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platinum and boron doped diamond (BDD).

In [5] electrochemical oxidation of toluene on glassy carbon electrodes in organic medium was investigated. Was shown, that electrochemical oxidation of toluene depends on the experimental time scale and involves different steps or reactions that could control the transformation.

Technologies of electrochemical oxidation allow to receive products with higher yield, for the majority of reactions are generally used a harmless solvents. Application of electrochemical methods for electrooxidation of organic compounds requires scrutinous study of the reaction mechanism and kinetic with identification of electrolysis products. Thus, electrooxidation is environmental friendly method and requires additional research.

References

- Sperry J. B., Wright D.L. The application of cathodic reductions and anodic oxidations in the synthesis of complex molecules Chem. Soc. Rev., 2006.– Vol.35.– P.605–621.
- 2. Steckhan E.E. Topics in current chemistry. Electrochemistry, Springer, NY, 1988.– Vol.3.
- Gandini, D.; Mahe, E.; Michaud, P. A.; Haenni, W.; Perret, A.; Comninellis, C. Oxidation of carboxylic acids at boron-doped diamond electrodes for wastewater treatment. Journal of Applied Electrochemistry, 2000.– Vol.30.
- 4. Oturan M.A., Brillas E. Electrochemical Advanced Oxidation Processes (EAOPs) for Environmental Applications. Portugaliae Electrochimica Acta, 2007.– Vol.25.
- Elia L.F.D., Ortiz R. Electrochemical oxidation of toluene on glassy carbon electrodes in organic medium. Portugaliae Electrochimica Acta., 2005.– P.481–490.

Reaction range definition of vacuum distillate cracking

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Catalytic cracking (CC) process is a basis of advanced refining of oil. CC is formation of high-octane gasoline and gas for petrochemical industries, for production of carbon black and coke from heavy raw material.

CC is related to heterogeneous catalysis. Study of the thermodynamics and kinetics is the way for its optimization. This approach allows estimating the process energy, the probability of chemical transformations, defining a set of products and their maximum yield. The basic kinetic parameters of a catalytic cracking process were calculated during the research using plant data. Diffusion coefficients were calculated to define the reaction range of the process. Olefin and paraffin formation reaction by cracking of high molecular paraffin (1) is considered. This type of interaction is more thermodynamically favorable for the system.

$$C_{n}H_{2n+2(HM)} = C_{n}H_{2n+2(MM)} + C_{m}H_{2m}$$
(1);

The molecular diffusion coefficient $D_i(2)$, the Knudsen diffusion coefficient $D_K(3)$ and the effective diffusion coefficient Deff are calculated by the formula (4):

$$D_{i} = \frac{0.43 \cdot 10^{-7} \cdot T^{1.5}}{P(V_{i}^{1/3} + V_{mix}^{1/3})} \cdot \left(\frac{1}{M_{i}} + \frac{1}{M_{mix}}\right)^{0.5}$$
(2)

$$D_k = 0.97 \cdot \frac{T}{M_i} \cdot 0.5 \cdot r \tag{3}$$

$$D_{eff} = D\left(1 - \exp\left(\frac{-D_k}{D}\right)\right) \tag{4}$$

Where r – pore radius (4 • 10⁻⁹), m; T – temperature (623–808), K; M – molecular weight (C_{13} – C_{40}), g/mol;

The Thiele parameter φ , which characterizes the reaction inside the catalyst grains, was calculated as following (5):

$$\varphi = L\left(\frac{k}{D_{eff}}\right) \cdot 0,5 \tag{5}$$

Where L – grain size of the catalyst (8 • 10⁻⁶), m; k – the reaction rate constant (0,1093), s⁻¹.

Efficiency factor varies from 0 to 1 and characterizes the efficiency of the inner surface of the catalyst grains.

For the catalyst grains of spherical shape is the following:

$$\eta = \frac{3}{\varphi} \left(\frac{e^{\varphi} + e^{-\varphi}}{e^{\varphi} - e^{-\varphi}} - \frac{1}{\varphi} \right)$$
(6)

Figure 1 shows linear dependency the Thiele parameter reduction from increase of the temperature process. Consequently, the diffusion complication of the process is reduced. Efficiency of the inner surface of the catalyst is consistently high and goes to the 100% value. This factor allows taking into account any complications of diffusion. Consequently, D >> k and the

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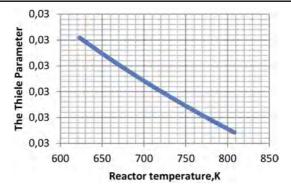


Fig. 1. The Thiele Parameter of HM paraffin cracking reaction dependence from the process temperature

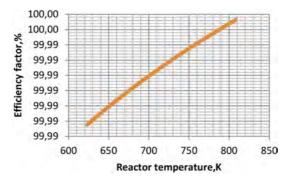


Fig. 2. The efficiency factor of HM paraffin cracking reaction dependence from the process temperature

reaction occurs in the kinetic range, from the conditions of $\phi \rightarrow 0$ and $\eta \rightarrow 1$. These results should be considered in the CC mathematical model. Chemical reactions on the catalyst surface are determined by a limiting stage of the process. The observed rate of the process depends on the temperature.

References

- Потехин В.М., Потехин В.В. Основы теории химических процессов технологии органических веществ и нефтепереработки: Учебник для вузов.– СПб: ХИМИЗДАТ, 2005.– 912 с.
- Ушева Н.В., Кравцов А.В. Макрокинетика химических процессов и расчет реакторов. Учебное пособие.– Томск: Изд-во Томского политехнического университета, 2013.– 100 с.