SCIENTIFIC FUNDAMENTALS OF RESOURCE-SAVING TECHNOLOGIES OF JELLY PRODUCTION

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INTRODUCTION

Modern conditions of the market economy present food manufacturers with the task of introducing new competitive resource-saving technologies with simultaneous improvement of consumer properties, increase in nutritional and biological value, extension of shelf life and expansion of product range.

Among the wide variety of food products, jelly products are especially popular with consumers. These are various candies, jellies, mousses, marmalade, marshmallows, cookies, and cakes, decorated with jelly semi-finished products, etc. These products have an attractive appearance, high taste, and are well absorbed by the human body. The texture of jelly products is provided by the introduction of various gelling agents into the recipe. They can be of plant origin products of seaweed processing (agar, carrageenans, alginates), from fruits and vegetables (pectins, starches), from plant seeds (various natural gums); animal (gelatin) and microbial (xanthan, xampan) origin. However, the production of these products is mostly carried out with the use of imported, and accordingly expensive, structure-forming agents.

The relevance of research lies in solving an important problem of the food industry – the rational use of food raw materials, including gelling agents of different origins, to create food products of increased nutritional value.

Recently, research in this direction has been carried out by such scientists as Antonella Dorokhovych[1], Pavlo Pyvovarov[2], Fedir Pertseviy[3], Viktoria Yevlash[4], etc.

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[1] Дорохович А. М. та ін. Використання гідроколоїдів у кондитерському виробництві. *Хлібопекарська і кондитерська промисловість України*. 2005. № 2. С. 9–11.

[2] Pyvovarov P. et al. Modelling of low-calorie pectin-based product composition. *Ukrainian Food Journal*. 2015. V. 4, № 1. P. 22–36.

[3] Pertsevoy F. et al. Modifying additives in jelly products. Publishing house of National University of Food Technologies, Kyiv, 2005, 260 pp.

[4] Yevlash V. et al. Development of scientifically grounded technologies of food products of increased nutritional value using structure formers of different origin. *Scientific Works of NUFT 2017*. Volume 23, Is. 5, Part 1. P. 115–123.

The analysis of literary data shows that the attention of scientists is focused on the development of technologies for jelly products with additives that correct nutritional value indicators. This involves not so much a reduction in the costs of structural formers, but a reduction in the sugar content, the creation of dietary products and the enrichment of products with proteins, vitamins, minerals, and ballast substances. To date, there are no complete theories and concepts in the literature that would make it possible to unambiguously predict the technological and consumer properties of jelly confectionery based on the knowledge of the molecular structure and the nature of the structuring agents used for their production. There are also no methods of quantitative determination of functional and physiological ingredients, adapted for confectionery products using structure-forming agents of various origins.

In connection with the above, the scientific substantiation, development and introduction of new resource-saving technologies of jelly products, which are based on the study of the functional and technological properties of raw materials, namely, structure-forming agents of various origins, and allow obtaining products with pre-forecasted characteristics are an urgent scientific and technical problem.

1. Molecular modeling of the processes of structure formation in aqueous solutions of collagen and agarose

The process of gel or structural formation is based on the formation of a spatial network between biopolymer molecules connected in individual "joints" by the forces of intermolecular interaction or chemical bonds of various nature.

According to the generally accepted concept[5], the mechanism of formation of agar hydrogels can be represented by two stages: 1) formation of double helices from individual chains of agarose; 2) association of double chains with the formation of coaxial associates (aggregates) with subsequent formation of three-dimensional structures (Fig. 1.1).

In aqueous solutions, gelatin (collagen), depending on the temperature and concentration, can exist in the form of: a) linear α-chains formed by repeating triads of amino acids, b) triple helices (tropocollagen molecules), c) coaxial associates of tropocollagen molecules having the ability to form three-dimensional structures (Fig. 1.2)[6].
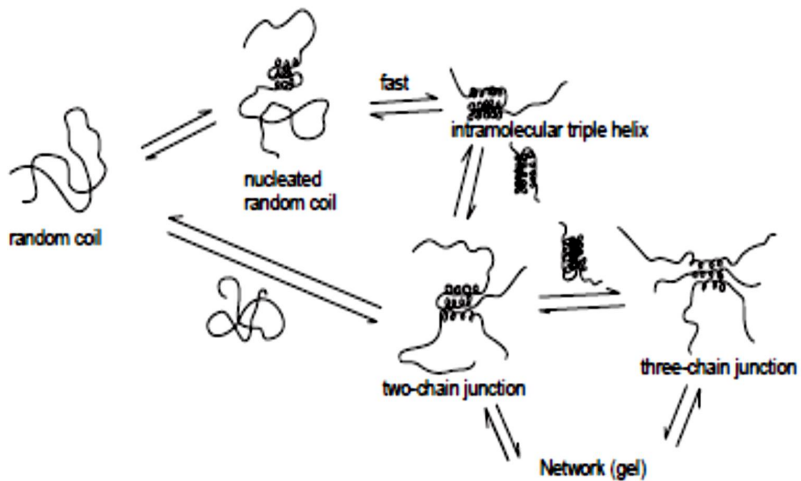
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[5] Rees D. A., Welsh E. J. (1977), Secondary and tertiary structure of polysaccharides in solution and gels, *Angew. Chem. Int. Ed. Engl.*, 15, pp. 214–224.

[6] Fiber, E. G., Franks, F., Phillips, M. C. & Suggest, A., Gel formation from solutions of single chain gelatin. Biopolymers, 14 (10), (1975) 1995–2005.
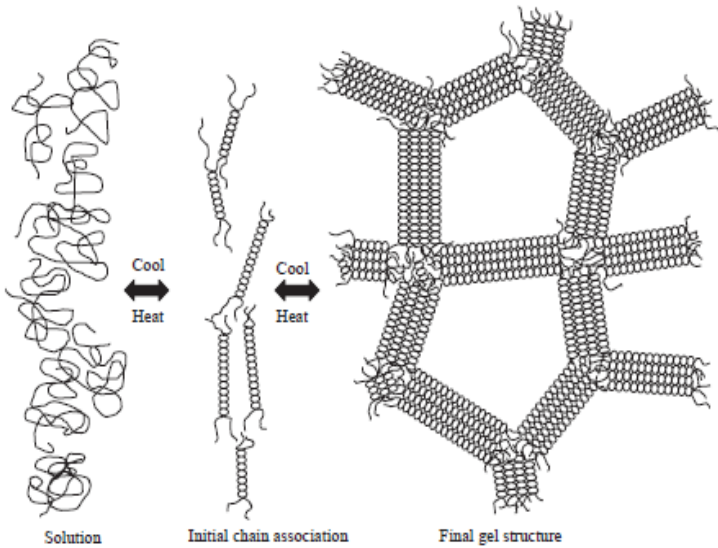
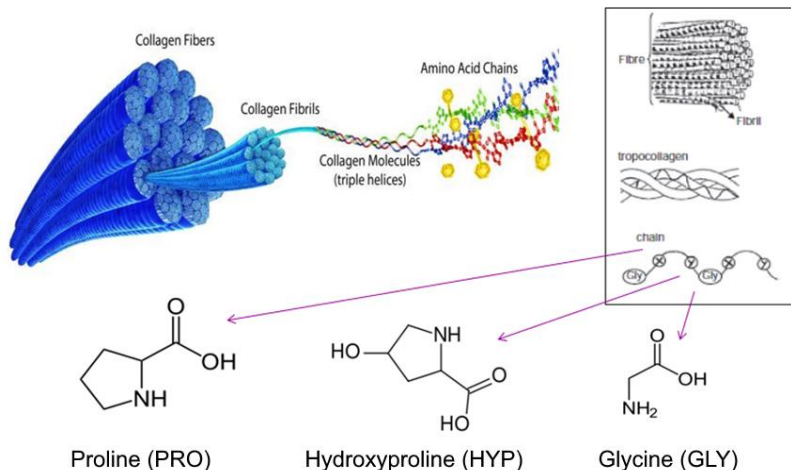**Fig. 1.1. Mechanism of agar structure formation**

Fig. 1.2. Mechanism of gelatin structure formation

A wide variety of gelatin types, depending on the raw material and production technology, is a widely known fact for experts in the field of

food technology[7]. In order to understand the influence of the composition of gelatin on the features of gelation, it is necessary to study this problem at the atomic-molecular level.

It is known that the structure of gelatin (collagen) is formed by repeating triplets of amino acids, which necessarily include glycine (GLY) and, most often, proline (PRO) and hydroxyproline (HYP)[8] (Fig. 1.3).

Fig. 1.3. The structure of gelatin (collagen)

Despite the significant success of recent years in studying the structure of gelatin (collagen) in the solid (crystal) state, individual stages of the mechanism of gel formation involving collagen remain unstudied at the atomic-molecular level. In addition, the study of intermolecular association involving spiral structures of collagen and agarose (the main component of sulfated polysaccharides of red seaweed) is of undoubted interest when they are used together as gelling agents.

Thus, the study of the two most popular gelling agents and their solutions at the molecular level, using the methods of quantum chemistry and molecular dynamic (MD) modeling, will provide a detailed quantitative description of the hydrogen bonds formed in the process of gelation, the

[7] Phillips G. O., Williams P. A. (2009), *Handbook of Hydrocolloids*, 2nd edition, Woodhead Publishing, Cambridge.

[8] Bhattacharjee A., Bansal M. (2005), Collagen Structure: The Madras Triple Helix and the Current Scenario, *IUBMB Life*, 57, pp. 161–172.

construction models of the supramolecular structure in the corresponding systems and prediction of their rheological properties.

The purpose of the study was to establish the features of intermolecular association (aggregation) in aqueous solutions of agarose (AG) and collagen (Col), as well as the role of hydrogen bonds at the atomic-molecular level using molecular modeling methods.

