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Computer Modelling of Organic and Inorganic Chemistry Processes

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***Abstract*—This article describes the modelling software complexes are described that allow to determine such parameters of technological processes that can not be directly measured, but knowledge of which is necessary for conducting chemical processes in optimal modes for a given quality of the product. The imitation modelling software of the polymerization of vinyl chloride, which allows determining the molecular mass distribution of polymer molecules, describes a program for modelling the electrolyzer parameters in the production of sodium hydroxide, chlorine and hydrogen, based on the temperature dependence of the current-voltage characteristic. The imitating modelling software of the polymerization process of vinyl chloride allows to determine the physical-chemical properties of polyvinyl chloride in the polymerization process, will help to ensure optimal modes of technological processes, to predict the change in parameters in the event of abnormal situations, which will increase the level of trouble-free functioning.In the training and monitoring modes of operation with the help of imitation software, it is possible to quickly assess the level of training of personnel, and also, if necessary, to conduct their training on the basis of the modules of virtual reproduction of the technological process included in it.Using the developed simulation-modelling software of the process of electrolysis of sodium hydroxide, chlorine and hydrogen production, it is possible to model the temperature dependence of the current-voltage characteristic, which helps to ensure optimal modes of technological processes, to predict the change in parameters in the event of abnormal situations, which will increase the level of trouble-free operation.**

Keywords— polymer, vinyl chloride, polymerization, initiator, medium molecular weight, sodium hydroxide, chlorine, hydrogen, temperature dependence

I. INTRODUCTION

An example of a technological process of organic chemistry is the production of polyvinyl chloride. The main raw material for the production of PVC is vinyl chloride (VC).At present, polyvinyl chloride is produced by three main methods for the polymerization of vinyl chloride: mass, emulsion, and suspension. The method of obtaining PVC affects its properties (molecular weight, particle size), the relative cost and the possibility of producing copolymers. The most widely used in the industry received suspension method, which accounts for more than 80% of the total production of PVC (polyvinyl chloride). This is primarily due to high productivity, relative ease of controlling thermal conditions and the possibility of modifying the properties of PVC. At the same time, this process is very close in mass to the process of polymerisation of vinyl chloride by the mechanism of formation of polymer particles, as well as by the kinetics. Therefore, the method of polymerization of vinyl chloride in suspension can be considered as a convenient for the practical implementation of the type of polymerization in bulk.

The PVC produced by the suspension method is a white powder with particle sizes from 50 to 350 microns (on average, 100-150 microns). PVC powder particles, often called grains, have a porous structure. Depending on the magnitude of the porosity, the bulk density of the grain is 1.1-1.3 g / cm^3 with a density of the polymer phase of 1.35 - 1.43 g / cm^3 of the determined molecular weight.

The technological process consists of four main stages: polymerization of vinyl chloride, PVC degassing, extraction of PVC from suspension, drying, and PVC classification. Of greatest interest is the first stage because of the significant impact on the quality of the products obtained. The main conditions for obtaining a polymer with the required properties are a correctly prepared polymerization recipe, maintaining the necessary technological regime throughout the polymerization process.

Polyvinyl chloride is a high molecular weight organic compound having the chemical formula (-CH_2-CHCl-) n, where n is the number of monomeric units (n = 150 - 2500).

An example of a technological process of inorganic chemistry is the production of caustic soda, chlorine and hydrogen.

The production of caustic soda (NaOH) was closely associated with the development of soda ash production. This relationship was due to the fact that soda ash served as a raw material for the chemical method of obtaining NaOH, which was caustified with lime milk in the form of soda solution. With the development of electrochemical methods for obtaining NaOH by electrolysis of aqueous NaCl solutions simultaneously with NaOH receive chlorine, which is widely used in the industry of heavy organic synthesis and in other industries.

Currently using three methods of obtaining: the process of obtaining using a diaphragm electrolyzer, in a membrane electrolyzer, mercury electrolyzers. With the help of a mercury electrolyzer, commercial (up to 50%) caustic soda (NaOH) is produced directly at the outlet of the electrolyzer.

This method allows to obtain a very pure and free from chlorine concentrated sodium hydroxide solution.

Pure sodium hydroxide NaOH is a white opaque mass that absorbs water vapor and carbon dioxide from the air.

