Abstract

Zeolite synthesis is one of a number of potential applications of fly ash for obtaining high-value industrial products from this waste material. Moreover, extend of international scientific and commercial interest in the zeolite molecular sieve is still increasing for its manifold applications in diversified areas. The wide variety of applications include separation and recovery of normal paraffins in hydrocarbons, catalysis in hydrocarbons, drying of refrigerants, separation of air components, recovering radio active ions from radio-active waste solutions, removing carbon dioxide and sulfur compounds from natural gas and so on. In view of its widespread applications, synthesis of zeolites from low cost (waste) material is of great commercial importance.

In the present investigation, efforts have been made to synthesize zeolite from fly ash using classical hydrothermal treatment method preceded by alkali fusion. The synthesis parameters were optimized to obtain X-type zeolite as the main product. Fly ash from different Indian thermal power stations have been used and highest conversion to X-type zeolite was observed for KTPS (Kolaghat Thermal Power Station, West Bengal, India) fly ash. Other fly ash samples were collected from DTPS (Durgapur Thermal Power Station, West Bengal, India) and NALCO (National Aluminum Company, Orissa, India) power stations. The original fly ash as well as the synthesized zeolites were characterized using various techniques such as XRD, SEM, XRF, FTIR and BET method of surface area measurement.

The synthesized zeolites were used as catalysts for cracking of n-heptane and alkylation of phenol with highly encouraging results.

Cracking of n-heptane was studied in a down flow fixed-bed reactor. Cracking reaction parameters as well as catalyst synthesis conditions were found to affect the n-heptane conversion and product selectivity. Cracking was conducted over synthesized zeolites derived from different fly ash samples and

the results were compared with commercially used catalyst. A mathematical model was developed, which includes a monomolecular cracking path based on Langmuir adsorption isotherm as well as a bimolecular path. Catalyst decay was accounted for using time-on-decay function. This model fits the experimental data very well.

Efficacy of the treated fly ash as a catalyst for alkylation of phenol with tert-butyl alcohol was first carried out in a batch system and then using a flow reactor. The synthesized zeolite showed better performance than commercial 13X zeolite. Phenol conversion was found to be higher on Hβ zeolite, but the interesting point is that the synthesized zeolite showed better selectivity for the desired product tert-butyl phenol (TBP). Hence, the effects of various reaction parameters on the conversion of phenol and selectivity of TBP and the kinetics were investigated with the synthesized catalyst. L-H-H-W surface reaction model was developed to interpret the kinetics of phenol alkylation in batch system and the model was also simulated for the flow system experimental data. In flow reactor, effect of various parameters, i.e., space-time, feed composition, and temperature were studied with different catalysts derived from fly ash.

The kinetic parameters of non-linear rare equations (in cracking and alkylation) were estimated by using Marquardt's routine, minimizing the error in-between the experimental and predicted rate of reaction. The activation energies and pre-exponential factor for there reactions were evaluated using Arrhenius equation. Thermodynamic properties such as heat of reactions, entropy change and Gibbs free energy for alkylation reaction were evaluated using different established techniques.

Key words: fly ash, zeolite, alkali fusion, hydrothermal treatment, characterization, X-ray diffraction, scanning electron microscopy, BET surface area, cracking, kinetics, kinetic modeling, n-heptane, alkylation, phenol, tert-butyl alcohol, tert-butyl phenol.