The following tasks were solved to achieve the set goal:

1) selection and validation of force field models of AG and Col molecules for MD modeling;

2) development of the MD method for modeling associative equilibria in aqueous solutions of AG and Col;

3) MD modeling and analysis of structural and energetic characteristics of H-bonds between Col molecules, as well as AG and Col molecules in the studied systems;

4) quantum-chemical analysis of detected hydrogen bonds.

The essence of the molecular dynamic (MD) modeling method[9] is the numerical solution of the Newtonian equations of motion according to the given model potentials of interaction, followed by the calculation of the average thermodynamic, structural and dynamic properties of the modeled system based on the set of instantaneous coordinates r(t) and velocities v(t) of all system particles. Since the velocities and coordinates of all particles in the system are known during MD modeling of the fluid, it is possible to calculate various distribution functions, correlation functions, both single-particle and collective, as well as thermodynamic parameters. In the MD modeling method, it is possible to calculate all the quantities considered by classical statistical mechanics, including those not studied by conventional statistical-mechanical methods.

The simulated system is usually represented by a cubic cell with an edge length L, which is calculated from the experimental density and a given number of particles (atoms, molecules, ions). Taking into account the significantly different dependence on the interatomic distance, in MD modeling the model interaction potential of any pair of particles (atoms) of the system is represented by the sum of the components of short-range and electrostatic interactions.

MD modeling is usually divided into three stages:

– initialization of the system (assignment of initial coordinates and velocities to all atoms (molecules) in the basic cell according to certain rules);

– balancing (bringing the system to a state of thermodynamic equilibrium);

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[9] Haile J. M. (1992), *Molecular dynamics simulation. Elementary methods*, New York, Wiley.

– conducting one or more consecutive launches (runs) with the calculation of all structural, dynamic and thermodynamic properties of the modeled system.

The following research algorithm was used in our work[10]:

– creation of linear α-chains of collagen;

– creation of tropocollagen molecules on their basis;

– creation of a model aqueous solution in the form of a MD cell with two tropocollagen molecules;

– MD modeling for the study of the dynamics of the association of tropocollagen molecules;

– further analysis of the topology of hydrogen bonds and their quantum-chemical analysis.
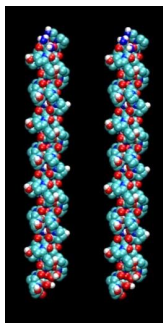
Structural elements for MD modeling of an aqueous solution of tropocollagen are shown in Fig. 1.4.
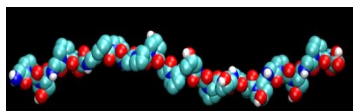
α-chain of the collagen molecule
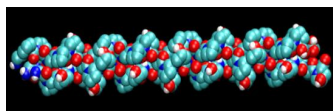
The triple helix of the tropocollagen molecule

The initial location of tropocollagen molecules in the MD cell
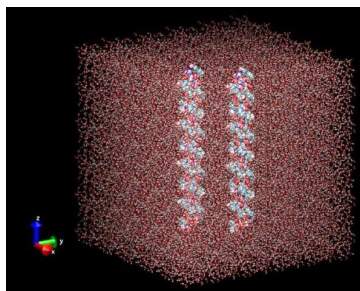
MD cell with 2 tropocollagen molecules and 32,560 water molecules

Fig. 1.4. Structural elements of tropocollagen for MD modeling

[10] Калугін О. М., Вовчинський І. С., Фощан А. Л., Губський С. М., Евлаш В. В. Методи молекулярного моделювання як інструмент для дослідження харчових драглів. Повноцінне харчування: інноваційні аспекти технологій, енергоефективного виробництва, зберігання та маркетингу: колективна монографія. Харків : ХДУХТ, 2015. С. 50–101.

A similar approach was used to study the association between tropocollagen molecules with the double helix of agarose (AG) in an aqueous environment (Fig. 1.5).

A single chain of the AG molecule

The double helix of the AG molecule

The initial arrangement of tropocollagen molecules and the double helix of agarose
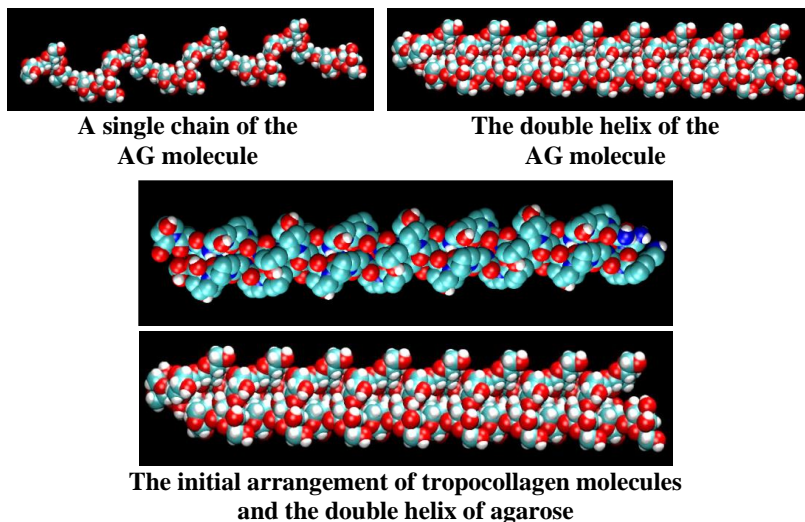
Fig. 1.5. Structural elements of agarose for MD modeling

The MD modeling carried out consisted of the following stages.

1. *Creation of the MD cell*[11]. After creating the model and adding – NH_2 and -COOH groups, two triple helices of tropocollagen were placed parallel to each other at a distance of 2.5 nm in the center of a $10\times10\times10$ nm cubic cell. Then it was evenly filled with 32,560 water molecules. The obtained geometry was used in the next stage. The choice of the collagen structure is due to the presence of the three most important amino acids in the composition, namely GLY, PRO and HYP, as well as acceptable sizes (the total number of simulated particles in the triple helix was 576). The GROMACS utility (namely pdb2gmx)[12] was used to create the force field model.

2. *Energy minimization*. The main goal of the energy minimization stage is to accelerate the thermodynamic equilibrium of the modeled system. Using the algorithm of the fastest descent, a more energetically

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[11] Lyssenko K. A., et all (2006), Water Clusters in Crystal: Beyond the "Hydrogen-Bonding Graphs", *ChemPhysChem*, 7, pp. 2453–2455.

[12] http://www.gromacs.org/

advantageous state of the system is found that meets the proposed conditions. The criterion for stopping minimization in this simulation was the absence of forces greater than 1000 KJ/mol/nm.

3. *Equilibration of the system with fixed heavy atoms of tropocollagen molecules in the microcanonical (NVT) ensemble.* After the minimization of the system energy was carried out, in order to bring the system to a state of thermodynamic equilibrium more quickly, MD simulation was carried out at a constant volume, temperature and number of simulated particles for 100 ps with a step of 2 fs. During the simulation, the heavy atoms of tropocollagen molecules (all but hydrogen atoms) were fixed in space using a special potential. In this way, molecules of the solvent – water – were able to occupy more favorable positions from the energetic point of view around the tropocollagen chains. A modified Berendsen thermostat with a constant value of 0.1 ps was used to maintain a constant temperature of 300 K. The criterion of variation was the system's potential energy, the absence of fluctuations and increasing/decreasing trends indicated that it is possible to proceed to the next stage of balancing.

4. *Equilibration of the system with fixed heavy atoms of tropocollagen molecules in the canonical (NPT) ensemble.* The geometry of the system obtained at the previous stage of equilibration was used as a starting point for equilibration in the canonical ensemble for 100 ps with a step of 2 fs. The main difference between this stage and the previous one is that the size of the simulated cell can be changed to reproduce the experimental pressure. In addition to the modified Berendsen thermostat, a Parrinello-Raman barostat was used, with a constant of 2 ps and a compressibility value for water. A slight change in the density of the system during the simulated stage indicates that the system can move to the final stage of equilibration.

5. *Equilibration of the system without spatial constraints in the NPT ensemble.* Equilibration in the canonical ensemble for 15 ns with a step of 2 fs is the final stage before studying the properties of the system. Over a period of time, the tropocollagen molecules stick together, forming hydrogen bonds between the triple helices. Minor fluctuations of such indicators as: potential energy of the system, density, and most importantly – a constant number of hydrogen bonds between the triple helices of tropocollagen indicated that the system has reached thermodynamic equilibrium and is suitable for calculating the studied properties.

6. *Modeling of the system for calculating the investigated properties.* Three consecutive (the final geometry of one simulation was the starting geometry for the next) simulations lasting 5 ns each were carried out in order to evaluate the energetic and structural characteristics of hydrogen

bonds in triple helices of tropocollagen. The simulation settings were similar to the final equilibration stage. Modeling of an aqueous solution containing one molecule of tropocollagen and a double helix of agarose was carried out according to a similar scheme. As a source of the structure of the double helix of agarose, data from the work[13] was used. Extremely important for MD modeling is the fact that this structure is potentially infinite and the relatively short translation vector of 0.19 nm allows you to flexibly select the length of the agarose chain depending on the available computational resources and other calculation needs.

Analysis of the dynamics of the intermolecular association (aggregation) of two collagen molecules showed that within several hundred picoseconds two tropocollagen molecules form a dynamically stable associate (Fig. 1.6).

Similar dynamics are demonstrated by molecules of tropocollagen and agarose double helix, placed in a model aqueous medium. They also form a co-axial associate within a fairly short time.

Thus, with the help of the MD modeling method, it is shown that the most important intermediate stage of gel formation involving collagen and agarose is the formation of coaxial associates (aggregates) of spiral molecules.

Analysis of the dynamic structure of tropocollagen molecules consisting of three α-chains of collagen (marked as A-B-C and D-E-F, respectively) in aqueous solution shows the special role of the network of hydrogen bonds between amino acid residues of α-chains[14] (Fig. 1.7, 1.8).