The development of computer simulation programs that mimic the processes of chemical technology is an urgent problem, the solution of which allows improving the quality of technological processes from the point of view of improving safety and reliability, ensuring energy and resource saving. The basis of mathematical models implemented in modelling software are the basic equations of thermodynamics and mass transfer, supplemented by characteristic empirical dependencies obtained experimentally on technological equipment. In the presented work, modelling software are described that allow to determine such parameters of technological processes that are not capable to direct measurement, but the knowledge of which is necessary for carrying out chemical processes in optimal conditions for a given quality of the products obtained. The article describes a simulation-modelling software of the polymerization process of vinyl chloride, which allows to determine the molecular weight distribution of polymer molecules [1, 2], describes the software for modelling the parameters of the electrolyzer in the production of caustic soda, chlorine and hydrogen, which is based on the temperature dependence of the current-voltage characteristic [3, 4].

II. Results and its discussion

The improvement and modernization of chemical-technological processes requires the appropriate development of computer-modeling systems that provide: determination of physicochemical parameters that cannot be directly measured during chemical transformations; definition and maintenance of optimal modes of technological processes, contributing to trouble-free operation.

The development of information technologies makes it possible to create computer-training complexes that allow one to acquire professional skills of managing technological processes, complementing the training of real-world objects that are not always available and do not exclude the creation of emergency situations.

The relevance of the research process of organic chemistry on the example of the production of polyvinyl chloride is primarily due to the volume of production of this product. Over 3000 types of products are obtained from this material, which are used for a wide variety of purposes and every year they conquer new applications. Therefore, the improvement of the technological process of obtaining PVC and the development of effective methods for managing the modes of carrying out chemical processes that ensure the production of a product with desired properties at the lowest possible energy cost is an urgent problem.

The relevance of the research process of inorganic chemistry on the example of the production of caustic soda, chlorine and hydrogen by the electrolytic method is due to the fact that caustic soda (caustic soda) is the most common alkali, the production and consumption of which per year is up to 57 million tons. In the chemical and petrochemical industry (they account for about 57% of the total Russian consumption of NaOH is used to neutralize acids and acid oxides, as a reagent or catalyst in chemical reactions, chemical analysis for titration, for etching aluminum and in the production of pure metals, in oil refining - for the production of oils.

One of the most common chemical production of organic synthesis is the process of polymerization of vinyl chloride (VC) by the suspension method [5, 6], therefore, computer simulation of this process is necessary to determine the physical-chemical parameters that are not directly measurable, determine and maintain optimal process conditions that promote failure-free operation. The simulation-modelling software of polymerization of vinyl chloride by suspension method is equipped with an interactive scheme (Fig. 1), two-and three-dimensional visualization mode of technological installations and equipment (Fig. 2), which allows the user to visually get acquainted with the design of devices and their characteristics.

From the analysis of experimental data [6], it follows that the process of heat release increases at the initial stage of polymerization, reaches a maximum value, and then decreases. The given heat flux curves (W / m2) are approximated by the following time dependencies (t, h).

At a concentration of trigonox, 0.062% of the mass.from VC:

$$Q = 0.0001t^6 + 0.003t^5 - 0.042t^4 + 0.270t^3 - 0.954t^2 + \\ + 1.876t - 0.336.$$

At a concentration of trigonox, 0.077% of the mass. from VC:

$$Q = 0.0001t^6 - 0.018t^5 + 0.186t^4 - 0.926t^3 + 2.360t^2 - \\ - 2.680t + 2.327$$

At a concentration of trigonox, 0.1% of the mass. from VC:

$$Q = 0.004t^6 - 0.100t^5 + 0.943t^4 - 4.483t^3 + 11.34t^2 - \\ - 14.30t + 8.501$$

These dependences are used in a simulator complex to control the flow rate of the refrigerant into the cooling jacket of the reactor to ensure isothermal process.

The change in heat flow in the polymerization process leads to a change in the temperature of the polymer-monomeric particles of vinyl chloride, which differs significantly from the temperature of the reaction medium T_c. From the solution of the stationary heat equation, for spherical polymer-monomer particles of radius R and heat transfer coefficient, it follows that the temperature is determined by the relation

$$T(r) = T_c + \frac{QR}{2\lambda}\left(1 - \frac{r^2}{R^2}\right), 0 \le r \le R,$$

