

ANNOTATION

General job description. The work is aimed at obtaining effective hydrogels for practical use by the method of radical copolymerization based on available industrial and natural monomers. To achieve this goal, N,N-dimethylacrylamide (DMAA) and N,N-dimethyl-N,N-diallylammonium chloride (DMDAH) and N,N-dimethylacrylamide (DMAA) and 2-acrylamido-2-propanesulfonic acid (AMPS) were used. The process of hydrogel synthesis and the kinetics of the copolymerization reaction were systematically studied. To do this, we studied the influence of a number of factors, namely temperature, the composition of a mixture of monomers, electrolytes, and the nature of initiators on the reaction of radical copolymerization. On the basis of these studies, the optimal conditions for obtaining hydrogels were found, and the composition and physicochemical properties of new hydrogels were determined by IR, ¹H NMR spectroscopy, and thermal analysis. In order to determine the possibility of water purification from toxic heavy metals by the obtained hydrogels, the sorption of lead (II) ions in hydrogel lattices was studied.

The relevance of research:

Hydrogels are of great interest due to their properties such as very high elasticity and swelling. Therefore, the demand for hydrogels is increasing every day. There are many types of materials from which hydrogels can be obtained, among which hydrogels based on N,N-dimethylacrylamide (DMAA) occupy a special place. This is due to the fact that DMAA polymerizes easily, is highly reactive, and is relatively inexpensive. DMAA, like other hydrogels, has a three-dimensional structure that can hold water for a long time.

Therefore, the preparation of new hydrogels based on N,N-dimethylacrylamide with a high ability to swell and the study of their properties is an urgent task.

The degree of development of the problem. Many scientists are conducting research on obtaining effective hydrogels based on N,N-dimethylacrylamide and solving problems of their practical use. In particular, much attention was paid to hydrogels used to purify water from paints and heavy metals, self-healing materials, and hydrogels to improve the mechanical properties of materials. But, despite this, it follows from a review of the literature that the search for and creation of new effective ways to improve the chemical stability and adsorption capacity of hydrogels remains important.

Scientific novelty:

- the kinetics of copolymerization reactions of N,N-dimethylacrylamide (DMAA) and N,N-dimethyl-N,N-diallylammonium chloride (DMDAAC) and N,N-dimethylacrylamide and 2-acrylamido-2-propanesulfonic acid (AMPS) was studied for the first time;

- the activation energy of the DMAA-DMDAAC copolymerization reaction was determined for the first time;

- for the first time, the regularities (rate equation) of changes in the rate of the DMAA and DMDAAC copolymerization reaction were determined;

- systematically studied the kinetics of obtaining hydrogels based on -N,N-dimethylacrylamide, the effect of temperature, the composition of the mixture of monomers, time, nature of the initiator, concentration on their conversion, and synthesized new hydrogels;

- on the basis of systematic studies, the optimal conditions for obtaining copolymers were determined, the composition, physicochemical properties of the obtained new hydrogels were determined by the methods of IR, ¹H-NMR spectroscopy, thermal analysis, and the mechanism of radical copolymerization was established;

- in order to determine the possibility of water purification from toxic heavy metals with the obtained hydrogels, the sorption of lead (II) ions into hydrogel networks was studied and a positive result was obtained.

The purpose of the study: obtaining and studying the properties of new hydrogels based on available industrial and natural monomers with a high swelling capacity and effective for practical use.

Research objectives:

- determination of the conditions for the synthesis of new effective hydrogels by the method of radical copolymerization based on available industrial and natural monomers;

- kinetics of the copolymerization reaction for obtaining hydrogels based on N,N-dimethylacrylamide, systematic study of the effect of temperature, composition of a mixture of monomers, time, nature of the initiator, concentration on their conversion;

- determination of the composition, physico-chemical properties of the obtained new hydrogels;

- testing the adsorption of heavy metals by synthetic water-absorbing composite materials in laboratory conditions;

Object of study: Industrial and natural monomers available for research and hydrogels synthesized on their basis,

Practical significance. Effective hydrogels and copolymers necessary for the treatment of agricultural or industrial wastewater have been synthesized.

Theoretical significance. Regularities of radical copolymerization of acrylamide derivatives, dependence of the properties of hydrogels synthesized on their basis on their composition, concentration, composition and structure of the binder have been established.

Provisions to be defended

- Copolymerization reactions of N,N-dimethylacrylamide and N,N-dimethyl-N,N-

diallylammonium chloride and N,N-dimethylacrylamide and 2-acrylamido-2-propane sulfonic acid have been determined.

- The influence of temperature, the composition of monomers, electrolytes, the nature of initiators, cross-linking agents on the reaction of radical copolymerization have been investigated;

- In the system N,N-dimethylacrylamide and N,N-dimethyl-N,N-diallylammonium chloride, the total polymerization rate R_p decreases with an increase in the amount of DMDAAC in the copolymer. Based on the straightline equation, it is shown that the value of the molar ratio of monomers is -0.86.