It should be noted that the stability of tropocollagen molecules (collagen triple helices) in the aqueous medium is ensured mainly by hydrogen bonds between the -NH groups of glycine of one of the α-chains of collagen and the oxygen atoms of proline of the other α-chain. The analysis carried out along the phase trajectory for 15 ns showed that on average, 15 to 20 strong hydrogen bonds are realized in the tropocollagen molecule over a length of approximately 9 nm (Table 1.1, 1.2).

[13] Arnott S., Fulmer A., Scott W. E., Dea I. C., Moorhouse R., Rees D. A. (1974), The agarose double helix and its function in agarose gel structure, *J.Mol.Biol.*, 90, pp. 269–284.

[14] Grabowski S. J. What Is the Hydrogen Bonding? Chem. Rev. 2011, 111, 2597-2625.
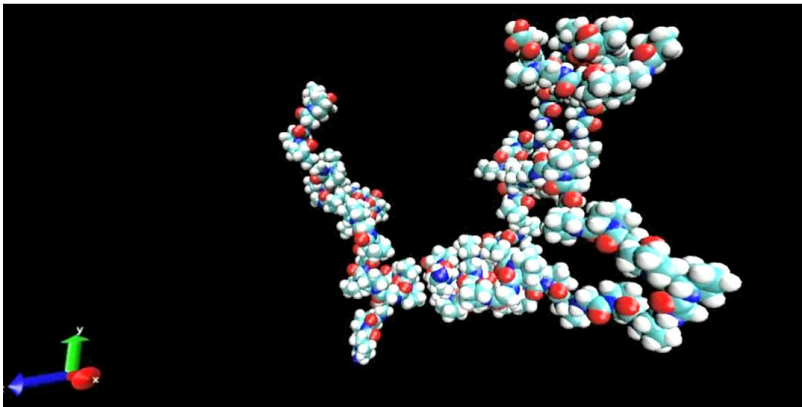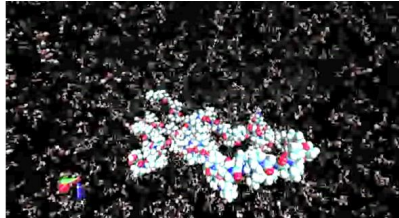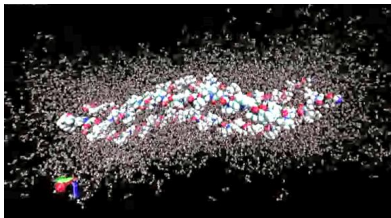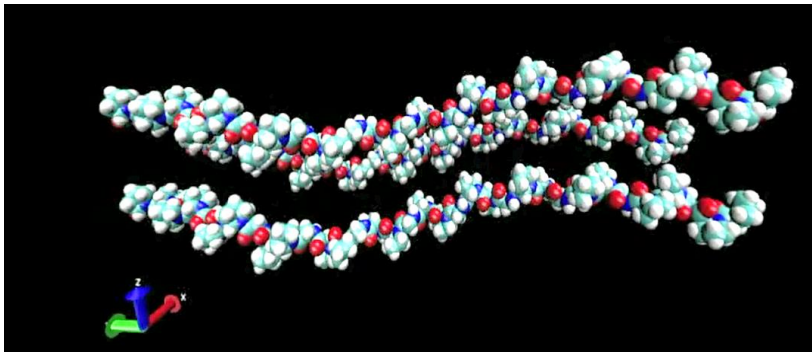
Fig. 1.6. MD simulation with two associated tropocollagen molecules and 32 560 water molecules
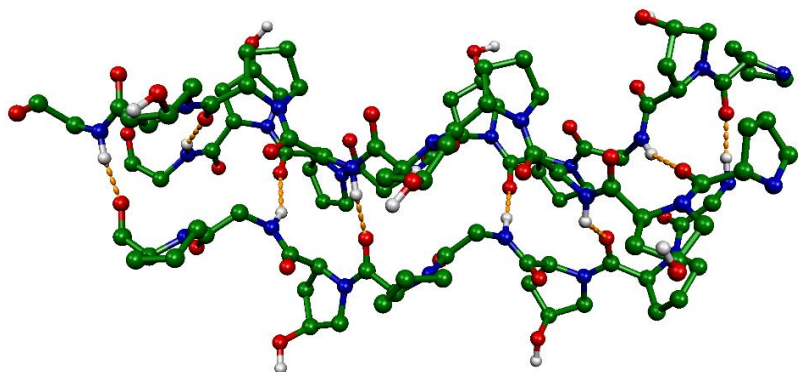
Fig. 1.7. A-B-C section of the tropocollagen molecule
Intramolecular hydrogen bonds are shown as dotted lines

Fig. 1.8. Section of D-E-F tropocollagen molecule
Intramolecular hydrogen bonds are shown as dotted lines

Table 1.1

Statistics of the formation of H-bonds (for 20 ns MD simulation) between α-chains inside the A-B-C tropocollagen molecule

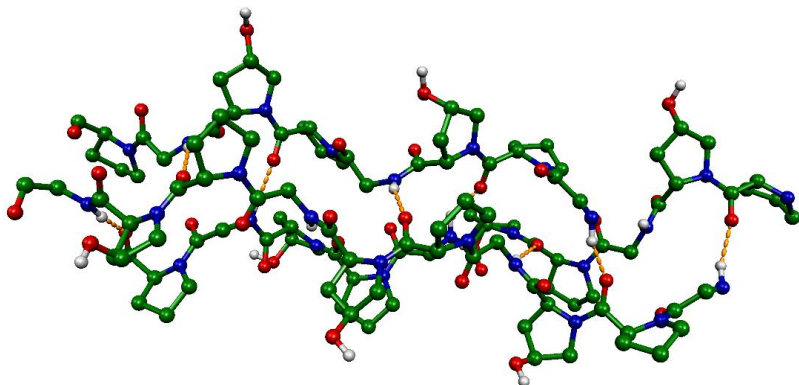| Interaction	Donor	Hydrogen	Acceptor
A-B	GLY7N	GLY7H	PRO5O
A-B	GLY10N	GLY10H	PRO8O
A-B	GLY13N	GLY13H	PRO11O
A-B	GLY19N	GLY19H	PRO17O
A-B	GLY22N	GLY22H	PRO20O
A-C	GLY4N	GLY4H	HYP3O
A-C	GLY16N	GLY16H	PRO14O
A-C	GLY19N	GLY19H	PRO17O
A-C	GLY22N	GLY22H	PRO20O
A-C	GLY25N	GLY25H	PRO23O
B-C	GLY4N	GLY4H	PRO5O
B-C	GLY7N	GLY7H	PRO8O
B-C	GLY10N	GLY10H	PRO11O
B-C	GLY13N	GLY13H	PRO14O
B-C	GLY16N	GLY16H	HYP18O
B-C	GLY19N	GLY19H	PRO20O
B-C	GLY25N	GLY25H	PRO26O

Table 1.2

Statistics of the formation of H-bonds (for 20 ns MD simulation) between α-chains inside the D-E-F tropocollagen molecule

Interaction	Donor	Hydrogen	Acceptor
D-E	GLY7N	GLY7H	PRO5O
D-E	GLY10N	GLY10H	PRO8O
D-E	GLY13N	GLY13H	PRO11O
D-E	GLY19N	GLY19H	PRO17O
D-E	GLY22N	GLY22H	PRO20O
D-E	GLY25N	GLY25H	GLY25O
D-F	GLY4N	GLY4H	PRO2O
D-F	GLY7N	GLY7H	PRO5O
D-F	GLY10N	GLY10H	PRO8O
D-F	GLY13N	GLY13H	PRO11O
D-F	GLY22N	GLY22H	PRO20O
D-F	GLY25N	GLY25H	PRO23O
E-F	GLY4N	GLY4H	PRO5O
E-F	GLY7N	GLY7H	PRO8O
E-F	GLY10N	GLY10H	PRO11O
E-F	GLY16N	GLY16H	PRO17O
E-F	GLY19N	GLY19H	PRO20O
E-F	GLY25N	GLY25H	PRO26O

At the same time, intermolecular association of tropocollagen molecules is carried out mainly due to hydrogen bonds between hydroxyproline residues of amino acids belonging to different tropocollagen molecules (Table 1.3).

A similar result was obtained from the analysis of associates of tropocollagen molecules with agarose molecules.

Table 1.3

Statistics of the formation of H-bonds (for 20 ns MD simulation) by tropocollagen molecules A-B-C and D-E-F

| Interaction	Donor	Hydrogen	Acceptor
ABC-DEF	HYP18OD1	HYP18HD1	HYP18O
ABC-DEF	HYP24OD1	HYP24HD1	HYP24OD1
ABC-DEF	GLY1N	GLY1H1	HYP3OD1
ABC-DEF	HYP6OD1	HYP6HD1	HYP6OD1
ABC-DEF	HYP24OD1	HYP24HD1	HYP24OD1

An important practical conclusion can be drawn from this: to improve the gel-forming properties of collagen or double systems based on agarose + collagen (gelatin), it is desirable to use collagen enriched with hydroxyproline residues.

In order to quantitatively assess the hydrogen bonds formed between tropocollagen molecules, their quantum-chemical analysis was carried out within the framework of Bader's quantum theory "Atoms in molecules" (QTAIM)[15].

Using the described approach, a selective analysis of two types of H-bonds formed between different amino acid residues of two tropocollagen molecules, glycine – hydroxyproline (Fig. 1.9) and hydroxyproline – hydroxyproline (Fig. 1.10) was carried out.

The quantitative characteristics of the corresponding hydrogen bonds in terms of quantum theory are given in the table. 1.4. According to the results of the quantum-chemical analysis of the relevant hydrogen bonds, it was established that the oxygen donor atoms of hydroxy-proline of one of the collagen α-chains of one molecule form, in addition to the classical (strong) H-bonds with NH (glycine) or OH (hydroxyproline) groups α-chains of collagen of another molecule also have weak hydrogen bonds with CH groups of the corresponding molecules, which explains the high dynamic stability of coaxial tropocollagen associates (aggregates) in aqueous solutions (Fig. 1.11).