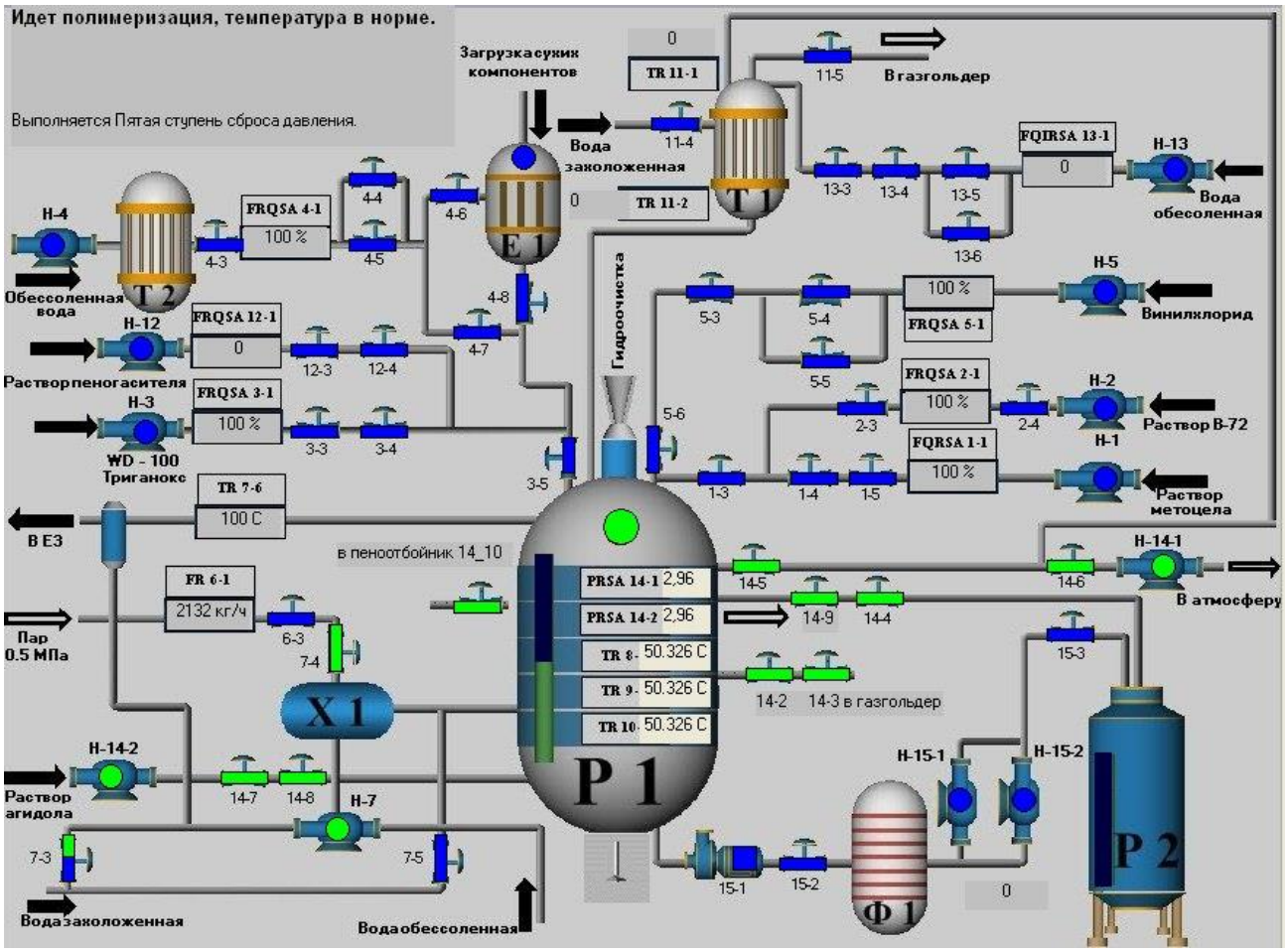

Fig. 1. Interactive scheme of a simulation-modelling software

Fig. 2. 3D model of a polymerization reactor

which shows that the temperature reaches the maximum value in the center at $r \to 0$.

The dependence of the temperature drop of the droplet on the average temperature in the reactor is determined by the equation:

$$\Delta T = \frac{QR}{2\lambda}$$

for polymer-monomer particles R = 100 μm and λ=1.25W/(m•K) is shown in Fig.3. It follows from the above graphs that the deviation of the temperature inside the drop from the temperature of the reaction mixture can reach ~ 10 °C, which affects the distribution molecular weight of polymer molecules.

