Structural and Texture Refinement of XRD Data of Fluid Catalytic Cracking Catalysts: A Prerequisite Results Requirement to Predict the Steaming Effect on Catalytic Performance

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ABSTRACT

Al-Bogami and Sitepu (2018) reported that the Brunauer-Emmett-Teller (BET) surface area decreased with steaming for fluid catalytic cracking (FCC) base catalyst based on Y zeolite while no significant change was observed with the FCC additive catalyst sample based on the ZSM-5 zeolite. Moreover, the steamed samples displayed a lower acidity compared to fresh samples, with more magnitude at the severe steaming condition. Subsequently, steaming reduced the conversion of vacuum gas oil, whereas steaming enhanced the selectivity toward the olefins' production and low coke formation. Additionally, sample X-ray powder diffraction (XRD) data confirmed the zeolite structure of both FCC catalysts: A base catalyst based on Y zeolite and an additive for olefins production based on the ZSM-5 zeolite samples was maintained after steaming at 750°C for 3 hours and 810°C for 6 hours [Al-Bogami et al. (2018). *Journal of Technology*. 2018 Winter Edition, 2-8]. However, they did not report the crystal structure and preferred orientation parameters derived from their XRD data.

In the present study, Rietveld refinement with the generalized spherical harmonic description for correction of the preferred orientation in powder diffraction analysis for both crystal structure refinement and quantitative phase analysis [Sitepu et al. (2005). *J. Appl. Cryst.* **38**, 158-167; Sitepu. (2009). *Powder Diffr.* **24**, 315-326] has been extended to describe crystal structure and texture in the all XRD data sets of the un-steamed (fresh) and steamed powders. The results revealed that the structural refinement parameters obtained from the Rietveld refinement with the generalized spherical harmonic description agreed well with the corresponding single crystal structure. Additionally, the generalized spherical harmonic description provides better results for the materials investigated in the present study than what the March model did. Therefore, the generalized spherical harmonic approach should be used for preferred orientation correction in XRD Rietveld analysis, for both crystal structure refinement and phase composition analyses. Finally, the transmission electron microscope (TEM) results will be discussed in this paper.

XRD − Rietveld