CREATION OF MIXED POLYFUNCTIONAL CATALYSTS FOR HYDRATION OF ACETYLENE IN VAPOR PHASE

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ABSTRACT

The catalytic properties of various substances in the transformation of acetylene depend on the mechanism of activation of reagents and the reactivity of intermediate substances. Acetylene chemistry uses metal complexes, acid-base catalysts, salts, and metal catalysts. A complex of mercury, cobalt, palladium, rhodium, chromium, titanium and other metals acts as a catalyst in the reactions of acetylene in the liquid phase.

Keywords: mercury, cobalt, palladium, rhodium, chromium, titanium

INTRODUCTION

The hydration reaction of acetylene is a complex sequential and parallel reaction, which includes the addition of a nucleophilic agent (water) to acetylene, isomerization, condensation (formation of aldol and croton aldehyde), ring formation (paraldehyde), decarboxylation and dehydrogenation. Such processes can be carried out in the vapor phase with the presence of polyfunctional catalysts. Based on the above, the role of each component in the activation of elementary steps in the formation of acetaldehyde and acetone is taken into account when choosing a catalyst. In this process, newly developed cadmium catalysts for the hydration of acetylene in the vapor phase direct the process towards the formation of acetaldehyde and zinc catalysts.

In order to obtain catalysts with high activity and stability for the hydration of acetylene in the vapor phase, more than 30 new catalysts have been created.To prove our point, we made a thermodynamic calculation of the acetone formation process.

$2C_2H_2 + 3H_2O \rightarrow CH_3COCH_3 + CO_2 + 2H_2$

We got the following values: ΔH^0_{298}= -334.4 kdJ/mol.

ΔS^0_{298}= -121,2 кдЖ/моль·град. ΔG^0_{298}= -367,5 кдЖ/моль.

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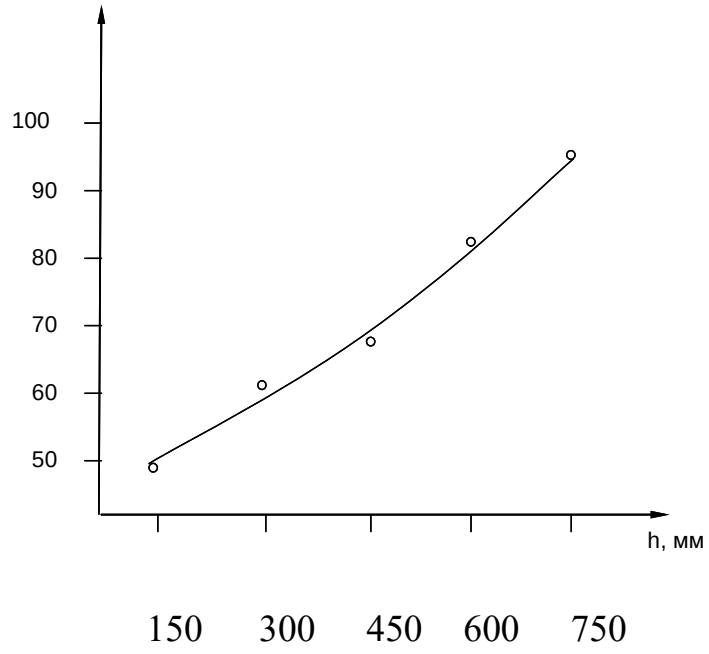
The obtained results showed that the process of acetone formation is irreversible and proceeds with the release of heat. It was found that the value of Gibbs energy decreases from 10800 kdJ/mol to 12404 kdJ/mol in the temperature range of 298 K–723 K. The effect of catalyst layer height on acetylene conversion was studied (Fig. 1).



1 – Picture. Variation of acetylene conversion according to the height of the catalyst layer.

As can be seen from Figure 1, the acetylene conversion increases as the height of the catalyst layer increases. This indicates that the process takes place in the internal diffusion layer. Acetylene conversion is significantly affected by the volumetric rate of acetylene.

Systematic studies are conducted to create mono- and bifunctional homogeneous and heterogeneous catalysts for the synthesis of acetaldehyde, acetone, and pyridine bases. Methods of analysis and verification of the obtained products and synthesized catalysts have been developed.

The composition of the catalyst for the release of acetaldehyde, including carriers, reaction temperature, volumetric rate and ratio of starting reagents, regeneration of the catalyst was also studied. When experiments are conducted in the temperature range from 320 to 440 ºC, the selectivity of acetaldehyde formation increases up to 360 ºC (67 %), and then sharply decreases. An increase in the conversion rate of acetylene was also found when the height of the catalyst layer increased from 150 mm to 750 mm.

When the volumetric rate of acetylene increases from 50 to 300 h-1, the acetylene conversion decreases to a certain extent, which is also shown by the mechanism of the process occurring in the internal diffusion field. Taking into account the above, more than 30 samples of catalysts for the synthesis of acetaldehyde, acetone, pyridine bases, and pyrroles were synthesized and their composition and textural characteristics were determined.

The regularity of catalysts consisting of zinc oxide and zinc fluoride was determined, in which the yield of acetylene increased from 20% to 69%. It is established that cadmium compounds direct the reaction to the formation of acetaldehyde, and zinc compounds direct the reaction to the formation of acetone.

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