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[15] Bader R F W 1990 In *Atoms in Molecules: A Quantum Theory* (Oxford: Clarendon Press)
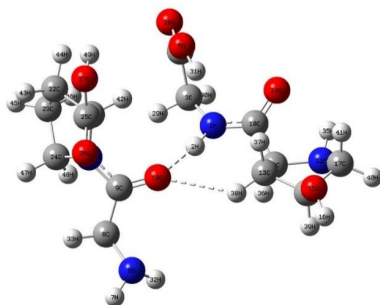
Fig. 1.9. An example of hydrogen bonds between amino acid residues glycine – hydroxyproline of two tropocollagen molecules
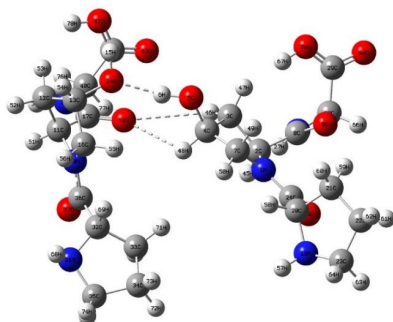
Fig. 1.10. Example of hydrogen bonds between amino acid residues hydroxyproline – hydroxyproline of two tropocollagen molecules

Table 1.4

Quantitative characteristics of hydrogen bonds shown in fig. 1.9 and 1.10, between amino acid residues of two tropocollagen molecules in terms of the quantum theory "Atom in molecules"

Atoms	ρ	$\Delta\rho$	Δq	l, нм
Gly-Hyp				
O10-H38	+0.003122	+0.022680	0.031077	0.271228
O10-H2	+0.034679	+0.144467	0.111862	0.175968
Hyp-Hyp				
Atoms	ρ	$\Delta\rho$	Δq	l, нм
O18-H48	+0.002721	+0.020243	0.004607	0.277263
O18-H46	+0.002549	+0.012544	0.021958	0.295039
H6-O14	+0.033367	+0.143695	0.082228	0.179223

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Hyp· · · Hyp			
Pair	ρ	Δρ	Δq	l, Å
O14-H6	+0.0334	+0.144	0.0822	1.792
O18-H48	+0.0027	+0.020	0.0046	2.772
O18-H46	+0.0025	+0.012	0.0220	2.950

Strong H-bonds

Weak H-bonds (C-H · · · O)

Gly· · · Hyp			
Pair	ρ	Δρ	Δq	l, A
O10-H2	+0.0347	+0.144	0.1119	1.760
O10-H38	+0.0031	+0.023	0.0311	2.712
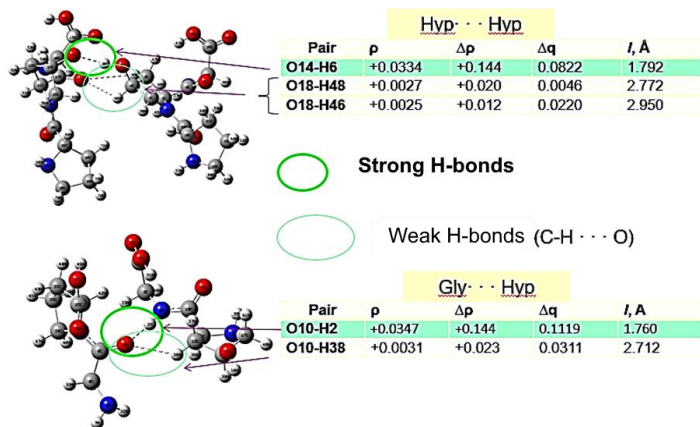
**Fig. 1.11. Scheme of the formation of strong
and weak hydrogen bonds**

Thus, the conducted dynamic modeling confirmed that the basis of gelation processes in aqueous solutions of collagen and agarose is the formation of intermolecular (interhelical) association of tropocollagen molecules with each other, and with tropocollagen molecules and double helices of agarose. It was established that the intra-helical stability of tropocollagen molecules in an aqueous medium is due mainly to the formation of glycine-proline interchain hydrogen bonds. The intermolecular association of tropocollagen molecules with each other, as well as between tropocollagen molecules and the double helix of agarose, is ensured mainly by hydrogen bonds with the participation of collagen hydroxyproline. Based on this result, it is recommended to use gelatin enriched with hydroxyproline for gel formation. Based on quantum-chemical calculations and the use of the theory "Atoms in molecules" it is shown that additional stabilization of intermolecular associates of tropocollagen and agarose is provided by the formation of weak hydrogen bonds C-H · · · O.

2. Empirical modeling of functional and technological properties of structure-forming agents of various origin

2.1. Study of the influence of the external force field on the functional and technological properties of gels

The construction of a spatial grid of gels occurs with the participation of van der Waals or molecular forces of various origins: hydrogen bonding,

electrostatic and hydrophobic interaction. Certain physical fields can influence these forces and change the properties of gels[16].

The effect of an ultra-high frequency (UHF) field of different power on the strength of agar, furcellaran and agaroid gels obtained from 1, 2 and 3 % solutions, respectively, was investigated.

The methodology of the experiment is as follows. After preliminary swelling and subsequent dissolution by heating in a water bath, solutions of appropriate concentrations were obtained. After that, they were cooled to 35…45 °C and processed in the microwave field with a frequency of 2450 MHz at different power for such a period of time that the solution did not heat up above 80 °C (1…10 min). The exposure time of polysaccharide solutions in the microwave field is selected experimentally according to the temperature of the solution. It depends on both the power of the field and the volume of the solution (Fig. 2.1.1).

After solidification, the strength of the gels was measured according to the method[17]. Untreated samples were taken as controls. The influence of the microwave field on the strength of gels is presented in Figures 2.1.2 and 2.1.3. Treatment of polysaccharide solutions with a microwave field leads to a significant (1.4…2.2 times) strengthening of the gels they form.
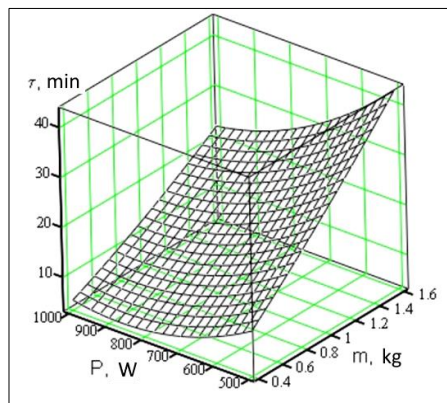
Fig. 2.1.1. The graph of the dependence of processing time on the mass of the solution and the heating power

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[16] Фощан А. Л. Деякі аспекти процесу структуроутворення у розчинах драглеутворювачів. *Прогресивні техніка та технології харчових виробництв ресторанного господарства і торгівлі* : зб. наук. праць ХДУХТ. Харків, 2005. Вип. 1. С. 343–348.

[17] Phillips O, Williams P. Bloom strength–standard method for characterizing gel strength. In: Handbook of Hydrocolloids. Taylor & Francis. 2000.
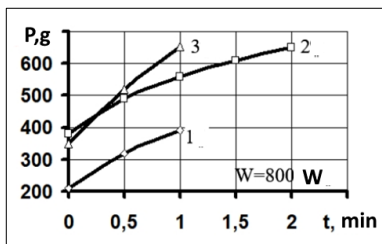
Fig. 2.1.2. Dependence of gel strength of agar (1), furcellaran (2) and agaroid (3) on heating time at heating power W=800 W

Fig. 2.1.3. Dependence of the strength of agaroid gels on heating power and time

In order to understand the effect of the microwave field on solutions of red seaweed polysaccharides, we used the method of turbidity spectrum analysis[18]. Its essence is that with the help of a photocolorimeter at different wavelengths λ (different light filters) the optical density D of the structure-forming solutions is measured. Turbidity of the solution τ is related to D dependence $\tau = 2.3\,D/l$, wh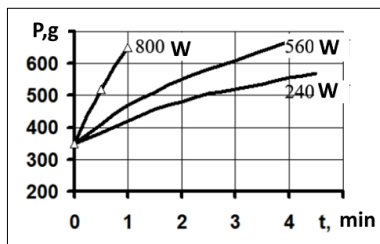ere l is the thickness of the cuvette. Turbidity is a function of λ at a given solution concentration C and temperature T. At small intervals λ $\tau \sim \lambda^{-n}$, where n is the wave exponent, which can be expressed in explicit form as $n = -\partial ln\tau / \partial ln\lambda$. n is a function of the relative size of the particles of the supramolecular structure (SMS) α and the relative refractive index m. ($\alpha = 2\pi r \mu_0/\lambda_{cp}$; $m = \mu/\mu_0$, where r is the radius of the SMS particles; μ and μ_0 are the refractive indices of the particles and water, respectively; λ_{cp} is the average value of the wavelengths in the section of the linear dependence $ln\,\tau$ from $ln\,\lambda$). Knowing n and m, α and the scattering coefficient k can be found from the Tables of characteristic light scattering functions. The radius of the particles r *(nm)* and their concentration N (cm^{-3}) are calculated according to the formulas:

$$N = 1.26 \cdot 10^{17}\,\frac{\tau_{cp}}{(\lambda')^2 \cdot k \cdot \alpha^2} \tag{2.1.1}$$

[18] S. Yu. Shchyogolev, V. I. Klenin, S. Ya. Frenkel. Solution of problems of analytical fractionation of polymers and copolymers by using a generalized material balance equation. *Acta Polymerica.* Vol. 34, Issue4 April 1983 PP. 237–237

$$r = \frac{\alpha \cdot \lambda_{cp}}{2 \cdot \pi \cdot \mu_0} \qquad (2.1.2),$$

where τ_{cp} is the average value of τ on the section of the dependence $ln\tau - ln\lambda$; $\lambda' = \lambda_{cp}/\mu_0$.

