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## Catalytic Synthesis Of Acetone From Acetylene

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### ABSTRACT

The vapour-phase hydration of acetylene with the formation of acetone on polyfunctional catalysts has been studied. The process parameters have been found that ensure the production of acetone with high selectivity and conversion of acetylene. As a result of studying the effect of temperature on the yield of acetone, it was found that in the temperature range of 360-5000C the dependence between the reaction yield and temperature is extreme and at 4500C the yield is maximum. Based on the study of the kinetic laws of the reaction, the mechanism of acetone formation in the presence of a given catalyst based on the kinetic equation of the reaction to obtain acetone by the catalytic hydration of acetylene and the results of experimental and qualitative and quantitative compositions of reaction products.

### KEYWORDS

Acetone, acetylene, vapour-phase, hydration, BET equation, diffract meter

### INTRODUCTION

Acetone is a valuable chemical product. It can be obtained by oxidative dehydrogenation of isopropyl alcohol, oxidation of propylene, decomposition of acetic acid and ethyl alcohol, oxidation of cumene, etc. [1-7]. Among the known processes for the production of acetone, the most promising is

the synthesis by hydration of acetylene in the presence of catalysts. The advantage of this method is the possibility of carrying out the process in existing installations for the production of acetaldehyde. On the other hand, the process of simultaneous production of acetaldehyde and acetone under the action

of polyfunctional catalysts and the implementation of the process by flexible technology are promising [8-12].

Currently, the acetic aldehyde is mainly obtained by two methods - hydration of acetylene and oxidation of ethylene [13-17].

The process of hydration of acetylene to acetaldehyde in the presence of catalysts has been studied quite well. Numerous catalysts have been proposed for this process [18-20]. Among the known catalysts for the hydration of acetylene to acetic aldehyde, the most active was the cadmium-calcium-phosphate catalyst (CCP), which is recommended for industrial use [18-21]. However, the cadmium-calcium-phosphate catalyst is not without its drawbacks. The average output of acetaldehyde per one pass of acetylene does not exceed 7.0%. The CCP catalyst is very sensitive to temperature changes, its service life before regeneration does not exceed 72-76 hours.

Hydration of acetylene in the presence of a catalyst can be carried out in order to obtain acetone. The advantage of this method is the possibility of carrying out the process in existing installations for the production of acetaldehyde. Replacing the cadmium-calcium-phosphate catalyst with a zinc-containing catalyst makes it possible to obtain acetone with good yield with minor changes in technology.

The production of acetone from acetylene in one phase by passing a mixture of acetylene with steam over catalysts at high temperatures is undoubted of considerable practical and theoretical interest [22].

## EXPERIMENTAL PART

Experiments on the catalytic hydration of acetylene and its derivatives in the gas phase were carried out on a reactor 25 mm in diameter and 1000 mm in height, made of stainless steel under stationary conditions. The qualitative and quantitative composition

of the reaction products was studied by gas-liquid chromatography under the following conditions: stationary phase 15% Apiezon-M in Cvetochrome, column thermostat temperature 800C, carrier gas flow rate - helium 60 cm<sup>3</sup> / min, detector-DIP. Quantitative analysis was carried out using the method of internal standards [23].

Specific surface area, crushing strength, total pore volume and ash content of the samples were determined.

The specific surface area was determined by the method of thermal desorption of nitrogen in a flow of a carrier gas - helium at the boiling point of liquid nitrogen; the experimental data were processed using the BET equation.

The phase composition of the samples was determined by the method of X-ray diffractometry, the shooting was carried out on a DRON-3M diffract meter on CuK $\alpha$ -radiation with a Ni-filter, the length of the X-ray radiation  $\lambda = 1,54 \text{ \AA}$ .

The specific surface area of the obtained catalyst was calculated by the BET method. Dispersed properties of the catalyst were studied using a scanning electron microscope (JSM-6510 LV). The catalytic activity of the obtained sample was studied using the acetylene hydration reaction. Acetaldehyde and acetone were synthesized as follows. Acetylene was saturated with water at a temperature of 70-800C and at a ratio of water: acetylene = (1:3)-(1:5) mol was passed through the catalyst bed at 3600C with a space velocity of 180-200 h<sup>-1</sup>. The vapour-gas mixture leaving the reactor was cooled in a refrigerator. The reaction products were trapped in water. The catalyst contains acetaldehyde, acetone, crotonaldehyde, paraldehyde, etc. In order to maintain the degree of acetylene conversion at least 80%, the reaction temperature was raised by 100C every 20 h. After 96-120 hours, the degree of conversion of acetylene decreases to 75-70%.

