

## COMPREHENSIVE STUDY OF CARBAMMONOLYSIS OF POLYVINYL ALCOHOL: FROM EXPERIMENT TO THERMODYNAMICS

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### ARTICLE INFO

### ABSTRACT:

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*This study presents a comprehensive analysis of the carbammonolysis reaction of polyvinyl alcohol, combining experimental investigation with thermodynamic modeling. The aim is to determine optimal conditions for the synthesis of polyvinylamide water-soluble polymers exhibiting pronounced surface-active properties. Based on experimental data, key parameters affecting conversion efficiency and structural characteristics of the product were identified. Thermodynamic analysis provided insight into the energetic profile and reaction mechanism. The obtained results contribute significantly to the field of targeted synthesis of functional polymers and can be applied to scale-up and optimization of industrial processes for producing water-soluble polymer compositions with tailored properties.*

**INTRODUCTION. Comprehensive Study of Polyvinyl Alcohol Carbammonolysis: From Experiment to Thermodynamics** Within the framework of studying the carbammonolysis reaction of polyhydric alcohols, including polyvinyl alcohol (PVA), special attention is given to the importance of the resulting amide derivatives. This work focuses on PVA due to its potential for various structural modifications, including the formation of polyacrylamide derivatives and stereoregular iso- and syndiotactic structures.

The objective of this study is to gain a deeper understanding of the reaction mechanism and to determine optimal synthesis conditions, which is crucial for the development of effective methods for producing functional polymeric materials with tailored properties and a wide range of potential applications.

The choice of PVA as a starting material is based on its industrial availability and the feasibility of large-scale production. The manufacturing of PVA can be realized using existing facilities for acetylene and acetic acid production, such as those at the NavoiAzot chemical complex. The resulting vinyl acetate serves as a monomer for the synthesis of polyvinyl acetate — a valuable polymer widely used in adhesives, coatings, linoleum, and other technical products.

These polymers can be further modified to enhance their properties, particularly through the synthesis of amide resins. Such materials are highly effective as structure-forming and stabilizing agents in dispersed systems and also function as complexing agents in the extraction of rare metals from industrial solutions.

The lack of accessible methods for producing water-soluble resins based on PVA presents a regional challenge, hindering the development and manufacture of a range of essential compounds. Therefore, alternative pathways for synthesizing amide resins via conjugated carbammonolysis reactions have been investigated, aiming to expand the product range and improve the performance of these important polymeric materials.

To study the carbammonolysis reaction, polyvinyl alcohol (PVA) with the following characteristics was used:

- Powder ranging from white to light yellow in color;
- Density ( $\rho$ ), g/cm<sup>3</sup>: 1.2–1.3;
- Refractive index ( $n$ ): 1.4950–1.5420.

Polyvinyl alcohol with these parameters is unstable; therefore, three fractions with distinct molecular weight distributions were obtained by ultracentrifugation of its solutions:

- PVA-I: 20,000–40,000 (30%),
- PVA-II: 40,000–75,000 (45%),
- PVA-III: 75,000–150,000 (25%).

These fractions are free from various inclusions, as they were separated by salting out using a calibrated salt.

**Table 1. Properties of PVA fractions**

Sample Name	Molecular Weight	Degree of Polymerization	Structure, %	Density, g/cm <sup>3</sup>	Refractive Index	Appearance
			<i>Cis-</i>	<i>Trans</i>		
				-		
PVA -I	20,000–40,000	680	87.0	13.0	1.085	1.4850
PVA -II	40,000–75,000	1350	40.5	59.5	1.170	1.5250
PVA -III	75,000–150,000	2700	22.1	79.9	1.215	1.5390

As shown in the table, the characteristic parameters of the PVA fractions are relatively stable, making them suitable for the carbammonolysis reaction. The experiment was conducted in sealed metal capsules with continuous agitation of the reaction mixture under thermostated conditions. The mixture included polyvinyl alcohol (PVA), carbon monoxide, and ammonia in a molar ratio of 1:1.2:1.4. The quantities of the gaseous reactants were calculated based on their partial pressures, and pressure control was performed visually.

A modified aluminum oxide was used as the catalyst. Analysis of the amide yield under various reaction conditions indicates that the reaction behavior depends on both pressure and temperature and exhibits a nonlinear pattern (see Fig. 1). It was found that PVA with lower molecular weight displays higher reactivity, resulting in an increased yield of the amide product.

Additionally, the amide derivatives obtained from this type of PVA contain a higher nitrogen content compared to those derived from higher molecular weight fractions. To determine the effect of reaction time on the carbammonolysis of PVA, the relationship between amide yield and autoclaving duration was examined under otherwise constant conditions (temperature, pressure, and reactant ratio).