- The order of the reaction respect to the initiator $R_p = [I]^{0.40}$. Reaction order respect to monomer concentration $R_p = [M]^{2.63}$;

- The kinetics of the DMDAAC-DMAA copolymerization reaction have been determined for the first time. The equation of kinetics of the DMDAAC-DMAA copolymerization reaction have been determined as $R_p = K[M]^{2.63}[I]^{0.40}$.

- Study of the kinetics of the copolymerization reaction. With an increase in temperature, the accumulation of radicals in the initiation stage increases, which led to an increase in the rate of polymerization. A graphical Arrhenius plot was obtained by plotting the logarithm of the rate constant K versus 1/T temperature. According to this Arrhenius graph, the activation energy of the polymerization rate reaction of N,N-dimethylacrylamide and N,N-dimethyl-N,N-diallylammonium chloride was 39.56 kJ/mol, the exponential factor A was equal to $1 \times 10^{12} \text{ sec}^{-1}$. It was close to the activation (37.38 kJ/mol) of copolymerization of DMDAAC and acrylamide, which has a composition similar to that of DMDAAC-DMAA copolymer studied in other works.

- The thermal degradation curve of copolymers of N,N-dimethylacrylamide and N,N-dimethyl-N,N-diallylammonium chloride was determined. The mechanism of the thermal degradation was scientifically proven and explained.

- The composition of new hydrogels, their physicochemical properties have been studied by IR, ^1H NMR spectroscopy and thermal analysis;

- The effect of monomer concentration on the conversion of H-AMPS and DMAA crosslinked copolymer was studied. Conversion increases with increasing monomer concentration. The higher the monomer concentration, the more active sites of free radicals are formed. The high reactivity of the DMAA monomer in the radical copolymerization reaction due to its resonance with the carboxyl group makes the monomers even more active at high monomer concentrations. At 10 M monomer concentration, there is a significant increase in polymer conversion ($p < 0.5$), while at 7.5 M and 5 M, polymerization conversion steadily increased ($p < 0.5$). It is clear from this figure that an increase in monomer concentration causes an increase in the rate of polymerization.

- The effect of initiators on the conversion of the copolymer was studied. It was

observed that the rate of polymerization increases when the concentration of the initiator is increased from 0.05% to 0.07%, and when it exceeds 0.1%, the conversion decreases. This phenomenon is fully explained in the research article.

- The influence of the concentration of the cross-linking agent on the degree of hydrogel swelling and the effect of pH on the degree of cross-linking swelling at different concentrations were systematically studied. As a result, it was found that the value of the degree of swelling is the highest when the concentration of the sewing agent is 0.74%. And when the pH value is 8, the hydrogel showed the highest degree of swelling.

- By studying the optimal temperature for hydrogel synthesis, it was determined that the optimal temperature for hydrogel synthesis is 60°C;

- The results of considering the possibility of using the obtained hydrogels in practice. Adsorption of Pb(II) ions at different times by the best swelling DMAA–AMPS hydrogel with high conversion was investigated. According to the research results, hydrogel showed the highest adsorption value in 4 hours.

- The kinetics of adsorption of Pb(II) ions was determined using pseudo-first-order and pseudo-second-order isothermal models. According to the research results, it was found that the adsorption of Pb(II) ions corresponds to the pseudo-first-order and pseudo-second-order models. However, a pseudo-first-order model was found to be more appropriate.

The contribution of a doctoral student to research work. The patterns of monomer copolymerization reactions, the kinetics and conversion of copolymerization reactions, the optimal conditions for the synthesis of hydrogels, the physicochemical properties, and the sorption of lead (II) ions into hydrogel networks were established by the researcher himself. The results obtained were discussed with the participation of a supervisor and a foreign consultant.

Publications. Based on the results of the study, 5 articles were published that fully correspond to the topic of the dissertation. Among them, two articles were published in journals submitted by the Committee for Quality Assurance in Education and Science of the Ministry of Education and Science of the Republic of Kazakhstan; three articles were published in journals included in the first (Q1) quartile of the SCOPUS indexing:

• *Polymers for Advanced Technologies*, 2020, 32(7), 2669-2675. (IF: 3.67; CiteScore 3.8; Percentile 76%; Q1). <https://doi.org/10.1002/pat.4999>

• *Polymers* 2021, 13, 3084. (IF: 4.3; CiteScore 5.1; Percentile 78%; Q1) <https://doi.org/10.3390/polym13183084>

• *Gels* 2021, 7, 234. <https://doi.org/10.3390/gels7040234> (IF:4.7; CiteScore 4.2; Percentile 65%; Q1)

Doctoral student identification number and Hirsch index in the SCOPUS and

Web of science databases.

✓ SCOPUS

ID:

<https://www.scopus.com/authid/detail.uri?authorId=57263784100>

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✓ H- index 3.