Then the reaction was stopped and the catalyst was regenerated in a known manner [3,4].

Subsequently, the effect of various parameters (temperature, space velocity, acetylene-water ratio) on the acetylene conversion and acetone yield was studied. As a result of studying the effect of temperature on the yield of acetone, it was found that in the temperature range of 360-5000C the dependence between the reaction yield and temperature is extreme and at 4500C the yield was considered maximum.

Recently, the sol-gel method has been intensively used for the synthesis of inorganic and organo-inorganic matrices at low temperatures. This method has a number of advantages: the simplicity of the used equipment of devices, efficiency, environmental safety, low cost, adaptability of technologies, and others. Nanocatalysts exhibit high catalytic activity, selectivity, stability (stability).

The prospect of using catalysts with nanoparticles in catalysis is associated with two features. First, as the particle size decreases, most of the atoms are located on the surface; therefore, the catalyst consisting of nanoparticles has a large surface and becomes very active in heterogeneous reactions.

Second, most of the properties of nanoparticles are related to their size (size

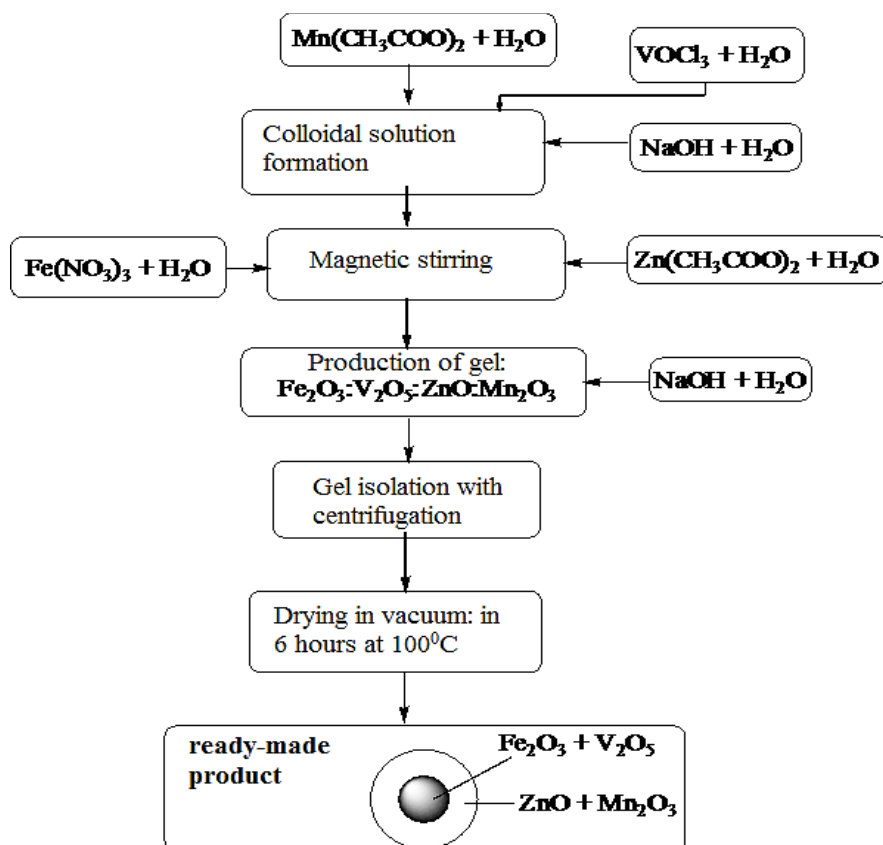
efficiency); therefore, changing the size of nanoparticles can control not only the activity but also the selectivity. As the catalyst particle size decreases, the reaction rate sharply increases.

Based on the foregoing, the study of the possibility of using Nanocatalysts based on the metals Zn, Mn, Fe, V and other elements with polyfunctional properties for the hydration reaction of acetylene and its derivatives is an urgent task.

