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*AIP Conf. Proc.* 3304, 040105 (2025)

<https://doi.org/10.1063/5.0269390>



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# Kinetics and Mechanism of Vapor Phase Vinyl Acetate Synthesis Reaction from Ethylene

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**Abstract.** Active and selective synthesis of vinyl acetate from ethylene was selected for the process of oxidative acetylation of ethylene with ethanoic acid in the presence of air oxygen, the substance that increases the speed of the chemical reaction was selected for the purpose of the development of the substance that increases the rate of the chemical reaction, and in order to control the catalytic properties of the included components, it was selected for the process of oxidative acetylation of ethylene with ethanoic acid in the presence of air oxygen, the rate of the chemical reaction the effect of the amount and ratio of individual components of the enhancer was studied.

**Keywords.** Ethylene, oxygen, ethanoic acid, vinylacetate, kinetic equation, mechanism.

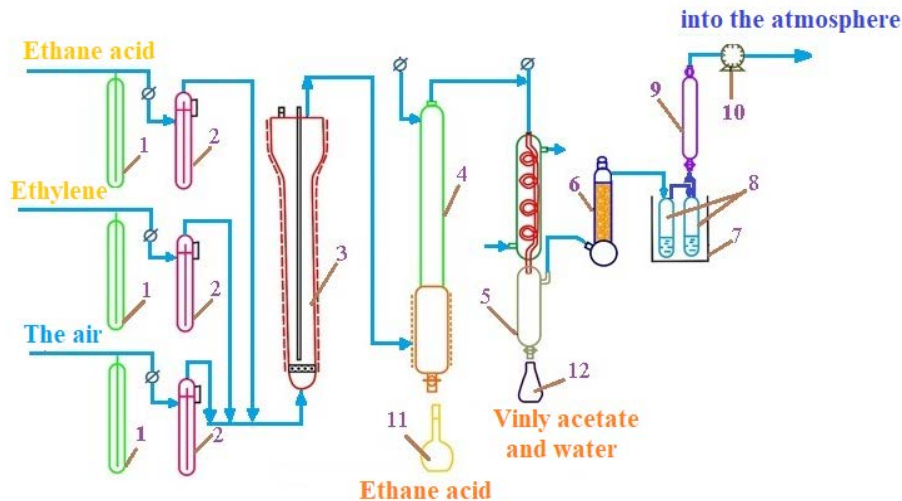
## INTRODUCTION

In industrial conditions and in experimental devices, despite the variety of retainers, catalytic systems based on silica gel and aluminum oxide are widely used [1-6]. Under the influence of ethylene selected for the oxidative acetylation process with ethanoic acid in the presence of air oxygen in a substance that increases the rate of the chemical reaction some properties of active centers, for example, the holder is selected for the process of oxidative acetylation of ethylene with ethanoic acid in the presence of air oxygen, the proton-acid properties of the surface, the coordination ability of the metal, or the parameters of the crystal lattice change due to the interaction with the substance that increases the rate of the chemical reaction [7-14]. In addition to palladium or its salts, selected for the process of oxidative acetylation of ethylene with ethanoic acid in the presence of air oxygen, the substance that increases the rate of the chemical reaction contains from 1 to 30% alkali metal acetates, among which the most widely used [15-21] accelerates the reaction and ethylene in air Potassium acetate is selected for the oxidative acetylation process with ethane acid in the presence of oxygen, and the substance that increases the rate of the chemical reaction and increases the selectivity is potassium acetate. It was found that the effectiveness of the promoter's effect depends on its content in the complex catalytic complex[22-26]. In many cases, the maximum activity of the substance that increases the rate of the chemical reaction is observed in a certain content, selected for the process of oxidative acetylation of ethylene with ethanoic acid in the presence of air oxygen [27-39].

Currently, the reaction of obtaining ethylene from methane in one step, while obtaining aromatic hydrocarbons and unsaturated lower molecular hydrocarbons from methane, as well as the synthesis of aromatic hydrocarbons from the propane-butane fraction and petroleum satellite gases are gaining importance. Therefore, the processes of catalytic aromatization of methane, propane-butane fraction and petroleum satellite gases, obtaining methanol and dimethyl ether from methane through synthesis gas, and obtaining lower molecular olefins from methanol and dimethyl ether are of great interest to world scientists, and scientific research in these areas is being intensively conducted[40 -60].

## EXPERIMENTAL PART

Oxidative acetylation of ethylene in the presence of air oxygen and acetic acid in a boiling-bed reaction rate-increasing substance reactor, which is a laboratory device, was studied in the laboratory.