We studied aqueous solutions of agar with a concentration of 0.2; 0.4; 0.7; 1.0 %. To prepare the solution, the polysaccharide was soaked in water at room temperature for a day, then dissolved at t=85…100⁰C. The resulting solutions were filtered, brought to the required temperature, the cuvette with the solution was kept for 30 minutes to establish equilibrium, and D was measured at different λ in a photoelectrocolorimeter. Part of the solution was kept in a 400 W microwave field for 3 minutes before thermosetting. Based on the results of measuring D and calculating τ, the dependence $ln\tau\text{-}ln\lambda$ was built. We calculate r and N according to formulas (2.1.1) and (2.1.2).

Fig. 2.1.4 shows the effect of agar concentration on r and N of SMS. The dotted line shows this effect after treatment of solutions with a microwave field. Both N and r increase as the concentration of the solution increases. The microwave field affects the interphase distribution of agar macromolecules. The size of joints – particles of SMS decreases, and their number increases.
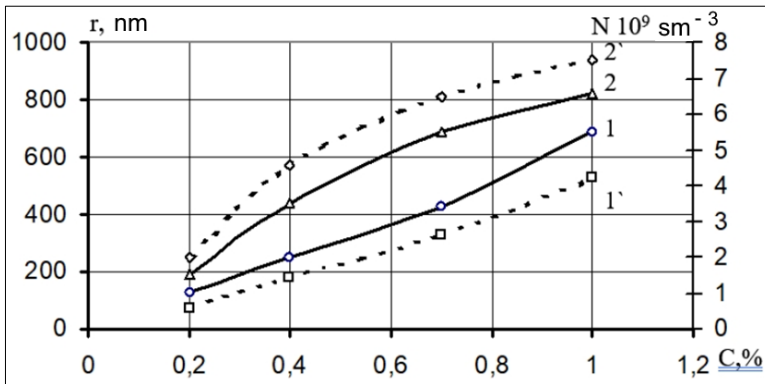
Fig. 2.1.4. Dependence of SMS on the structure former concentration at 20°C
1 – r=f(C); 1' – r=f(C) after microwave; 2 – N=f(C); 2' – N=f(C) after microwave

According to the theory of structure formation[19], at high temperatures, polysaccharide molecules are in solution in the form of globules. As the solution cools, the molecules straighten out, twist into spirals, double spirals, which group together to form particles. All fragments of the dissolved substance: spirals, double spirals and particles participate in building the gel structure. As shown earlier, treatment of agar solutions with a microwave field strengthens the gel structure. Comparing the data of the study of the influence of the microwave field on the strength, we can conclude that the greater the concentration of SMS particles and the smaller their size at a given concentration of the structure former, the stronger gels are formed.

Heating of solutions in an alternating electromagnetic field is caused by the presence of polar molecules, groups of atoms, and ions. Forced oscillations of these particles transform the energy of the field into heat. In solutions of polysaccharides, hydrated polar groups of atoms, which are in both ionized and non-ionized states, can partially lose their hydrated shells, which greatly facilitates intra- and intermolecular interactions and conformational transformations of macromolecules. All this should increase the number of double helices and strengthen the network of gels, which is observed.

In the process of manufacturing jelly products, an important technological parameter that affects the quality of finished products is the solidification temperature of the jelly mass and the melting temperature of jelly. In order for jelly products to retain their shape and have a good marketable appearance, it is necessary that the melting temperature of the jelly mass be as high as possible. This can be achieved by increasing the concentration of the structure former, which will lead to an increased expenditure of this expensive and scarce raw material.

Since the treatment of solutions of red seaweed polysaccharides by the microwave field leads to an increase in the strength of the gels, it would be reasonable to assume that such treatment can also change the melting and solidification temperatures. That is why the study of these indicators is of practical interest.

Figure 2.1.5 (a) shows the results of the study of the melting temperatures of untreated and treated agar gels in the microwave field depending on the concentration of the structure former. It can be seen that treatment of agar solutions with a microwave field leads to an increase in the melting temperature of gels in comparison with the untreated sample at the same concentration of the structure former.

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[19] Rees D. A. Conformational analysis of polysaccharides / V. I. Chem. Soc. B / 1970. № 5. P. 877.

An important characteristic of the state of the gel structure is the average energy of a single link joint of the gel network, or the melting enthalpy of the gel, which characterizes the energy of disintegration of the joints of the gel network. The relationship between this value and the melting temperature of gels is described by the Eldridge-Ferry equation:

$$\Delta H = -R \frac{\Delta \ln C}{\Delta T_m^{-1}} \qquad (2.1.3)$$

where ΔH is the bond disintegration energy, R is the universal gas constant, C is the concentration of the structure former, Tm is the melting temperature of gels of a given concentration.

In fig. 2.1.5 (b) the curves of the dependence of $ln\ C$ on $1000/Tm$ are given, calculated according to the data shown in fig. 2.1.5 (a).
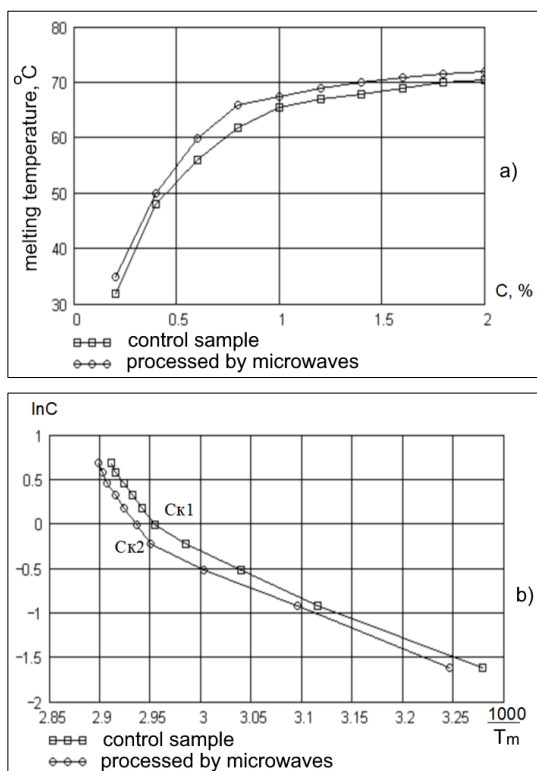
Fig. 2.1.5 Dependence of the melting temperature of agar gels on the concentration of the structure former (a) and the dependence of _ln C_ on the inverse melting temperature _Tm_ (b)

These dependences represent curves with a characteristic break. The concentration at which a break in these curves is observed is called the critical concentration, Ck, and characterizes the transition from a molecular structure to a supramolecular one. The molecular structure of gelatin is characterized by weak bonds. Connections between individual units of such a structure arise because of the interaction of molecules or double helices through hydrogen bonds or with the participation of water. When the concentration of the structuring agent in the solution is higher than Ck, their aggregates take part in the formation of the structure of the dredges, along with individual double helices. The structure of gels becomes supramolecular, and a larger number of bonds is involved in the formation of a single node of the gel network. It can be seen that the processing of agar solutions in the field of microwaves leads to a decrease in the critical concentration of the transition of the molecular structure of the gel to the supramolecular one (Ck1>Ck2).

The slope of the curves lnC – 1000/Tm, according to the Eldridge-Ferry equation (2.1.3), allows you to calculate the energy value of a single bond node of the gel network ΔH. The values of ΔH are in Table 2.1.1.

Table 2.1.1

Value of the energy of a single bond node of the gel network

Agar	ΔH_1, kJ/mol	ΔH_2, kJ/mol
Control sample	38	130
Processed in the microwave field	40	150

The molecular structure of gels is characterized by weak bonds and, therefore, a small value of the melting enthalpy of the gel (ΔH_1). When the concentration of the structuring agent in the solution is higher than Ck, in the formation of the structure of gels, along with individual double helices, a larger number of bonds, characterized by a higher melting enthalpy (ΔH_2), is involved. The value of ΔH_1 is approximately the same for both the treated solution and the untreated one. However, the value of ΔH_2 for the sample treated in the microwave field is greater, which indicates the formation of stronger bonds between polysaccharide macromolecules.

Thus, the treatment of structure-forming solutions with a microwave field leads to strengthening of the gel structure, and thanks to this, it makes it possible to reduce the cost of the structure-forming agent in the production of jelly products and leads to a decrease in the cost of finished jelly products.

2.2. Study of the influence of the addition of sodium alginate and calcium chloride on the properties of gels of sulfated polysaccharides from red seaweed

One of the ways to reduce the costs of structure-forming agents in the production of jelly products is the introduction of various additives into the recipe mixture, which lead to an increase in the structure-forming ability of red seaweed polysaccharides. This allows you to save some amount of gelling raw material without deteriorating the quality of the finished product[20, 21, 22].

Alginic acid and its salts are widely used in the economy. Sodium alginate is most often used. Sodium alginate is a salt of alginic acid, which in the form of mixed salts of calcium, magnesium and other metals makes up the main part of the cell walls of brown seaweeds of the kelp family. The chemical structure of sodium alginate, like the chemical structures of many other algal polysaccharides, is variable and depends on the type of algae and other factors. The structural formula of sodium alginate has the following form:
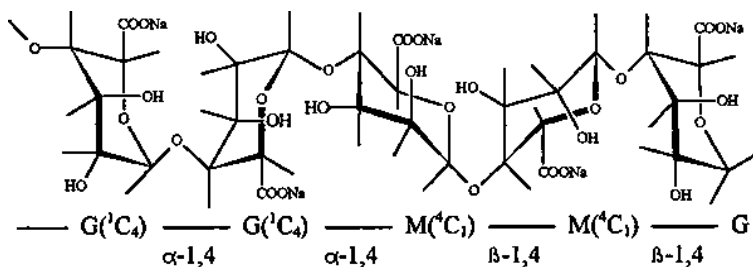
Macromolecules are built from two components – residues of L-guluronic and D-mannuronic acids, which have a linear structure and are connected by (1→4) bonds connecting individual monosaccharides. Water molecules binding alginate molecules are not shown in this structural formula.

