

Kinetics of Isopropyl Alcohol Conversion over Oxide Catalysts with Oxidation-Reduction Properties

Wincenty Turek¹, Agnieszka Wolna¹, Mieczyslaw Lapkowski^{1,2},

¹Institute of Physical Chemistry and Technology of Polymers, Silesian Technical University, Strzody 9, 44 100 Gliwice, Poland, ²Institute of Coal Chemistry, Polish Academy of Sciences, 44 121 Gliwice, Poland

Introduction

The objective of the studies was to obtain kinetic equations of parallel reactions and the overall kinetic equation of isopropyl alcohol conversion over Co_3O_4 . Selectivities towards propene, acetone, activation energies and reaction orders of parallel reactions and for the entire process were calculated.

Results and discussion

Conversion of isopropyl alcohol is often used as a test reaction to investigate the activity of various catalysts [1]. Two parallel reactions proceed during isopropyl alcohol conversion: dehydration to propene and dehydrogenation to acetone [1-3]. Selectivities of these reactions are a useful measure of oxidation-reduction and acid-base properties of the catalyst surface [2,3].

The experiments were performed to obtain kinetic equations of parallel reactions and for the entire process of isopropyl alcohol conversion. The kinetics was determined over Co_3O_4 . The catalyst was prepared by heating cobalt (II) hydroxide at 833 K for 6 h. The purity of the catalyst was verified by X-ray diffraction measurements. The diffraction pattern of Co_3O_4 contained all peaks characteristic of this oxide while other peaks, which could suggest the presence of impurities, were absent. Hence, the sample was pure regular Co_3O_4 (spinel).

Kinetic measurements were performed using the differential method in a glass reactor with the internal diameter of 18 mm. The reaction substrate - isopropyl alcohol was diluted with nitrogen. During the measurements of activation energy the mole fraction of isopropyl alcohol was 0.0179. For the determination of kinetic equations the mole fraction of the alcohol was changed between 0.0141 to 0.0228. In all experiments the flow rate through the reactor was 20.0 dm^3/h . The reaction conversion levels were in the range 5÷15 %. In all measurements approximately 2.027 g of the catalyst with grain size between 0.49 and 0.75 mm were used.

Table 1. The selectivity of isopropyl alcohol conversion

Selectivity (%)					
450 (K)		465 (K)		480 (K)	
Propene	Acetone	Propene	Acetone	Propene	Acetone
0.11	99.89	0.18	99.82	0.28	99.72

Previous kinetic investigations of isopropyl alcohol conversion indicate that the selectivity strongly depends on redox and acid-base properties of the catalyst surface. It suggests that the kinetic equation of the reaction can be determined by the properties of the surface of the catalyst over which the reaction proceeds. In our studies the catalyst with strong oxidation-reduction properties was used.

The kinetic results of isopropyl alcohol conversion are shown in Fig. 1 and Fig. 2.

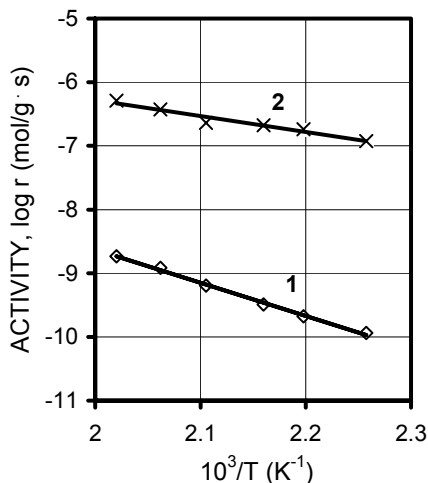


Fig. 1. Arrhenius plots of isopropyl alcohol decomposition. 1 – Propene, 2 – Acetone

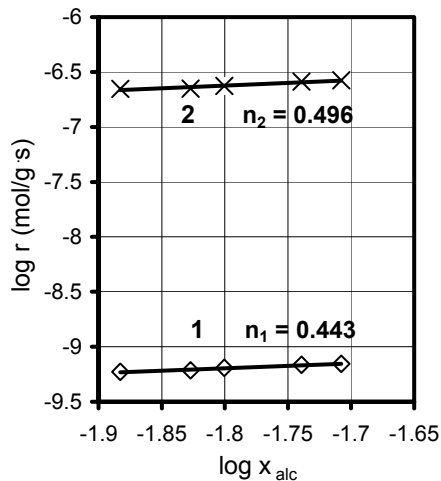


Fig. 2. The rate of reaction as a function of the isopropyl alcohol mole fraction x_{alc} . 1–Dehydration, 2–Dehydrogenation

It was found that the reaction rate does not depend on the concentration of the products. The values of activation energy are: for dehydration $E_{a(1)} = 102.0$ kJ/mol and for dehydrogenation $E_{a(2)} = 45.5$ kJ/mol. The results concerning reaction selectivities are given in Table 1.

The kinetic equations of isopropyl alcohol conversion can be expressed as:

$$r = k \cdot p_{alc}^n$$

where: r – reaction rate, k – rate constant, p_{alc} – partial pressure of isopropyl alcohol,

n – reaction order.

The reaction order for the conversion process is $n = 0.50$, for dehydration $n_1 = 0.44$ and for dehydrogenation $n_2 = 0.50$.

As a result of the low significance of the dehydration reaction in the conversion process of isopropyl alcohol over Co_3O_4 the overall reaction order is the same as for the dehydrogenation reaction.

References

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