**FIGURE 1.** Laboratory apparatus for studying the catalytic oxidative acetylation reaction of ethylene with acetic acid in the presence of atmospheric oxygen in the vapor phase

1-Manostats; 2-Rheometers; 3-Reactor; 4-Evaporation column; 5-Refrigerator; 6-Drying column; 7-Dewar's container; 8-Toluene trap; 9-Gas pipette; 10-Gas clock; 11-acetic acid collector; 12- Vinyl acetate collector

The initial gas-ethylene, acetic acid, air and, if necessary, oxygen-through the drying system, cleaning and dosing of additives (1,2) are introduced into the lower part of the reactor after initial mixing (3). In the reactor, a quartz tube with a diameter of 42 mm and a length of 1.2 m is equipped with an electric heater. At the bottom of the reactor, the Shotta reactor is placed, and it performs the function of ensuring equal distribution of the supplied gas. In the upper part of the reactor, there is a width, which is used for better separation of dusts of the substance that increases the reaction rate and the carried particles. The temperature of the reaction zone is measured by a moving thermocouple. A substance that increases the reaction rate is placed in the reactor, the volume of the substance that increases the reaction rate is changed from 100 to 840 ml. Depending on the conditions, the combustion of the substance that increases the reaction rate and the heating of the system to sufficient temperatures were carried out using an electric heater. At the same time, air was supplied to the reactor to form a boiling bed. When the temperature was raised to 180oC, the system providing the initial reagent ethylene and acetic acid was started. The device was idle for 1-1.5 hours until a stationary mode was formed, and then the experiment was started. During the experiment, the specified regions are entered in the required amount, along with the participation of carbon monoxide. The mixture of reaction gases from the reactor (3) enters the quartz purification column.

Methods of determining the granulometric content of a substance that increases the rate of reaction. This method used a vibrating machine using mesh sizes of 20µm, 30µm, 40µm, 50µm, 60µm, 80µm to analyze the analysis based on the transfer of particles of specific mass-reacting agent through the mesh and measurement of the mass of the sample retained on the mesh. A 0.5g accelerator suspension is placed on the top of the grid (80µm). A set of nets is attached to a vibrating machine. When the vibrating process is stopped, the machine is stopped and the nets are pulled out separately. The mass fraction of the substance fraction that increases the reaction rate is calculated by the following formula 20µm (X1).

$$X_1 = \frac{m_1 \cdot 100}{m}, \% \quad (1)$$

where m1 is the mass remaining in the substance. m is the mass of the substance that increases the reaction rate.

If the fraction of the substance increasing the reaction rate is less than 30 µm, the mass fraction (X2) is expressed by the following formula.

$$X_2 = \frac{(m_1 + m_2) \cdot 100}{m}, \% \quad (2)$$

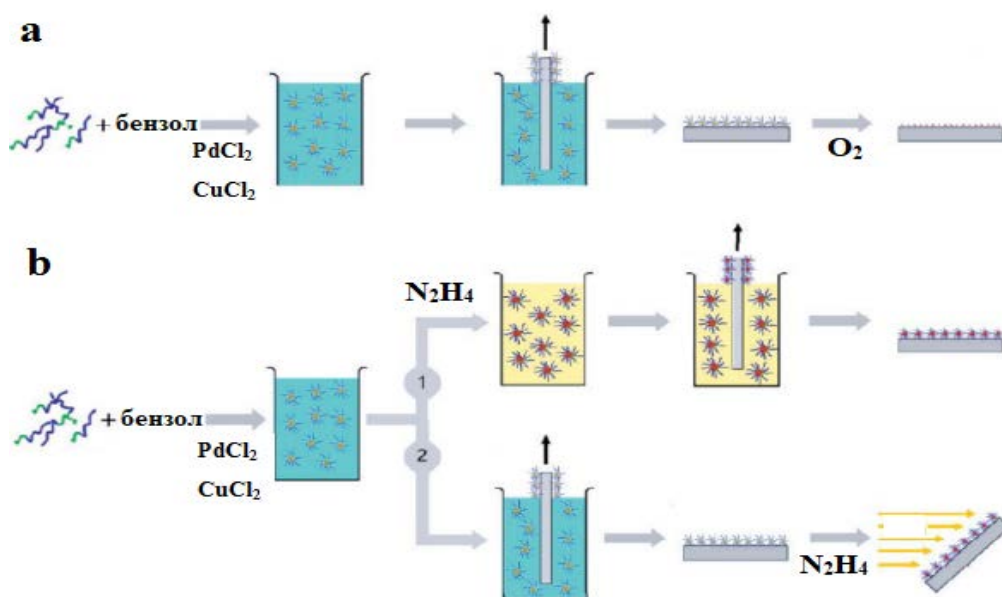
where is the residual mass on the -20µm grid.