[20] Перцевий Ф. В., Савгіра Ю. О., Фощан А. Л., Гринченко О. О., Пивоваров П. П., Гарнцарек Б. Ч. Технологія переробки продуктів харчування з використанням модифікаторів : монографія. Харків : ХДТУСГ, 1998. 178 с.

[21] Перцевий Ф. В., Фощан А. Л., Савгіра Ю. О., Гринченко О. О., Пивоваров П. П. Виробництво желейної і збивної продукції з використанням модифікаторів : монографія. Дніпропетровськ : Пороги, 2003. 201 с.

[22] Pertsevoy F., Savgira Yu., Foshchan A., Ukrainets A., Garncarek B., Miskiewicz T. Modifying additives in jelly products (Модифікуючі добавки в желейній продукції) : монографія (англ. мовою). Київ : Бізнесполіграф, 2005. 260 с.

Numerous toxicological studies carried out in the world have confirmed the harmlessness of sodium alginate and the possibility of using alginates as a food additive[23]. At the same time, acceptable human doses of sodium alginate were established, amounting to 50 mg/kg body weight per day.

Alginates are effective sorbents. They can be used as a food treatment and preventive supplement[24] to remove heavy metals, radionuclides, slags and toxins from the body. In addition, they are used in the treatment of gastrointestinal diseases: chronic colitis, gastritis, duodenal ulcer, chronic hepatitis; in diseases of the liver, pancreas and cardiovascular system.

In the manufacture of food products, alginates are used to preserve the consistency of the product during freezing and thawing, ensure the production of viscous media that quickly form gels, stabilize the system, add hardness, reduce the release of moisture, for thickening and stabilization[25].

Based on the above, we assumed that the introduction of alginates into the recipe mixture of jelly products will allow to significantly change the structural and mechanical properties of jelly, strengthen their structure, which will lead to a reduction in the cost and saving of expensive jelly-forming agents. For this purpose, we studied the influence of sodium alginate and calcium chloride on the structural and mechanical properties of agar, agaroid, and furcellaran gels.

Increasing the strength of gels is equivalent to the possibility of reducing the consumption of gelling agents. Such structural and mechanical indicators as strength, elasticity, plasticity, elasticity are related to the organoleptic evaluation of the finished product. Characterization of structural and mechanical properties of products in terms of elastic-plastic-strength indicators makes it possible to solve a few important practical tasks: they can be used for directed control of the technological process of obtaining products with specified properties. In addition, it is known that the strength and structure of gels are largely determined by the nature of the bonds that unite macromolecules into a structural network, as well as by all kinds of conformational transformations capable of giving the gel pronounced elastic-elastic or plastic-viscous properties. From this point of

[23] K. Y. Lee and D. J. Mooney, "Alginate: Properties and biomedical applications," *Progress in Polymer Science* (Oxford), vol. 37, no. 1. Elsevier Ltd, pp. 106–126, 2012.

[24] Phillips, M. M., Rimmer, C. A. Functional foods and dietary supplements. *Anal Bioanal Chem*, 405, 4323–4324 (2013).

[25] Фощан А. Л., Овсяникова Л. Г., Перцевий Ф. В. Використання альгінату натрію для удосконалення технології кулінарної продукції. *Прогресивні ресурсозберігаючі технології та їх економічне обгрунтування у підприємствах харчування та економічні проблеми торгівлі* : зб. наук. праць ХДУХТ. Харків, 2003. С. 456–462.

view, the study of the influence of introduced additives on the structural and mechanical properties of gels is of great theoretical interest.

We chose such a research path, according to which it was first necessary to find the optimal concentrations of the proposed additives and their ratio, which lead to an increase in the structure-forming ability of polysaccharides. The mechanical strength of dredges was taken as the criterion. Then investigate the influence of additives in the established concentrations on the structural and mechanical properties of gels, and thus on the character of the bonds of the elements of the spatial structure of the gel.

The first stage of the research was the study of the strength of agar, furcellaran and agaroid gels in the presence of sodium alginate and calcium chloride. The concentration of gelling agents was chosen experimentally: agar – 1 %, furcellaran – 2 %, agaroid – 4 %. At lower concentrations, the gels had insufficient mechanical strength, and a long time was required for structure formation, at higher concentrations, the solubility of polysaccharides deteriorated, and heterogeneous gels were formed.

Admissible concentrations of added additives: no more than 1 % for sodium alginate and no more than 3 % for calcium chloride $CaCl_2$.

Solutions and gels were prepared as follows. A certain amount of gelling agent was poured with the required amount of distilled water with a temperature of 20 ^{0}C and left to swell for 1.5…2 hours. Then the gelling agent was dissolved by boiling in a water bath in reflux flasks. After that, hot water solutions of polysaccharides were poured into cups for solidification, which were placed in a desiccator over water to avoid the formation of a gel crust on the surface.

Sodium alginate was introduced at the swelling stage of the gelling agent in the form of a 5 % solution, and calcium ions (in the form of a 2.8 % $CaCl_2$ solution) into the polysaccharide solution cooled to 70 °C, because at higher temperatures, the destruction of the molecules and the decrease in the strength of the samples are observed.

Experimental data on the effect of additions of sodium alginate and calcium chloride on the change in the strength of gels of 1 % agar solution, 2 % furcellaran solution and 4 % agaroid solution are shown in Fig. 2.2.1–2.2.3.

It can be seen from the graphs that the effect of additives on the strength of sulfated polysaccharide gels depends on the concentration of the additive and the nature of the gelling agent. The concentration at which the maximum strengthening of the system is observed is 0.5…1 % of sodium alginate. At the same time, the strength of the system increases by 15 % for agar, 17 % for furcellaran and 18 % for agaroid in comparison with the control sample. When introducing calcium chloride with a concentration of

0.08…0.1 %, (corresponding to 0.03…0.04 % Ca^{2+} ions) for agar, 0.18…0.20 % (0.06 …0.07 % Ca^{2+}) for furcellaran and 0.2…0.22 % (0.07…0.08 % Ca^{2+}) for agaroid, the gel strength of these polysaccharides increases by 17, 20 and 25 %, respectively.

The increase in strength when sodium alginate is introduced into the system is probably due to the fact that small amounts of sodium alginate in polysaccharide solutions lead to conformational changes of macromolecules, as a result of which a stronger three-dimensional network of gelling is formed.

(a)   *(b)*
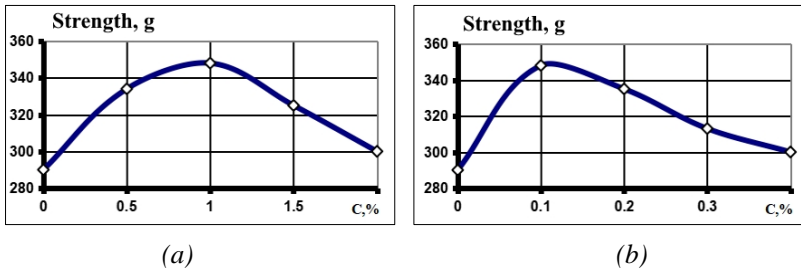
Fig. 2.2.1. Dependence of the strength of gels of 1 % agar solution on the concentration of sodium alginate (a) and calcium chloride (b)

(a)   *(b)*
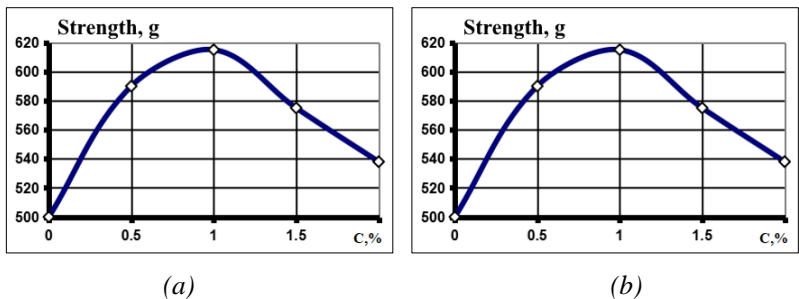
Fig. 2.2.2. Dependence of the strength of gels of 2 % furcellaran solution on the concentration of sodium alginate (a) and calcium chloride (b)

314

(a)   *(b)*
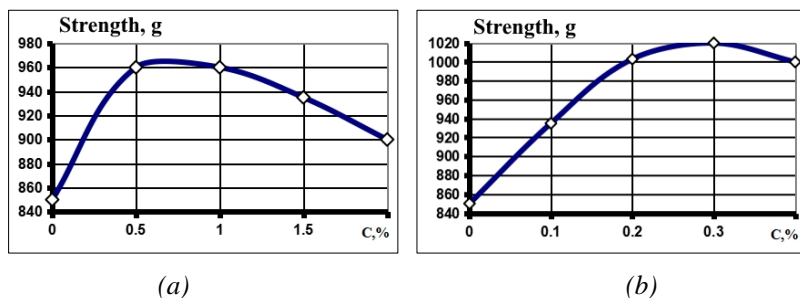
Fig. 2.2.3. Dependence of the strength of gels of 4 % agaroid solution on the concentration of sodium alginate (a) and calcium chloride (b)

Gels that form sulfated polysaccharides together with sodium alginate belong to the type in which the polymer structures of different ingredients do not mix. This leads to the accumulation of sodium alginate molecules in the mesh of the structure former. The consequence of this can be the strengthening of the intermolecular interaction of the gelling agent at certain concentrations of the second component with a corresponding increase in the strength of the gel. A further increase in the alginic acid salt concentration causes partial salting out of the gelling agent. As a result, the amount of charge of polysaccharide molecules decreases. Decreasing the charge of molecules below the optimal value leads to the predominance of the forces of molecular attraction over the forces of electrostatic repulsion. As a result, weak gels are formed.

