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Molecular Simulation of NO, NH3 Adsorption in MFI and H-ZSM5

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Abstract : Due to developing the industries, the emission of pollutants such as NOx, SOx, and CO2 are rapidly increased. Generally, NOx is attributed to the mono nitrogen oxides of NO and NO2 that is one of the most important atmospheric contaminants. Hence, controlling the emission of nitrogen oxides is urgent environmentally. Selective Catalytic Reduction of NOx is one of the most common techniques for NOx removal in which Zeolites have wide application due to their high performance. In zeolitic processes, the catalytic reaction occurs mostly in the pores. Therefore, investigation the adsorption phenomena of the molecules in order to gain an insight and understand the catalytic cycle is of important. Hence, in current study, molecular simulations is applied for studying the adsorption phenomena in nanocatalysts applied for SCR of NOx process. The effect of cation addition to the support in the catalysts' behavior through adsorption step was explored by Mont Carlo (MC). Simulation time of 1 Ns accompanying 1 fs time step, COMPASS27 Force Field and the cut off radios of 12.5 Å was applied for performed runs. It was observed that the adsorption capacity increases in the presence of cations. The sorption isotherms demonstrated the behavior of type I isotherm categories and sorption capacity diminished with increase in temperature whereas an increase was observed at high pressures. Besides, NO sorption showed higher sorption capacity than NH3 in H–ZSM5. In this respect, the Energy distributions signified that the molecules could adsorb in just one sorption site at the catalyst and the sorption energy of NO was stronger than the NH3 in H-ZSM5. Furthermore, the isosteric heat of sorption data showed nearly same values for the molecules; however, it indicated stronger interactions of NO molecules with H-ZSM5 Zeolite compared to the isosteric heat of NH3 which was low in value.

Keywords : Monte Carlo simulation, adsorption, NOx, ZSM5
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