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EMPIRICAL MATHEMATICAL MODEL OF PROCESS OF HETEROGENEOUS CATALYTIC OLIGOMERIZATION OF C_9 FRACTION OF DIESEL FUEL PYROLYSIS LIQUID PRODUCTS

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Synthesis of cooligomers from ethylene productions by-products is the most reasonable way of their utilization. C_9 fraction of diesel fuel pyrolysis liquid products is object of our research. Cooligomers obtained from this fraction have wide application. Our approach consists in synthesis of these products by heterogeneous catalytic oligomerization. Number of zeolites and clay materials having been previously activated by acid were investigated as heterogeneous catalysts. Activated bentonite clay was found to be the most effective catalyst of investigated ones. Cooligomers production in its presence was studied in following range of conditions: the catalyst content in reaction mixture 1-15% $_{\text{by wt.}}$, temperature 313-413 K and oligomerization duration 1-6 hrs. Based on the experimental results the empirical mathematical model of the process, as a set of regression equations, was constructed. Such model allows to determine the process optimum conditions, as well as to predict yields and properties of cooligomers obtained under conditions different from studied. The latter is very important and convenient for design of this process technology. In given case we have three-parameter mathematical model, where parameters are the catalyst content (C_{cat}, % $_{\text{by wt.}}$), temperature (T, K) and duration (τ, hrs.). Response functions are the cooligomer yield (η, % $_{\text{by wt.}}$) and properties: average molar weight (M, g/mole), bromine number (BN, gBr_2/100g) and colour (C, mg I_2/100ml). Coefficients of regression equations were calculated by solution of system of equations formed based on experimental data. The Mathcad 14 software was used for this aim. The empirical mathematical model of heterogeneous catalytic oligomerization of C_9 fraction in presence of activated bentonite clay as a catalyst is

$$\eta = -91.769 + 0.892 \cdot C_{cat} + 0.278 \cdot T + 1.083 \cdot \tau \quad (\Delta\eta = 1.67\ \%_{\text{by wt.}},\ \delta\eta = 6.45\%)$$

$$M = 6280 + 291.16 \cdot C_{cat} + 17.202 \cdot T - 2898 \cdot \tau - 4.733 \cdot C_{cat}T + 166.819 \cdot C_{cat}\tau - 10.925 \times$$

$$\times T\tau + 0.776 \cdot C_{cat}T\tau + 2.158 \cdot C_{cat}^2 + 0.07 \cdot T^2 + 17.453 \cdot \tau^2 \,(\Delta M = 23.4\text{ g/mole}, \delta M = 3.50\%)$$

$$BN = 7.846 + 1.857 \cdot C_{cat} + 0.047 \cdot T + 9.684 \cdot \tau + 0.003951 \cdot C_{cat}T - 0.9 \cdot C_{cat}\tau + 0.01 \cdot T\tau$$

$$(\Delta BN = 2.9\ gBr_2/100g,\ \delta BN = 3.90\%)$$

$$C = -18.789 + 2.116 \cdot C_{cat} - 7.393 \cdot T + 562.283 \cdot \tau + 0.518 \cdot C_{cat}T - 61.267 \cdot C_{cat}\tau + 1.008 \cdot T\tau$$