From fig. 2.2.1–2.2.3 (b) an increase in the strength of gels is observed when a small amount of calcium chloride is introduced. The maximum strength was observed for 1 % agar gels at 0.08…0.1 % $CaCl_2$, (corresponding to 0.03…0.04 % Ca^{2+} ions), for 2 % furcellaran gels at 0.18… 0.20 % $CaCl_2$ (0.06…0.07 % Ca^{2+}), for 4 % agaroid gels at 0.2…0.22 % $CaCl_2$ (0.07…0.08 % Ca^{2+}). A further increase in the concentration of iron chloride leads to a gradual decrease in the strength of the gels.

The concentration of calcium ions at which the maximum strength of the gels is observed increases from agar to furcellaran and then to agaroid. Similarly, the content of sulfate groups SO_3M (M metal ion) in polysaccharides, capable of dissociating in water with the formation of high molecular weight polyanions, changes. Calcium ions added to solutions of polysaccharides reduce the charge of their molecules, shielding the charge of anions, and thus reduce the repulsive forces between molecules. Which leads to the formation of stronger gels. Calcium chloride supplements are most effective on polysaccharides that have a lower structure-forming ability.

Polysaccharide gels containing calcium chloride as an additive have greater strength compared to gels containing sodium alginate. This is probably explained by the fact that Ca^{2+} calcium ions, along with the simple shielding of the charge of sulfate groups, can form bridging bonds of the ionic type that connect the polymer chains of the polysaccharide.

When the additives are jointly introduced into polysaccharide solutions, the strength of the obtained gels is significantly higher than the strength of samples with only one additive. Thus, the strength of the 1 % agar solution is 25 % higher than the strength of the control sample, the strength of the 2 % furcellaran solution is 30 %, and the strength of the 4 % agaroid solution is 44 %, respectively (Fig. 2.2.5).

In fig. 2.2.4 shows graphs of curves of equal strength values of agar, furcellaran and agaroid gels depending on the concentration of added additives. These curves were constructed by mathematical processing of experimental data (table 2.2.1).
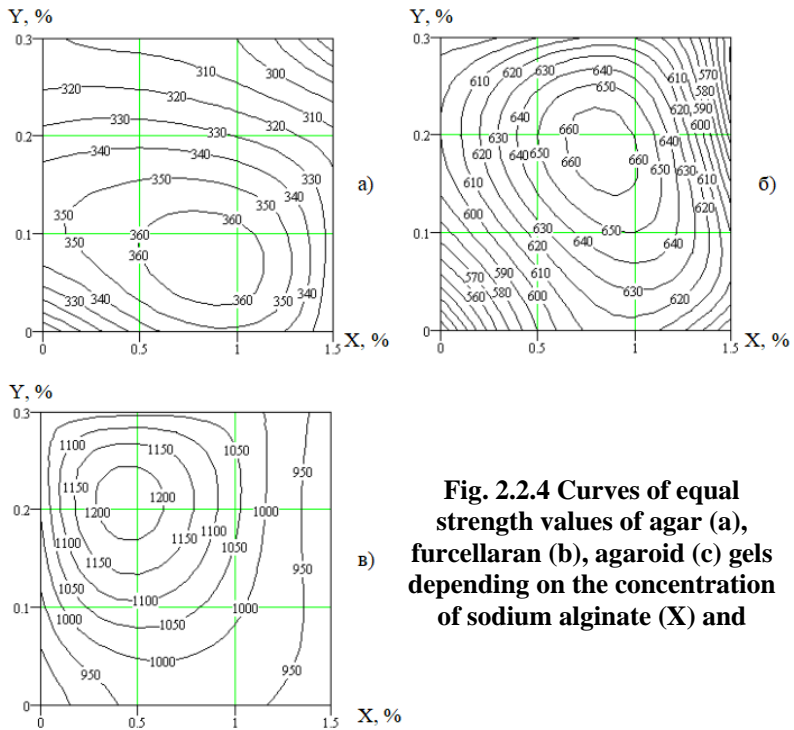
Fig. 2.2.4 Curves of equal strength values of agar (a), furcellaran (b), agaroid (c) gels depending on the concentration of sodium alginate (X) and
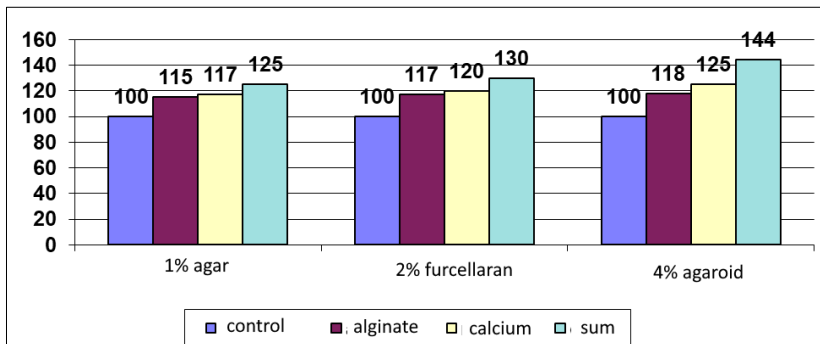
Fig. 2.2.5. Relative strength of gels (%) depending on the added additive

Strength of polysaccharide gels (g) depending on the concentration of additives

Concentration of calcium chloride, %	Concentration of sodium alginate, %			
	0	**0,5**	**1,0**	**1,5**
	1 % agar			
0	290	334	348	320
0,1	348	360	363	325
0,2	333	336	330	313
0,3	313	307	300	260
	2 % furcellaran			
0	500	590	615	570
0,1	575	625	650	600
0,2	600	650	660	555
0,3	585	600	610	530
	4 % agaroid			
0	850	960	960	935
0,1	935	1088	1012	945
0,2	1003	1224	1063	940
0,3	1020	1037	1020	918

The mechanical properties of gels play an important role not only in their production, but also in their consumption. The product is subjected to various types of deformations and failures (compression, tension, shear), which act in combination or separately. Therefore, it is of practical interest to study the effect of additives introduced on such characteristics of gels as resiliency, plasticity, elasticity. Gels of red seaweed polysaccharides contain in their structure a significant number of aggregates of molecular spirals, and to a greater extent exhibit resilience-elastic properties. Plastic properties are less developed. When the ultimate shear stress is exceeded, the system collapses.

The introduction of calcium chloride into solutions of polysaccharides leads to an increase in elasticity and a decrease in the elasticity of their gels. This is probably caused by the fact that calcium ions are able to form intermolecular bonds of the ionic type that bind polymer chains. The formation of such bonds increases the rigidity of polymer chains, which is expressed in a decrease in resiliency and an increase in the elasticity of gels. The addition of sodium alginate leads to a significant increase in the plasticity of polysaccharide gels.

Thus, our research allowed establishing the dependences of the strength of agar, furcellaran, and agaroid gels at different mass concentrations of sodium alginate and calcium chloride. It was determined that by combining the mass fractions of these components, it is possible to change the resilience-plastic-elastic properties of gels, as well as to vary their strength in the range of 360–1020 g, which will make it possible to obtain gels with previously known structural and mechanical characteristics[26].

3. Technologies of jelly products with low content of structural raw materials

On the basis of the scientific concept, which consists in the fact that by adding various low-molecular additives, combining structure-forming agents of different origin and the influence of an external electromagnetic field, it is possible to control the processes of gel formation and, thus, ensure the proper quality of jelly products, while reducing the cost of structure-forming raw materials, was developed and tested and the technology of jelly products, such as: "Chocolate-marshmallow", "Chocolate-jelly" cakes, was introduced into the production.

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[26] Control of the gelling process in production of jelly products / Foshchan A. L. Eastern-*European Journal of Enterprise Technologies*, № 2 (8), 2004. P. 38–42.

3.1. Technology of production of "Chocolate-jelly" cake with the use of microwave field

For the prototype was taken the traditional recipe of the "Chocolate-jelly" cake[27], which is a body glazed with chocolate glaze, consisting of two outer jelly layers and an inner layer of whipped mass. The main raw materials for making a cake are sugar, food agar, apple puree, egg whites, dyes, food flavorings, citric acids, vanillin, chocolate glaze, starch syrup, essences.

According to the traditional recipe and taking into account the results obtained, a recipe was developed for the "Chocolate-jelly" cake with a reduced amount of gelling agent, given in Table 3.1.1. The difference between the new recipe and the traditional one is to reduce agar consumption by 40 %.

On the basis of the studies carried out to develop a new recipe, the technology was improved and a technological scheme for the production of the "Chocolate-jelly" cake was developed (Fig. 3.1.1).

The production technology of the "Chocolate-jelly" cake consists of the following operations:

– preparation of raw materials;
– preparation of agar-sugar-treacle syrup for the lower and upper layers;
– preparation of whipped mass for the middle layer;
– pouring syrup into molds and its gelling agent;
– drying of bodies;
– icing and cooling of cakes;
– packaging;
– marking;
– transportation and storage.

The body of the "Chocolate-jelly" cake on agar consists of three layers: the bottom and top – jelly, having different colors, and the middle – whipped layer – white. Jelly layers, depending on taste and color, are flavored with various essences:

– raspberry or strawberry (red);
– orange or tangerine (orange color);
– lemon or apricot (yellow);
– pear or pineapple (green);
– blackcurrant or cherry (lilac color);
– apple or vanilla (white).

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[27] Павлов О. В. Збірник рецептур борошняних кондитерських і здобних булочних виробів: навчально-практичний посібник / О. В. Павлов. 2-ге видання, доповнене. Київ : ПрофКнига, 2019. 340 с..

