Complete Oxidation of n-Hexane and Toluene on Perovskite-type Catalysts

Tzvetomila Lazarova[1], Maya Markova-Velichkova[1], Georgi Ivanov[1], Daniela Kovacheva[1] and Anton Naydenov[1]

[1] Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria. *E-mail:* markova@svr.igic.bas.bg

A series of perovskite-type catalysts ($LaFeO_3$, $LaCoO_3$, $YFeO_3$ and $YCoO_3$, supported on α-Al_2O_3 spherical particles) were synthesized via sucrose assisted solution combustion method. A catalytic activity with respect to the complete oxidation of hydrocarbons (n-hexane and toluene) was studied. The phase formation stages as well as the surface morphology and catalyst evolution were studied before and after the reaction using different instrumental methods as XRD and XPS. In order to establish the reaction mechanism, an additional experiments on so-called "depletive" oxidation were performed. Based on the experimental results the mechanisms of Elley – Rideal and Mars – van Krevelen were considered as non probable. Power law kinetic and four mechanistic models (Langmuir – Hinshelwood, bimolecular reaction, surface reaction being the rate-determining step) were fitted with the experimental data by applying of an integrated computer program for simultaneous solving the material balance in an isothermal PFR (plug flow reactor) and numerical nonlinear optimization procedure, based on iterative reducing the gradients. Aliphatic hydrocarbon (n-hexane) was found to be difficult to oxidize, while with aromatic compound (toluene) a promising activity was observed with $LaFeO_3$ sample, while the lowest activity being observed with $YFeO_3$. This fact is associated with the lowest crystallite size of $LaFeO_3$ catalyst assuming highest surface area of the active phase. It was concluded that the reaction proceeds via LH – mechanism with dissociative adsorption of oxygen.