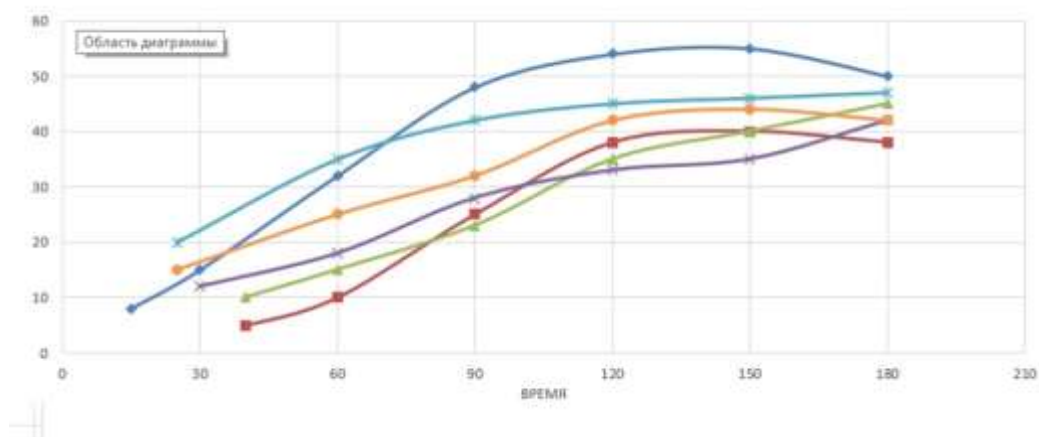


Fig. 1. Dependence of the yield of polyvinylamides on the conditions of carboammonolysis of PVO with different molecular weights.

As shown in Figure 2, the yield of the amide product increases functionally up to a certain maximum, after which it begins to decline. This behavior can be attributed to a side reaction involving the mutual condensation of macromolecular structures, leading to a gradual decrease in the concentration of polyvinylamide in the system. Such polymer-analogous transformations are commonly observed in reactions involving acrylate-based polymers and their derivatives.

The reaction product was purified using a water-acetone decontamination method, which effectively removed impurities. Residual condensation products and by-products were repeatedly washed with xylene until all contaminants were eliminated, resulting in a final product of high purity.

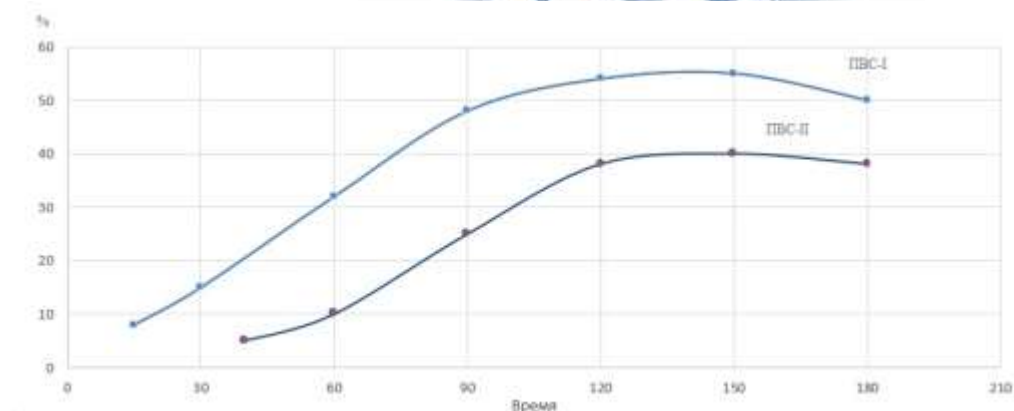


Fig. 2. Dependence of the yield of polyvinylamide on the duration of the carboammonolysis reaction with other parameters remaining constant.