Sol-gel technology is one of the methods for producing Nanocatalysts based on the synthesis of inorganic and inorganic-organic hybrid materials from colloidal particles. The use of the sol-gel method in petrochemical synthesis can ensure the production of crystalline nanoparticles and lower the synthesis temperature of a single-phase product. Therefore, at present, studies devoted to the synthesis of Nanocatalysts for petrochemical synthesis are relevant. Proceeding from this, we studied the process of acetylene hydration to obtain acetaldehyde, acetone, or their mixture in the presence of mixed polyfunctional Nanocatalysts [24].

Scheme of the synthesis of nanoparticles with the composition

Fe<sub>2</sub>O<sub>3</sub>: V<sub>2</sub>O<sub>5</sub>: ZnO: Mn<sub>2</sub>O<sub>3</sub> with a core-shell structure:



The specific surface area of the obtained catalyst was calculated by the BET method, and the average mesopore size was calculated by the VUA method. The phase composition was studied by X-ray diffraction on a DRON-3 diffract meter (CuK $\alpha$  radiation). Dispersed properties of the catalyst were studied using a scanning electron microscope (JSM-6510 LV). The catalytic activity of the obtained sample was studied using the acetylene hydration reaction.

The reactions of catalytic hydration of acetylene were carried out in a reaction glass tube 2 cm in diameter, the length of the catalyst layer was 60 cm, and the catalyst volume was 90 cm<sup>3</sup> (the true volume of the catalyst was 25 cm<sup>3</sup>).

The qualitative and quantitative composition of the reaction products was studied by gas-liquid chromatography under the following conditions: stationary phase 15% Apiezon, M in Cvetochrome, column thermostat

temperature 800C, carrier gas flow rate — helium 60 cm<sup>3</sup> / min, detector-DIP. Quantitative analysis was carried out by the method of internal standards.[25]

Subsequently, the effect of various parameters (temperature, space velocity, acetylene-water ratio) on the acetylene conversion and acetone yield was studied.

As a result of studying the effect of temperature on the yield of acetone, it was found that in the temperature range of 360-500C the dependence between the reaction yield and temperature is extreme and at 450C the yield is maximum.

To maintain the conversion of acetylene at a constant level of 80-85%, it is necessary to increase the temperature by 100C every 15-20 hours.

**Effect of temperature on reaction yield.** The newly formed composition has a high activity and productivity

$(\text{Fe}_2\text{O}_3)_x(\text{V}_2\text{O}_5)_y(\text{ZnO})_z(\text{Mn}_2\text{O}_3)_k$  when the effect of temperature on the yield of

acetone in the presence of a catalyst was studied, it was found that the optimum temperature for the hydration reaction of acetylene was 425°C (Table 1).

**Table 1.**

**Effect of temperature on acetylene conversion, acetone yield and process selectivity.  $(\text{Fe}_2\text{O}_3)_x(\text{V}_2\text{O}_5)_y(\text{ZnO})_z(\text{Mn}_2\text{O}_3)_k$**

№	Temperature, °C	Total conversion of acetylene, %	The yield of acetone, %	Selectivity, S %
1	280	18.2	10.0	54.90
2	330	33.5	20.6	61.2
3	350	48.5	32.6	67.2
4	375	52.4	41.7	73.4
5	400	65.8	58.5	88.9
6	425	94.8	86.4	91.1
7	450	86.5	70.8	81.8
8	475	90.8	68.4	75.3

The table shows that when the temperature reaches 425°C, the yield of acetone is 86.4%, and the selectivity of the process to acetone is 91.1%.

**Effect of volumetric velocity on acetylene conversion and acetone yield**

The effect of volumetric velocity on acetone yield and acetylene conversion was also studied, and the experimental results are presented in Table 2. As the volume rate of acetylene increases, its overall conversion decreases, as shown in Table 2.

**Table 2.**

**Effect of volumetric velocity on acetaldehyde yield and acetylene conversion. (cat №4; T= 4250C)**

Volumetric velocity hour <sup>-1</sup>	The rotation rate of acetylene, %		S, %
	General	Acetone	
40	98.2	34.3	34.9
60	97.6	44.8	45.9
80	96.5	55.7	57.7
100	95.2	68.8	72.3
120	94.8	86.4	91.1
140	92.6	69.4	74.9
160	90.2	50.8	56.3
180	87.7	38.2	43.6

Influence of reagent ratios on acetylene conversion and acetone yield. The effect of C<sub>2</sub>H<sub>2</sub>: H<sub>2</sub>O mole ratios on acetone yield and

acetylene conversion was also studied. The results of the experiment are presented in Table 3.