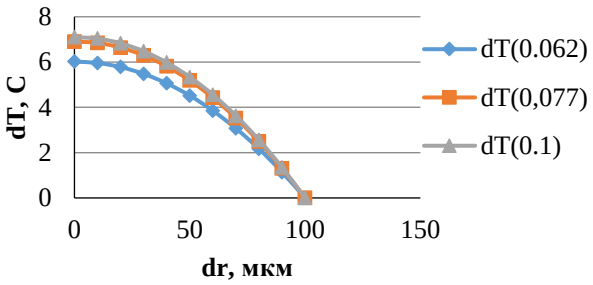

Fig. 3. Dependence of temperature deviation in a polymer drop on the radius at various initiator concentrations

Modeling software allows you to explore the process of polymerization at different temperatures and hydrodynamic modes of mixing determine the size of the polymer-monomer particles in the polymerization process, and the molecular weight of the molecules. From the experimental data [5], it follows that the molecular weight of polymer molecules is determined by the temperature of the polymerization process (Fig. 4) and varies widely from $250 \cdot 10^3$ at a polymerization temperature of 50 C to $70 \cdot 10^3$ at a temperature of ~ 73°C. Such a temperature dependence of the molecular weight will affect the molecular weight distribution of the molecules inside the polymer-monomeric vinyl chloride particle in the polymerization process, given that the central part of the polymer-monomeric vinyl chloride particle has a higher temperature and, therefore, a lower molecular weight than the peripheral regions.

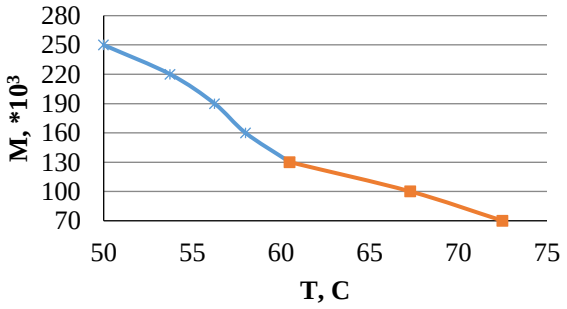

Fig. 4. The dependence of the average molecular weight of the polymer on temperature

Simulation-modelling software allows you to determine the mass fraction of molecules with different molecular weight in the polymer particle.

In fig. 5shows the dependence of the volume fraction of molecules with different molecular masses in a polymer particle with a radius of ~ 100 μm at different concentrations of the initiator of the polymerization process. It can be seen from the figure that when the temperature of the medium in the reactor is 50 °C in polymer particles, the molecular weight of molecules will vary widely from $170 \cdot 10^3$ to $250 \cdot 10^3$, while the proportion of molecules with relatively low molecular weight does not exceed 10%. The main proportion of molecules ~ 70% will be in the molecular weight of the molecules corresponding to the temperature of the medium in the reactor-polymerizer.

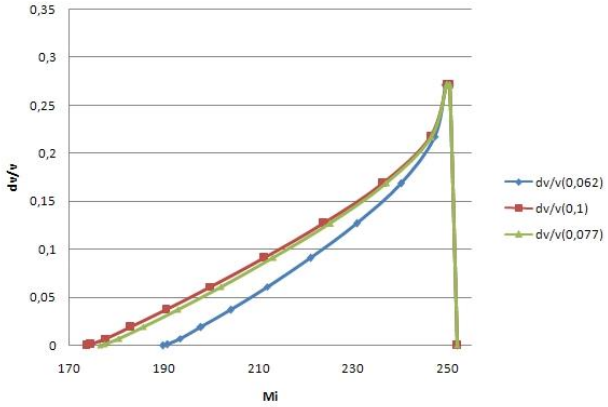

Fig. 5. The dependence of the volume fraction of molecules with different molecular weight at different concentrations of the initiator

The modeling software includes technical calculators for calculating reactor productivity and component loading, which make it possible to determine time-varying technological parameters during the simulation of various process modes.

From the above analysis, it follows that due to the thermal effect of the polymerization reaction, the temperature of the polymer-monomeric particles of vinyl chloride is different from the temperature of the medium in the polymerization reactor. It was determined that the temperature inside the particles increases according to a parabolic law, reaching a maximum value in the center. The temperature deviation from the average in the reactor is proportional to the size of the polymer-monomer particles and can reach ~ 10 ° C.

