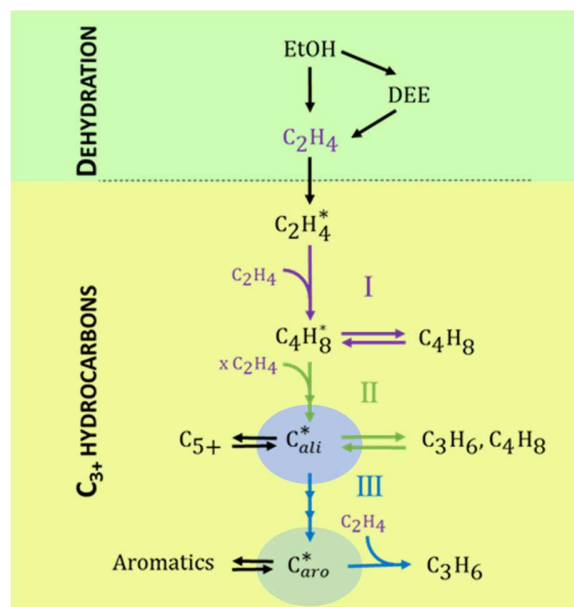


Figure 1. Reaction mechanism for the conversion of ethanol to hydrocarbons

[1] Sun, J. and Wang, Y., ACS Catal. 4 (2014) 1078-1090.

[2] Van der Borght, K. Galvita, V.V. Marin, G.B., Appl Catal A-Gen. 492 (2015) 117-126.

[3] Gleaves, J.T. Yablonsky, G. Zheng, X. Fushimi, R. and Mills, P.L., J. Mol. Catal. A: Chem. 315 (2010) 108-134.