If the fraction of the substance increasing the reaction rate is less than 40  $\mu\text{m}$ , the mass fraction is determined by the following formula.

$$X_3 = \frac{(m_1 + m_3) \cdot 100}{m}, \% \quad (3)$$

where is the mass remaining on the -20 and 30 $\mu\text{m}$  grids. By this method, the percentage of mass in the remaining fractions was determined.

Methods of conducting and processing the experiment. The required amount of reaction rate-increasing substances with sizes of 100-300 microns are introduced into the reactor. Heating of the reactor to a temperature sufficient to form a boiling bed was carried out simultaneously with the introduction of air into the reactor. When the required temperature is reached, the introduction of all components begins and the reactor is started for 1.5-2 hours until a stationary mode is formed, then the device is connected to the experiment through a 3-way tap. At the end of the experiment, the reactor is connected to the "sbros", all the supplied gases are stopped except for air, and the substance that increases the reaction rate is blown in for one hour. Blowing is stopped when the temperature of the reactor reaches room temperature. Synthesis method of nanoreaction rate-enhancing substance containing PdCu.



**FIGURE 2.** Methods used to obtain bimetallic PdCu nanoparticle arrays: (a) oxygen plasma; (b) Reduction with hydrazine in solution or in hydrazine vapor.

The resulting colloidal Pd nanoparticles stabilized with polyvinylpyrrolidone were precipitated with acetone under stirring, followed by redispersion of the precipitate in ethyl alcohol. Pd nanoparticle reaction rate enhancers placed on high silica gel YuKTs carrier were obtained as follows. The desired volume of the colloidal solution was added to pre-dried high silica gel supports at 300 °C in a ready-made catalyst containing 0.4% Pd and 4% Cu and dried at 85-80 °C with occasional stirring, avoiding boiling of the solution. It was further dried at 160 °C for 4 h.

The composition and concentration of acid centers was determined by the Bates method. The sample was suspended in 0.05 N NaOH solution for one day, after which the sample was filtered and a given volume of hydrochloric acid was added to the filtrate. The resulting sample was potentiometrically titrated with 0.05 N sodium hydroxide solution.

## RESULTS AND DISCUSSION

The addition of 3-5% Cu to the chemical reaction accelerator was selected for the oxidative acetylation process of ethylene with ethanoic acid in the presence of air oxygen, to obtain a chemical reaction accelerator and its activity. ethylene has been shown to allow an increase of  $\approx 30\%$  with almost no increase in burning rate.

A significant increase in the experimental values of  $W_{CO_2}$  rates for a series of reactions in the study of the effect of copper is explained by the use of the above-mentioned reason - the use of samples of chemical reaction accelerators selected for the process of oxidative acetylation of ethylene with ethanoic acid in the presence of atmospheric oxygen, prepared with a technology violation. Thus, the  $W_{CO_2}$  rates differ from the calculated experimental values by a constant magnitude, which indicates that additional reactions of ethylene combustion occur in the trap rather than in the active palladium centers. The last value was selected for the process of oxidative acetylation of ethylene with ethanoic acid in the presence of air oxygen in order to find the most effective samples, mathematical models were used to optimize the composition of the substance that increases the rate of the chemical reaction.

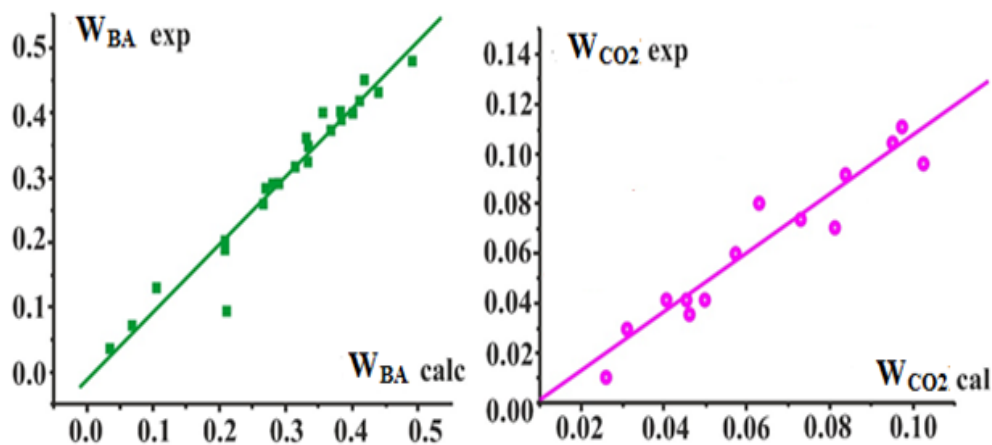


FIGURE 3. Correlation dependences of experimental and calculated values of reaction rates