The heterogeneity of the temperature field inside the polymer monomer particles in the reactor-polymerizer leads to the expansion of the spectrum of the distribution of molecular masses of the polymer in the region of smaller values. The share of molecules with a relatively low molecular weight does not exceed 10%. The main proportion of polymer molecules ~ 70% will be in molecules with a molecular mass corresponding to the temperature of the medium in the reactor.

Modeling software “Polymerization of vinyl chloride by suspension method” allows not only to simulate the polymerization process of vinyl chloride, but also using the module “Functional automatization scheme” (FSA) included in the program, to familiarize and study the system of automatic control and monitoring of the process as a whole, and its individual control circuits. The FSA contains the necessary database of instrument characteristics with a detailed description of their purpose and technical parameters.

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The use of the developed simulation and simulation complex will make it possible to determine the physicochemical properties of polyvinyl chloride, which are not available for direct measurement during the process (size of polymer particles, temperature distribution, and molecular mass spectrum), will help ensure optimal chemical transformations, predict changes in parameters when deviating from normal operation mode.

One of the common processes of inorganic synthesis is the process of obtaining sodium hydroxide, chlorine and hydrogen by electrolytic method in electrolyzers with a mercury cathode [7-8]. Therefore, the development of modelling programs for this process seems relevant.

The first stage of the process of obtaining caustic soda with the formation of chlorine gas and sodium amalgam is carried out in the electrolyzer, then the amalgam is fed into the decomposer, where caustic soda and hydrogen are obtained, and mercury is circulated by the pump.

In the electrolysis cell, the cathode is circulating mercury, and the anode, as a rule, is made of ruthenium and titanium oxides deposited on a titanium base.

The main target process at the anode is the discharge of chlorine ions

$$2Cl^- - 2e = Cl_2$$

At the same time, side processes can occur at the anode and in the volume of electrolyte as a result of electrochemical and chemical reactions with the loss of the target electrolysis products and current:

The depolarization of sodium ions at the cathode is associated with the ability of sodium to easily form amalgam in various stoichiometric ratios, which dissolves well in excess of pure mercury and diffuses from its surface into the deep layers. The faster in the process of electrolysis is the depletion of the surface of the mercury cathode by sodium as a result of diffusion, the higher the effect of depolarization. Since the discharge rate of sodium ions is usually ahead of the rate of its diffusion in the mercury layer, the concentration of amalgam over time can increase to a value at which the concomitant increase in cathode potential will make it possible to discharge hydrogen ions. Therefore, during the industrial implementation of the process, the concentration of amalgam (0.2 ~ 0.3%) is limited and it is continuously removed from the electrolysis zone. It is equally important that the surface of mercury be smooth and homogeneous.

The main process on the cathode of a mercury electrolyzer, meeting the goals of industrial electrolysis, is the discharge of sodium ions.

$$Na^+ + e(nHg) = Na(Hg)_n$$

At the cathode, the occurrence and adverse reactions are possible. So with a small interelectrode distance, to which, in order to save electricity, they strive in practical conditions, the anode electrolyte layers saturated with chlorine can reach the cathode, where chlorine will be restored.

This entails a loss of current, therefore in industrial electrolysis it is necessary to create conditions that suppress the possibility of cathode reduction of chlorine. These conditions affecting the solubility of chlorine in the electrolyte are determined by the concentration of the electrolyte and the temperature. The higher the electrolyte concentration by NaCl and the process temperature, the lower the solubility of chlorine.

On the other hand, increasing the temperature contributes to the process of decomposition of the amalgam by water contained in the electrolyte, which reduces the current output at the cathode, as well as at the anode. This is due to the fact that the alkali formed during the decomposition of amalgam will interact with the acid electrolyte to form chlorate and perchlorate. Direct interaction of chlorine dissolved in electrolyte with sodium amalgam with loss of chlorine and alkali current outputs is also possible.

$$Cl_2 + 2NaHg_n = 2NaCl + 2nHg$$

As follows from the stoichiometry of chemical reactions and the law of conservation of electric charge, a charge of 1000 Ah (3.6×10^6 C) passes through the electrolyzer and releases 1,323 kg of chlorine (Cl), 0.0376 kg of hydrogen (H_2) and 1,492 kg of sodium hydroxide (NaCl).

Thus, the charge rates for the charge are:

for chlorine, $K_{Cl} = 3.675 \cdot 10^{-7}$ kg / C;

for hydrogen, $K_H = 1.044\ 10^{-8}$ kg / C;

for caustic soda $K_{NaOH} = 4{,}144\ 10^{-7}$ kg / C.