**Table 3. Influence of c<sub>2</sub>h<sub>2</sub>: h<sub>2</sub>o mole ratios on acetone yield.**

**( T=4250C, catalyst №4; )**

№	C <sub>2</sub> H <sub>2</sub> :H <sub>2</sub> O mol ratio	Acetylene conversion, %		Selectivity S%
		General	Acetone	
1	4:1	44.8	22.3	49.8
2	3:1	65.7	46.8	71.0
3	2:1	78.6	71.4	78.1
4	1:1	86.2	71.8	83.3
5	1:2	94.8	86.4	91.1
6	1:3	88.5	79.8	90.7
7	1:4	93.4	72.5	77.6

Kinetic model and mechanism of the catalytic hydration reaction of acetylene. It is known from the scientific literature that there is no single view on the kinetic laws of this process and the mechanism of the process. Therefore, to study the kinetic laws of the catalytic hydration reaction of acetylene, the effect of water and acetylene partial pressures on the rate of acetone formation at a temperature of 400-4750C in the range of 250C and a

volumetric velocity (on acetylene) of 120 h<sup>-1</sup> was studied.

The effect of the partial pressures of the reagents on the kinetic laws of the process was carried out by changing the partial pressure of one reagent while maintaining the partial pressures of the remaining reagents at a constant rate. In order to keep the linear velocity of the initial mixture constant, the

required amount of pure argon gas was sent to the reaction zone (field) as needed. The catalyst volume was adjusted accordingly to maintain a constant rate of acetylene flow. As a result of studying the effect of partial pressures of acetylene and water on the kinetic laws of the reaction, it was found that the yield of acetone increases with the decrease of the partial pressure of acetylene. At this time, the total conversion of acetylene

increases, while the selectivity of the reaction relative to acetone decreases.

Based on the study of the kinetic laws of the reaction, the following kinetic equation for the reaction of obtaining acetone by the catalytic hydration of acetylene was proposed:

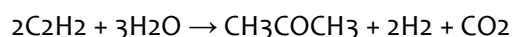
$$K_p = \frac{P_{C_3H_6O} \cdot P_{CO_2} \cdot P_{H_2}^2}{P_{C_2H_2}^2 \cdot P_{H_2O}^3}$$

The relationship between  $\lg K_p$  and temperature is expressed as follows:

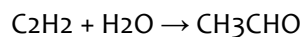
$$\lg K_p = \frac{17637}{T} - 2,611 \lg T + 1,356 \cdot 10^{-3} T - 0,092 \cdot 10^{-6} T^2 - \frac{0,223 \cdot 10^5}{T^2} - 3,794$$

Based on the results of the experimental and qualitative and quantitative compositions of the reaction products, the following scheme of the mechanism of acetone formation in the presence of a given catalyst is proposed:

The formation of acetone can be expressed in the form of the following sum equation:



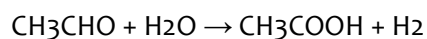
The formation of acetylene is explained by the following reliable mechanism: first acetylene is hydrated and acetaldehyde is formed:



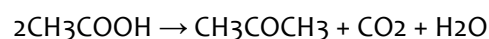
Acetaldehyde reacts with water vapour to form acetone:



The formation of acetic acid as a result of the reaction can also be considered as the result of the following reaction:



Some of the acetic acid formed is converted to acetone by the release of carbon dioxide and water:



The above method of obtaining acetone is a promising method for Uzbekistan.

## CONCLUSION

The vapour-phase hydration of acetylene with the formation of acetone on polyfunctional catalysts has been studied. The process parameters have been found that ensure the production of acetone with high selectivity and conversion of acetylene. As a result of studying the effect of temperature on the yield of acetone, it was found that in the temperature range of 360-5000C the dependence between the reaction yield and temperature is extreme and at 4500C the yield is maximum.

Based on the study of the kinetic laws of the reaction, the mechanism of acetone formation in the presence of a given catalyst based on the kinetic equation of the reaction of

obtaining acetone by the catalytic hydration of acetylene and the results of experimental and qualitative and quantitative compositions of reaction products.

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