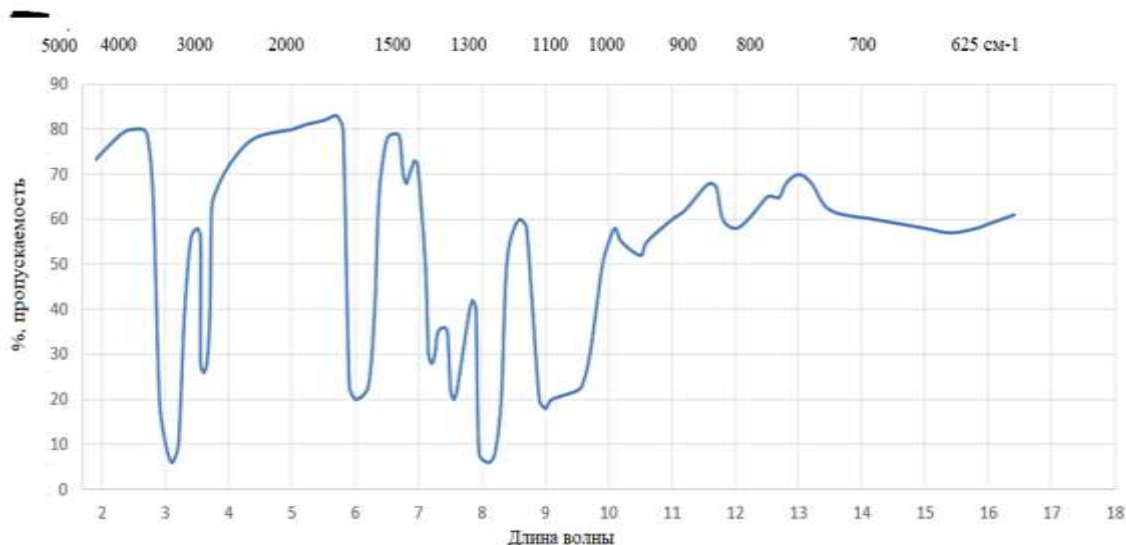


Fig. 3. Infrared spectra of PV

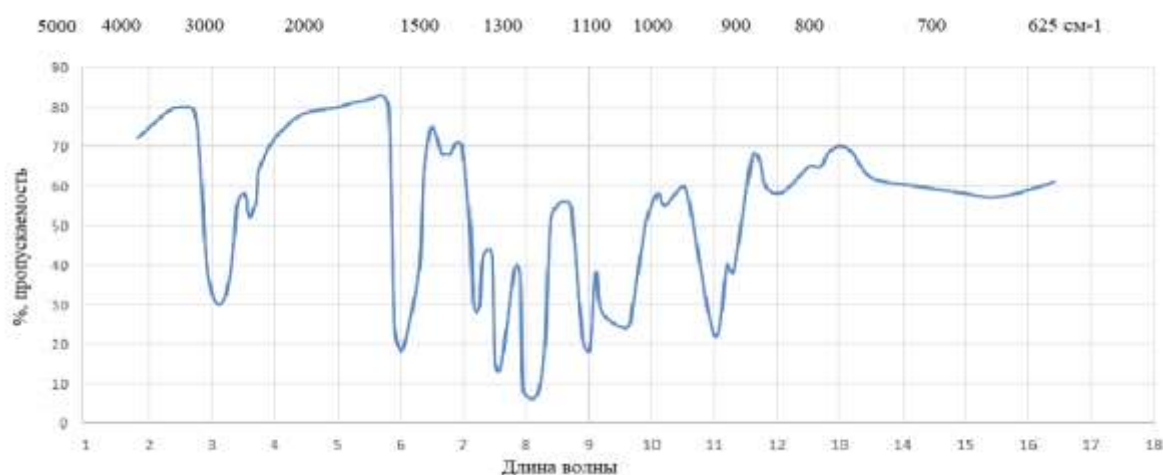


Fig. 4. Infrared spectra of PVA

This section analyzes the results of spectral analysis of polyvinylamide, conducted using a UR-20 spectrometer. The IR spectra presented in Figures 3 and 4 display characteristic features of both polyvinyl alcohol and amide groups.

Figure 3 shows distinct absorption bands corresponding to  $-\text{OH}$ ,  $-\text{CH}_2$ , and  $-\text{CH}-$  functional groups, which are typical for the structure of polyvinyl alcohol (observed at 3.0, 3.4, 8.14, 8.80, 9.16, and 10.9  $\mu\text{m}$ ). A decrease in the intensity of bands associated with

C=C bonds is also noted, indicating the chemical transformation of the original polymer into a polyvinylamide structure.

Figure 4 reveals absorption bands characteristic of amide groups, such as those of  $\text{C=O}$  and  $\text{NH}_2$ , along with a noticeable reduction in the intensity of  $\text{OH}$ -related bands. These spectral changes confirm the successful formation of polyvinylamide from polyvinyl alcohol.

Overall, the obtained spectroscopic data provide compelling evidence for the progression of the carbammonolysis reaction and the formation of the amide product, demonstrating structural modifications at the molecular level.

The obtained corresponding acrylamides were analyzed to determine their characteristic parameters (Table 2).

**Table 2.** Physicochemical characteristics of polyvinylamides

Title	Degree of Polymerization	Hydroxyl Number, mg KOH	Amide Number	Density, g/cm <sup>3</sup>	Appearance
PVA A-I	820	188	64	1.110	White amorphous powder
PVA A-II	1570	170	72	1.195	Same as above
PVA A-III	3500	125	85	1.255	Pale red amorphous powder

Analysis of the data presented in Table 2 indicates that the degree of polymerization of acetylated polyvinyl alcohol (APVA) increases compared to that of unmodified polyvinyl alcohol (PVA). Simultaneously, the hydroxyl number decreases, while the amide number increases with the growing degree of polymerization. These trends suggest the feasibility of synthesizing resins containing both hydroxyl and amide functional groups through the carbammonolysis of polyvinyl alcohol.

The resulting amide derivatives of PVA exhibit characteristics typical of water-soluble polymers. Additionally, the carbammonolysis reaction itself is accompanied by structural transformations of the polymer chain, leading to a further increase in the degree of polymerization. These findings highlight the potential of carbammonolysis as a viable route for producing functionalized, water-soluble polymers with broad application prospects.

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