To create a computer-simulation complex that simulates the functioning of an electrolyzer, a mathematical model is needed that relates technological (current, voltage, temperature, etc.) parameters to the electrolyzer design.

To determine the influence of the design parameters of the electrolyzer on the performance and determine the cost of electricity, it is necessary to establish the dependence of the electric current on the technological parameters. The electric current between the anode and the cathode of the electrolyzer is determined by the ratio

$$I = en_{Na}\upsilon_{Na}S + en_{Cl}\upsilon_{Cl}S \qquad (1)$$

where n_{Na}, n_{Cl} is the concentration of sodium ions and chlorine in the electrolyte; υ_{Na}, υ_{Cl} - the speed of the directed movement of ions; S is the anode area of the electrolyzer.

In the electric field between the anode and the cathode, Na^+ ions move toward the mercury cathode, and Cl^- ions toward the anode. To determine the velocities υ_{Na}, υ_{Cl}, the equations of motion are used taking into account the forces of the electric field and viscous resistance:

$$m_{Na}\frac{d\upsilon_{Na}}{dt} = eE - F_{Na} \quad (2)$$

$$m_{Cl}\frac{d\upsilon_{Cl}}{dt} = eE - F_{Cl} \quad (3)$$

where m_{Na} is the mass of the solvated Na ion;

m_{Cl} is the mass of the solvated Cl ion;

Electric field strength in the gap between the anode and cathode

$$E = \frac{U}{d}$$

U - potential difference (voltage);

d is the distance between the anode and the cathode.

Viscous resistance forces during the motion of solvated ions Na^+, Cl^-

$$F_{Na} = 6\pi\mu\ r_{Na}\upsilon_+$$

$$F_{Cl} = 6\pi\mu\ r_{Cl}\upsilon_-$$

μ is the coefficient of dynamic viscosity of the electrolyte;

r_{Na}, r_{Cl} — characteristic radii of solvated ions;

m_{Na}, m_{Cl} are the masses of solvated ions.

The radii of the solvated elements can be estimated by the formula

$$r_{Na} \approx r_{Cl} = R_C = \left(\frac{ep_e}{6\pi\varepsilon_0 kT}\right)^{\frac{1}{2}}\left[1+\frac{3\pi\varepsilon_0 kTp_e}{2e^3}\right]^{\frac{1}{2}} + \frac{p_e}{2e}$$

in which $e = 1.6 \cdot 10^{-19}$ C is the elementary charge;

p_e is the dipole moment of water molecules (H_2O);

$\varepsilon_0 = 8.86 \cdot 10^{-12}$ F / m is the electric constant;

$k = 1.38 \cdot 10^{-23}$ J / K - Boltzmann constant;

T is the absolute constant temperature of the electrolyte.

From the solution of equations (2) and (3), it is possible to determine the velocities of the directional motion of sodium and chlorine ions in the interelectrode space.

$$\upsilon_{Na} = \frac{eU}{6\pi\mu\ r_{Na}d};\upsilon_{Cl} = \frac{eU}{6\pi\mu\ r_{Cl}d} \quad (4)$$

The current between the anode and cathode is determined by the ratio

$$I = \frac{e^2S}{6\pi\mu\ d}\left(\frac{n_{Na}}{r_{Na}} + \frac{n_{Cl}}{r_{Cl}}\right)U \quad (5)$$

Given that the concentration of sodium ions and chlorine in the electrolyte solution is almost the same and is determined by the concentration of NaCl in brine, the latter ratio can be represented as

$$I = \frac{n_i e^2 S}{\mu d}\cdot\left(\frac{\varepsilon_0 kT}{6\pi\ ep_e}\right)^{\frac{1}{2}}U \quad (6)$$

rom the last equation it follows that the dependence of the current in the electrolyzer is determined by both the design parameters, in particular, the anode and cathode area S, the distance between the electrodes d, and technological parameters: n - brine concentration n_i and its temperature T, μ - dynamic viscosity. Formula (6) also makes it possible to determine the temperature dependence of the volt-ampere characteristic of the electrolyzer with regard to the change in the viscosity of the electrolyte with a change in temperature (Fig.6). Knowing the dependence of the current on the design and technological parameters, it is possible to determine the performance of the electrolyzer and the specific energy consumption G (J / kg) (Fig.s 7, 8).

$$G_{Cl} = \frac{U}{k_{Cl}};G_H = \frac{U}{k_H};G_{NaOH} = \frac{U}{k_{NaOH}} \quad (7)$$

where U is the voltage between the electrodes of the electrolyzer.

