Kinetic Modeling of Gas-oil Catalytic Cracking Reactions

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Introduction

Modeling microreactors for predicting the kinetics of cracking reactions and deactivation in FCC catalysts is relevant for its application to the simulation of the processing of vaccum gas oil in industrial riser reactors, and for ranking industrial catalysts in terms of yield, product selectivity and conversion. Under typical short-contact time operating conditions (3-10 s), the analysis of the interaction between mass transfer, cracking reactions and deactivation on conversion and selectivity becomes important. In this work, the estimation of the kinetics of cracking reaction and deactivation is based on a mechanistic model that predicts products distribution and coke deposition in FCC catalysts, which accounts for interfacial and intraparticle mass transfer interactions coupled to cracking reactions and coke deposition [1]. The model describes an isothermal ideally mixed fluidised bed microreactor where surface reactions and coke deposition occur on a single-pore microsphere cracking catalyst. The kinetics, described in terms of LHHW expressions, consider the cracking of vacuum gas oil in terms of 6 lumps: vacuum gas-oil (A), light cycle-oil (B), gasoline (G), Gas LP (D), Dry gases (E), and Coke (CS); the adsorption of lumps A, B, G and D, and the fraction of free active sites, as shown in Fig. 1. To close the mass balance, the model also describes the stripping stage of the adsorbed lumps, after the cracking stage. Finally, the model assumes that diffusion of all lumps takes place in the Knudsen regime.

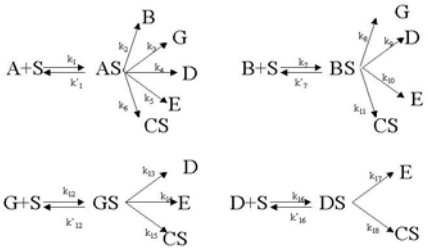

Figure 1. Schematic representation of the six-lump model.

Experimental

The experiments were conducted on an ACE-R™ confined fluidized bed micro-reactor, using a vacuum gas-oil and an equilibrium FCC catalyst from a commercial unit. In all experiments the mass of catalyst employed was 9 g, and the gas-oil feed rate was 0.02 g/s, for times on stream: 45, 60, 75, 90 and 120 sec. The reactions were carried out at temperatures of: 520°C, 535°C, 550°C and 565°C. Gas products

were analysed by gas chromatography and simulated distillation methods. The amount of coke on the catalyst was determined via IR analysis of the CO_2 produced by coke burning in air at 695 ºC.

Results and Discusion

Figure 2 shows the comparison between experimental and predicted temporal profiles for products distribution, based on the estimation of all kinetic parameters for the case of 520°C. Similar results were obtained for all temperatures. Figure 3 shows the predictions of catalyst deactivation at different temperatures as a function of the amount of coke-on-catalyst, using the same value for parameter α in the deactivation expression used in the model [2]. Other results, like the prediction of the stripping of adsorbed lumps (not shown) are included in the model. Good agreement was obtained between predictions and experimental observations.

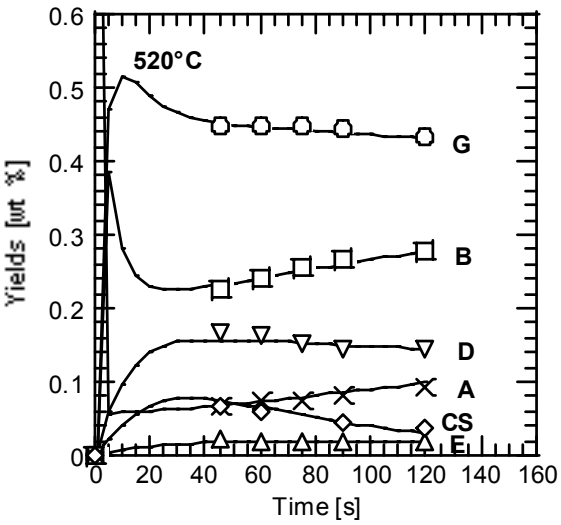

Figure 2. Comparison of experimental (symbols) versus predicted (continuous lines) temporal profiles at 520°C.

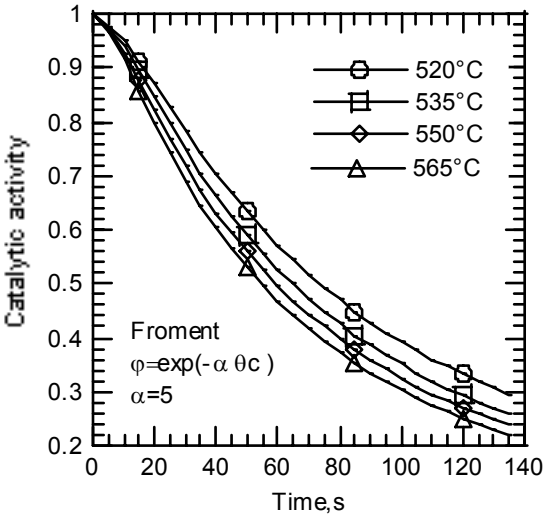

Figure 3. Prediction of catalyst activity versus times on stream at different temperatures.

1] López-Isunza F., Moreno M., Quintana R., Moreno J., Hernández F., Stud. Surf. Sci. Cat. **133** (2001), 509-514.

[2] Froment G. F., Bischoff K. B., *Chemical Reactor Analysis and Design*, John Wiley, New York, 1979.