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Theoretical Estimation of Intracrystalline Diffusivities of Olefins in MTO Catalysts

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Highlights

1. Intracrystalline diffusivities of olefins were estimated by SV (Solid Vibrational) model.
2. Effective vibrational frequencies are calculated by curvature of potential well.
3. Selectivity of propylene in both catalysts increases with temperature.
4. Ethylene to propylene diffusivity ratio obtained in ZSM-5 is 2.3 while in SAPO-34 is 35.6.

Abstract

Light olefins are considered symbolic petrochemicals applied in many chemical industries. Conventionally, they are produced from petroleum feedstock via steam cracking of naphtha and fluidized catalytic cracking. Since last two decades, methanol to olefins (MTO) has been paid much attention, and regarded as a promising alternative route for olefins production over microporous zeolite catalysts.

Olefin product distribution in MTO process is delineated by kinetic and diffusion mechanisms inside the micropores of catalyst. A bunch of studies has been carried out on the mechanism in different zeolites. In this work, we have focused on the molecular movements within the crystal. The rationale behind this work is to uncover the molecular interactions with the lattice of zeolite catalyst in the intracrystalline pores.

Two well-known microporous catalysts i.e. ZSM-5 and SAPO-34 are used for this study. We have considered only adsorbate and oxygen interactions present inside the lattice. It is observed that adsorbate-adsorbent interactions are dominant inside micropores while adsorbate-adsorbate interactions are negligible. Activations energies of olefins consist of intermolecular interactions and soft harmonic interactions present inside the channel intersections. Intermolecular interactions are calculated by three different classical methods i.e. LJ 12-6, LJ 9-6 and Buckingham ex-6. In ZSM-5, LJ 12-6 model gives satisfactory approximations while for SAPO-34, Buckingham ex-6 model is best choice. While soft harmonic calculations inside cage are carried out by Schrodinger Wave equations in the light of harmonic oscillator principles. Activation energy results reveal that instead of having same kinetic diameters, higher olefins have different energies. Due to the difference in molecule length, the rotational and vibrational movements are highly restricted in the lattice structure. Molecules having smaller kinetic diameters than channel, have strong attractions towards channel and can pass easily through it. While larger molecules stay most of the time in the channel intersections and cages of catalyst. In addition, solid Vibrational model is used to address intracrystalline diffusivities of C₂= - C₇= olefins within temperature range 673-873 K. This model defines that even at higher temperatures, molecules retain their solid property and vibrate with the zeolite lattice. It was analyzed that temperature has ascending effect on the diffusion selectivity of propylene. That's why ethylene to propylene ratio decreases with increase in temperature and concentration of propylene in product stream of MTO enhances.

References

- [1] C. Wang, et. al., Insight into the topology effect on the diffusion of ethane and propene in zeolites: A molecular dynamic simulation study, *Journal of Energy Chemistry*, 22(2013), 914-918.
- [2] J. Xiao, J. Wei, Diffusion mechanism of hydrocarbons in zeolites-I. Theory, *Chemical Engineering Sciences*, 47 (1992), 1123-1141.

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