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SUPPLEMENTARY MATERIAL TO

Kinetic study of propane aromatization over Zn/HZSM-5 zeolite under conditions of catalyst deactivation using genetic algorithm

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TABLE S-I. Propane conversion, aromatics selectivity and yield on the ion exchanged and impregnated Zn/HZSM-5 catalysts for propane aromatization. (reaction conditions: T=560 °C, space velocity=500 $cm^3\ g_{cat}^{-1}\ h^{-1}$, TOS=0.5 h, P=1 atm, feed composition=50 mol% propane)

Catalyst	Propane conversion, %	Aromatics selectivity, %	Aromatics yield, %
Ion Ion exchanged Zn/HZSM-5 with 0.01 M solution of zinc nitrate	55.1	59.7	32.9
Ion exchanged Zn/HZSM-5 with 0.02 M solution of zinc nitrate	63.2	63.6	40.2
Impregnated Zn/HZSM-5	64.8	67.0	43.4

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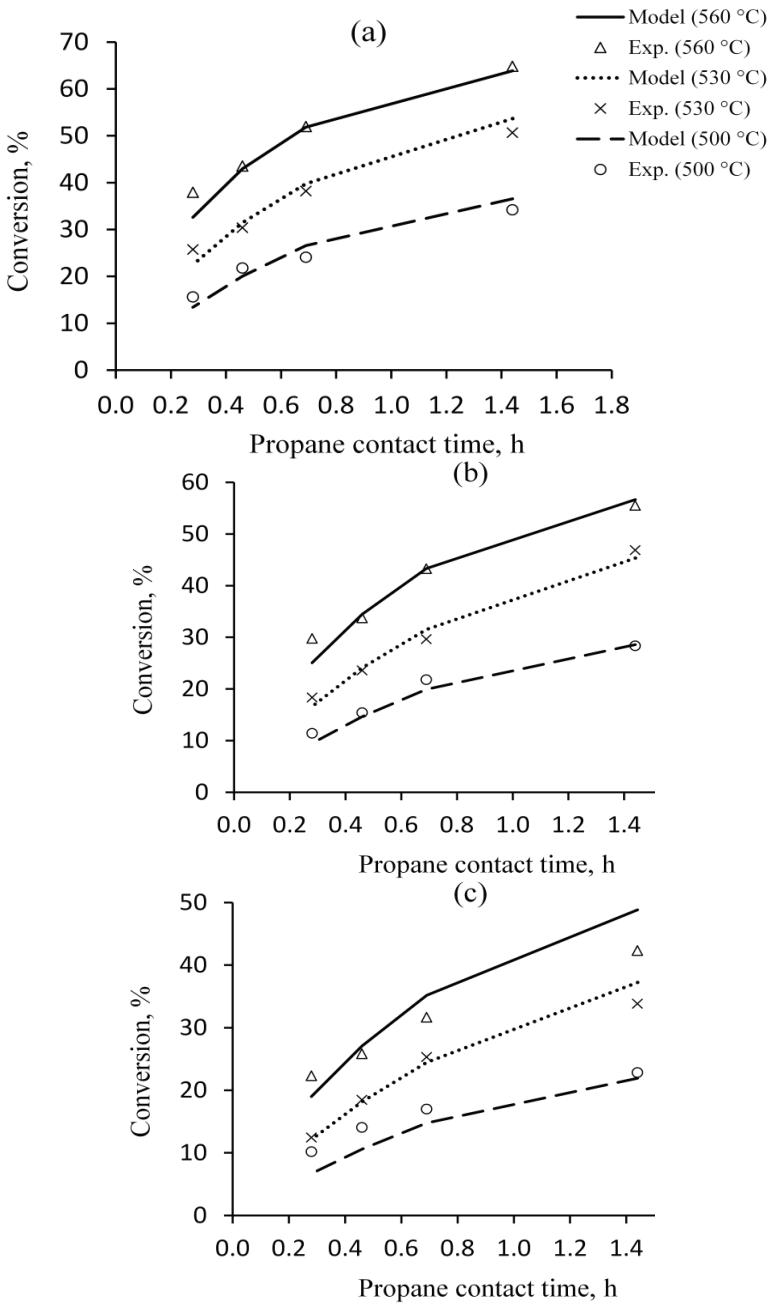

Fig. S-1. Effect of contact time on propane conversion at different temperatures and (a) TOS=0.5 h, (b) TOS=11 h, (c) TOS=21 h.

$$R_i = (\sum_{j=1}^{n} \upsilon_{ij} r_j) a \quad \text{(S-1)}$$

$$R_A = (-k_1 C_A^{P_1} - k_2 C_A^{P_2}) a \quad \text{(S-2)}$$

$$R_B = (k_1 C_A^{P_1}) a \quad \text{(S-3)}$$

$$R_C = (k_2 C_A^{P_2} - k_3 C_C^{P_3}) a \quad \text{(S-4)}$$

$$R_D = (k_3 C_C^{P_3} - k_4 C_D^{P_4} - k_5 C_D^{P_5}) a \quad \text{(S-5)}$$

$$R_E = (k_5 C_D^{P_5} - k_6 C_E^{P_6}) a \quad \text{(S-6)}$$

$$R_F = (k_6 C_E^{P_6} + k_4 C_D^{P_4}) a \quad \text{(S-7)}$$

Where r_j is the rate of reaction step j, mol g^{-1} h^{-1}, υ_{ij} is the stoichiometric coefficient of lump i in the reaction step j, n is the number of reaction steps. In the kinetic studies of the lumping model for propane aromatization, a non-selective kinetic deactivation was considered, in which a same activity was used for all the reaction rates of a lumped component i.

$$C_3H_8 \longrightarrow C_3H_6 + H_2, \Delta H^{o}_{r,500^{\circ}C} = 128.9\,\text{kJ mol}^{-1} \quad \text{(S-8)}$$

$$C_3H_8 \rightarrow C_2H_4 + CH_4, \Delta H^{o}_{r,500^{\circ}C} = 79.5\,\text{kJ mol}^{-1} \quad \text{(S-9)}$$

$$2C_3H_8 \rightarrow C_6H_6 + 5H_2, \Delta H^{o}_{r,500^{\circ}C} = 316.3\,\text{kJ mol}^{-1} \quad \text{(S-10)}$$