

## **Naphtalene derivatives in the MTO process from a molecular modeling perspective: reactive species or cokes?**

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Currently, basic chemicals in polymer industry are mainly produced by thermal cracking of petroleum, but a promising alternative has been found: methanol-to-olefins (MTO). Methanol can be made from natural gas via syngas, but also from biomass. Molecular modeling of the MTO process has been a challenging topic, yet the reaction mechanism of the active route is starting to get unraveled based on the ‘hydrocarbon pool’ hypothesis [1], where aromatic species play a fundamental role as co-catalytic species within the zeolite pores and cages.

All catalysts face the problem of deactivation due to coke formation [2]. This is a major threat for the application of the process and the need for a reliable kinetic model of the coke deposition to optimize the reaction conditions is, therefore, high. Experimentally, it is found that the deactivation is a result of the presence of voluminous polyaromatic compounds in the cages of the catalyst. For SAPO-34, which has a chabasite topology, this are phenantrene- and pyrene-like species, which show no activity towards olefin production. The topology of the catalyst is a crucial aspect regarding the coking issue: ZSM-5 only shows a blocking of the channels in the external cups, while a chabasite topology is subject to internal coking [3].

As of yet, the boundary region between active hydrocarbon pool species and deactivating coke remains uncharacterized. In this contribution, this question will be answered for naphtalenic compounds by remodeling the active route for ethylene and propylene production and comparing the activities with the original side-chain mechanism [1]. An other topic of examination is the influence of the formation of such compounds on the propene/ethene selectivity ratio [4]. And finally, the chemical composition of the catalyst, which clearly has an influence on the activity and coking rate of the catalyst [5] will be investigated by comparing the behavior of naphtalenic molecules in SSZ-13 chabasite and SAPO-34.

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