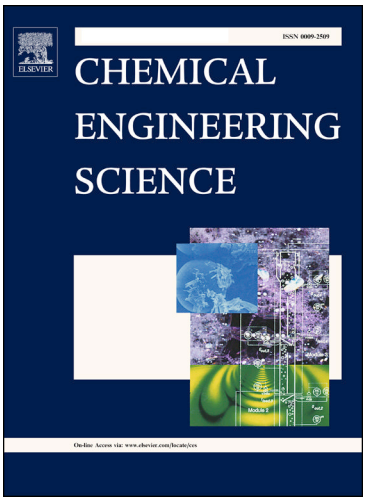

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Monitoring the Progress of Catalytic Cracking for Model Compounds in the Mid-Infrared (MIR) 3200-2800 cm^{-1} Range

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Abstract

Hydrocarbon species concentrations in the gas phase are of critical importance to elucidate catalytic cracking kinetics and riser/downer fluid dynamics. In this respect, Mid-Infrared (MIR) spectroscopy provides a singular approach to monitor chemical species conversions at various reaction times. In the MIR, the Absorption Cross Section Coefficients and Integrated Absorption Band Intensities can be related to the number of C-H bonds present in the different chemical species. The proposed methodology is based on a Group Contribution Method (GCM), which accounts for the additive contribution of molecular functionalities related to the C-H bonds present in hydrocarbons. This allows absorption spectra predictions in 3200−2800 cm^{-1} region. This Group Contribution Method can be applied in conjunction with a helium-neon (HeNe) laser, with a 2949.85 cm^{-1} wavenumber (3.39 μm wavelength). The technique is validated using both 1-hexene and 1,3,5-TIPB catalytic cracking data. The importance of the proposed method is shown in the context of using a CREC Riser Simulator, a mini-fluidized laboratory scale unit invented at CREC-UWO (de Lasa, 1991). Hydrocarbon species are MIR monitored in the outer CREC Riser Simulator annulus. The data obtained can be used to extrapolate gas phase hydrocarbon conversions and fluid molar densities in risers and downers. This information can be also used to accurately predict fluid dynamics in FCC catalytic cracking units.

Keywords

Mid-infrared, catalytic cracking, reaction conversion, HeNe laser