Since the rate of formation of reaction products in the reactor is constant, the output of vinylacetate (or  $CO_2$ ) over time is equal to the rate of formation of reaction products multiplied by this time, that is,  $n = W \cdot t$ , where the output of the indicated products in one hour is equal to the reaction rate:

$$n/t = W \cdot t/t = W$$

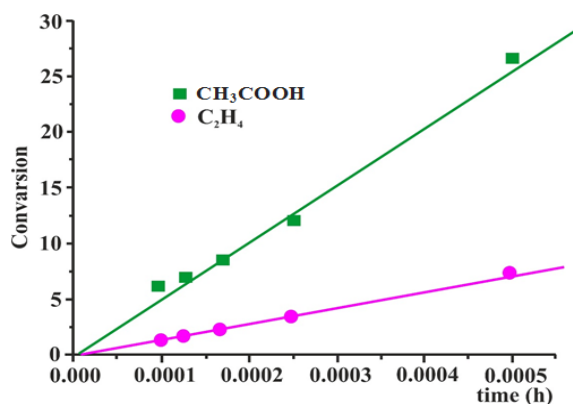


FIGURE 4. Dependence of conversion of reagents on the time of BGA in the reactor (contact time).

Now, all rates of product formation and selectivity can be expressed by the following equations in this range of changes in volumetric rates of delivery:

$$W_{BA} = 0,4(1+2,2 \cdot 10^{-5} \cdot V) \text{ mole/hour}; \quad W_{CO_2} = 0,09(1-3 \cdot 10^{-5} \cdot V) \text{ mole/hour}$$

$$S = \frac{0,4(1+2,2 \cdot 10^{-5} \cdot V)}{0,09(1-3 \cdot 10^{-5} \cdot V)}$$

where  $V$  is the BGA volumetric rate ( $h^{-1}$ )

All the studied reactions occur in the kinetic domain through subtle diffusion effects, which only begin to affect the increase in the residence time of the BGA in the reactor.

A decrease in the oxygen content to 1.0% in the specified parameters does not lead to a significant increase in the carbon monoxide content.

No inhibition of the reaction by oxygen is observed. The reaction rate equations will look like:

- as a function of the mole fraction of oxygen in ethylene:

$$\text{WBA} = (6.54 \pm 0.5) \cdot [\text{O}_2 \text{ fraction}] \text{ mol/h}$$

$$\text{WSO}_2 = (0.92 \pm 0.07) \cdot [\text{O}_2 \text{ fraction}] \text{ mol/h}$$

- as a function of oxygen partial pressure:

$$\text{WBA} = (1.07 \pm 0.07) \cdot [\text{R}(\text{O}_2)] \text{ mol/h}$$

$$\text{WSO}_2 = (0.156 \pm 0.01) \cdot [\text{R}(\text{O}_2)] \text{ mol/h}$$

Using the obtained equations, the calculated selectivity of vinylacetate formation on ethylene ( $S_{\text{his}} = S_{\text{al}}$ ) describes well the experimental values.

The relationship between vinyl acetate yield and  $\text{SO}_2$  formation is linear. Formation rates of reaction products were calculated from the constructed kinetic curves.

Thus, in the conditions of these experiments, the reaction rates are determined by the following equations:

Formation of vinyl acetate:

$$\text{WBA} = \exp(8.63) \cdot \exp(-4086/T^\circ\text{K}) \text{ mol/hour}$$

$$\text{WSO}_2 = \exp(20.1) \cdot \exp(-9810/T^\circ\text{K}) \text{ mol/hour}$$

## CONCLUSION

As a result of the experiments, a laboratory installation was carried out for the catalytic reaction of ethylene hydroxyacetylation with atmospheric oxygen in the presence of ethanol acid in the vapor phase in a reactor with a boiling catalyst. It has been proven that the agent chosen for the oxidative cross-hydroxyacetylation process reduces the efficiency of the chemical reaction and blocks active centers.

The desired volume of colloidal solution was added to pre-dried silica gel supports at 300 °C over the prepared catalyst containing 0.4% Pd and 4% Cu and dried at 85–80 °C with occasional stirring to avoid boiling. Solution and drying at 160 °C. And they dry again for 4 hours.

Methods for determining the particle size distribution of the catalyst in the catalytic reaction of ethylene oxyacetylation in the presence of atmospheric oxygen and acetic acid in the vapor phase were determined by sorbent studied and the results were obtained.

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