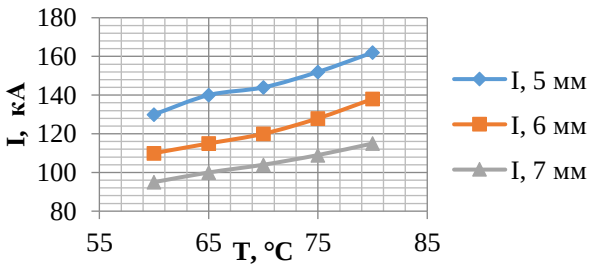

Fig. 6. Dependence of current strength on the electrolyzer as a function of temperature at fixed values of the interelectrode distances and voltage of 3.65 V

From formula (6) it follows that for a given current value in the electrolyzer, the voltage on the electrodes is determined by the formula

$$U = \frac{\mu d}{n_t e^2 S}\cdot\left(\frac{6\pi\ ep_e}{\varepsilon_0 kT}\right)^{\frac{1}{2}}I \quad (8)$$

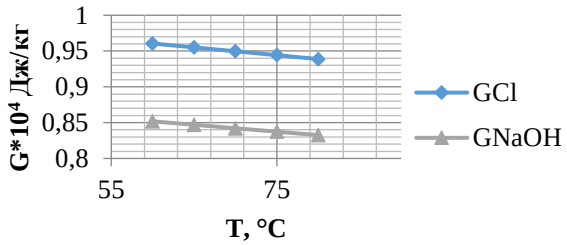

Fig. 7. The specific cost of energy G for chlorine and caustic soda

From the formula (8) it is seen that with an increase in the electrolyte temperature, the voltage decreases.

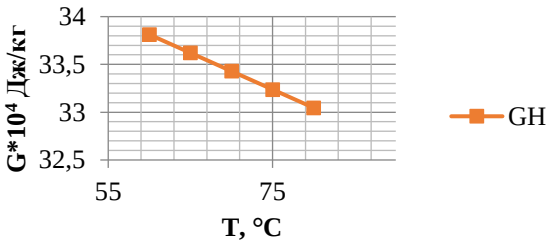

Fig. 8. Specific energy consumption G for hydrogen

Fig.9shows the temperature dependence of the voltage at fixed values of the current at an interelectrode distance of 5 mm.

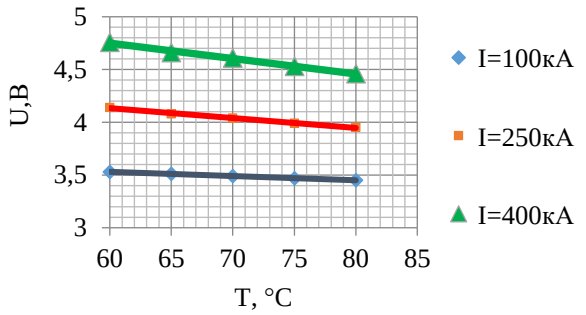

Fig. 9. The dependence of the voltage on the cell from the temperature at fixed values of the current strength and the interelectrode distance of 5 mm

The dependences are implemented in the simulation stage “Electrolysis stage of the production of caustic soda, chlorine and hydrogen”.

In the course of research, it was found that with an increase in the electrolyte temperature, the dynamic viscosity decreases, and the diameters of the solvated ions decrease, which leads to an increase in conductivity and an increase in current in the electrolyzer at a given voltage between the anode and cathode.

III. Conclusion

Computer simulation of technological processes is an integral part of the technological regulations, allowing the processes under optimal conditions, ensuring product quality and trouble-free operation. The main advantage of mathematical modelling is that it is possible to determine with the necessary accuracy such process parameters that are not amenable to direct measurement, but the knowledge of which is necessary to ensure the quality of the resulting product, saving energy and material costs.

When modelling polymerization processes, it is important to take into account the temperature distribution inside the polymer-monomer particles that affect the molecular weight distribution of the polymer molecules.

When describing electrolysis processes, it is necessary to take into account the temperature dependence of the current-voltage characteristic, which determines the energy costs of the process. All the factors listed above lead to the conclusion about the prospects and the need to develop computer simulation programs that adequately describe real chemical-technological processes.

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