Table 3.1.1

The recipe for the "Chocolate-jelly" cake with a reduced amount of gelling agents

Raw materials	Mass fraction of dry substances, %	Raw material consumption, kg			
		for 1000 kg of semifinished product		for 1000 kg of finished products	
		actually	in dry matter	actually	in dry matter
Chocolate glaze	99,10	302,75	300,03	306,40	303,60
Granulated sugar	99,85	440,20	439,54	445,48	444,81
Syrup	78,00	142,58	111,21	144,30	112,55
Apple puree	10,00	26,01	2,60	26,17	2,62
Agar	85,00	6,12	5,20	5,22	4,44
Citric acid	91,20	6,89	6,28	6,29	5,74
Vanilla essence	0,00	0,30	0,00	0,30	0,00
Essences are different	0,00	0,23	0,00	0,23	0,00
Different dyes	0,00	0,74	0,00	0,74	0,00
Total	-	952,82	864,86	935,13	873,76
Yield	81,60	1000,00	816,00	1000,00	816,00

The cake making technology is as follows. Agar is soaked in water in cloth bags and washed in running water. After that, the calculated amount of water is added and heated in the microwave field. Granulated sugar is added to the agar solution. Heat and stir constantly until sugar dissolves. Then add molasses without stopping heating and stirring. The resulting agar-sugar-syrup is cooled to 60–65 °C and part of it is taken to obtain a whipped (middle) layer of the cake body. In the rest, add dye, citric acid, essence and pour into molds (bottom layer). After hardening, a white whipped layer is poured onto it. After the structure formation of the middle layer, a jelly top layer is poured and the molds with the bodies are kept at a temperature of 18–21 °C for 6–8 hours to strengthen the layers of the bodies.

Dried bodies are glazed with chocolate glaze. The last tempering at a temperature of 31–32 °C. After glazing, the cakes are cooled to 8–12 °C for 30–60 minutes. Finished products are packaged and labeled.

The difference of the proposed technology lies in the use of a microwave field in the preparation of agar-sugar treacle syrup to dissolve swollen agar, which makes it possible to reduce the prescription amount of gelling agents and reduce the cost of the product.

Water — Preparation

Agar — Preparation

Sugar — Preparation

Starch syrup — Preparation

Applesauce, TSS=10 % — Preparation

Chicken egg — Preparation

Vanillin — Preparation

Soaking t=10–25 °C
τ=(1–1.5)x360 s

Washing
t=10–25 °C

Warming up in the
microwave field t=85 °C

Separating yolks
from whites

Egg
white

Mixing

Cooking (dissolving sugar)

Agar-sugar syrup,
TSS=71–72 %

Cooling, TSS=78–79 %

Agar-sugar-treacle syrup,
TSS=71–72 %

Cooling, t=65–70 °C

1 3   2   6

Whipping,
τ=(7–15)x60 s

5

Dye — Preparation

Mixing

Preparation — Vanilla essence

Preparation — Citric acid

4

Pouring and proofing,
t=35–40 °C; τ=(3–4)x360 s

1, 3

Body formation

2

Whipped mixture,
TSS=57–59 %

Drying shell,
t=18–2; τ=(6–8)x360 s

Removing from the mold

Chocolate glaze

Glazing — Tempering,
t=31–32 °C — Sifting, d=
=2x10⁻³ m; 90 %

Cooling,
t=8–12 °C; τ=(0.5–1)x360 s

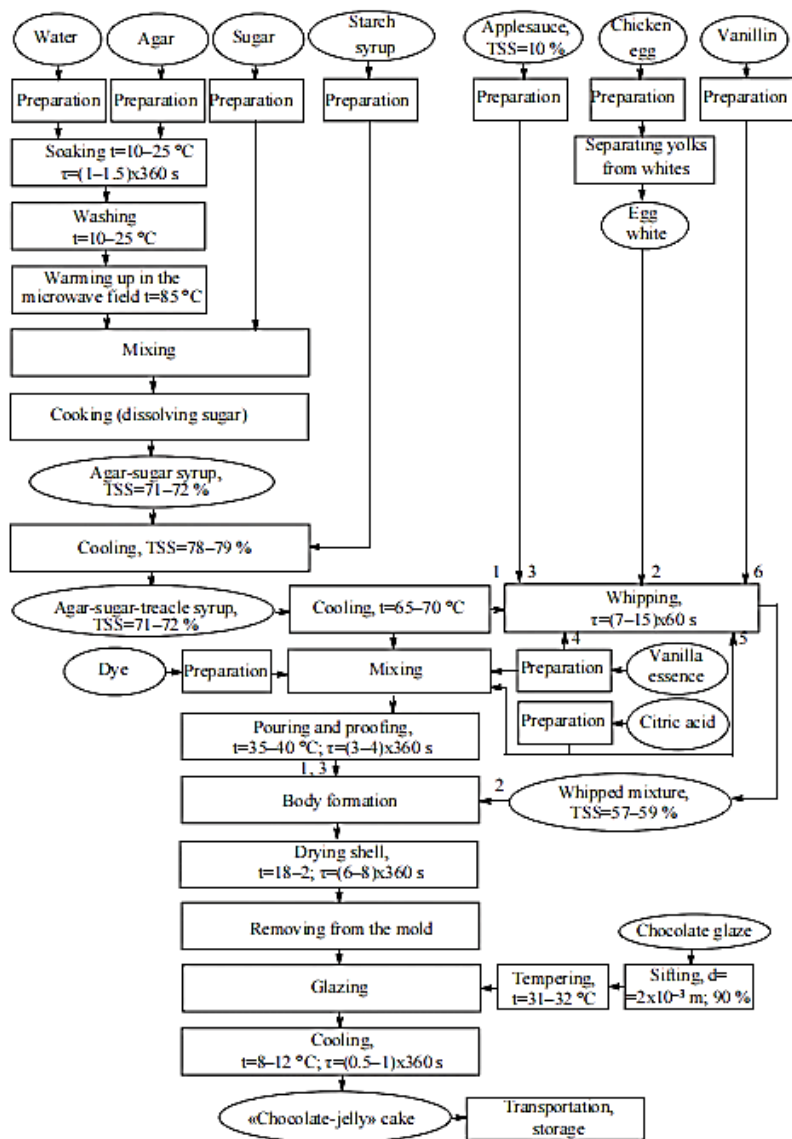«Chocolate-jelly» cake — Transportation,
storage

**Fig. 3.1.1. Technological scheme for the production of the
"Chocolate-jelly" cake with a reduced number of jelling agents**

The use of the microwave field provides for minor changes in the instrumentation of the technological process. The parameters of the technological process do not differ from the traditional ones, so the new technology can be introduced into production without complications.

The organoleptic characteristics of the "Chocolate-jelly" cake showed their full compliance with the requirements of regulatory documentation for this type of product.

Thus, the use of a microwave field to dissolve agar during the preparation of agar-sugar-molasses syrup in the "Chocolate-jelly" cake technology allows you to reduce the recipe amount of agar by 40 % and obtain products with high quality indicators.

3.2. Technology of production of cake "Chocolate-marshmallow" with use of sodium alginate and calcium chloride

The production process of the "Chocolate-marshmallow" cake consists of the following operations: preparation of raw materials; soaking and washing agar; preparation of agar-molasses syrup; preparation of apple-sugar mixture; preparation of marshmallow mass; pouring marshmallow mass into molds and proofing; icing with chocolate glaze and cooling; packaging; labeling; transportation and storage.

The main raw materials for the preparation of the "Chocolate-marshmallow" cake are: white sugar, chocolate glaze, apple puree, starch molasses, egg white, agar, citric acid, vanilla essence.

In the recipe of the cake, the dosage of gelling agent is 6 kg/1000 kg of finished products. In order to reduce the consumption of gelling agent in the formulation, we suggested partially replacing agar with sodium alginate. During a complex of experimental studies, it was established that the use of the model system: "water – agar – sodium alginate – calcium chloride" leads to a strengthening of the jelly structure.

Considering the obtained results, we have developed a recipe for the "Chocolate-marshmallow" cake based on a complex gelling agent, which is shown in table 3.2.1.

The difference of the new recipe lies in the reduction of agar consumption by up to 50 %, the use of a complex gelling agent agar – sodium alginate – calcium chloride, which makes it possible to obtain high-quality products of adequate strength. The technological scheme for the production of new products is shown in Fig. 3.2.1.

The preparation of a cake according to this technology involves the preparation of sodium alginate by a soaking operation. The difference of the proposed technology is the addition of swollen sodium alginate at the stage of preparation of agar-sugar-molasses syrup. The sequence of

operations of the technological process of cake preparation was left unchanged. This will provide an opportunity to quickly implement the proposed technology in any confectionery production.

Table 3.2.1

**"Chocolate-marshmallow" cake recipe based on
a complex gelling agent**

Raw materials	Mass fraction of dry substances, %	Raw material consumption, kg			
		for 1000 kg of semifinished product		for 1000 kg of finished products	
		actually	in dry	in kind	actually
Chocolate glaze	99,10	353,48	353,30	358,30	355,10
Granulated sugar	99,85	432,40	431,75	438.37	437,71
Syrup	78,00	90,59	70,66	91,84	71,64
Apple puree	10,00	236,36	23,64	239,86	23,99
Egg white	12,00	42,18	5,06	42,50	5,10
Agar	85,00	3,00	2,55	3,02	2,57
Sodium alginate	85,00	3,00	2,55	3,02	2,57
Calcium chloride	96,00	0,29	0,28	0,30	0,30
Citric acid	91,20	5,00	4,56	5,01	4,57
Vanilla essence	0,00	0,65	0,00	0,65	0,00
Total	–	1166,95	894,35	1182,87	903,55
Yield	86,68	1000,00	866,80	1000,00	866,80

The organoleptic evaluation of the "Chocolate-Marshmallow" cake showed their full compliance with the requirements of the regulatory documentation for this type of product.

Thus, the use of complex gelling agent agar – sodium alginate – calcium chloride in the technology of the "Chocolate marshmallow" cake allows you to reduce the recipe amount of agar by 50 % and obtain products with high quality indicators. In addition, the use of a complex gelling agent allows you to reduce the cost of products due to a decrease in the cost of the gelling agent.
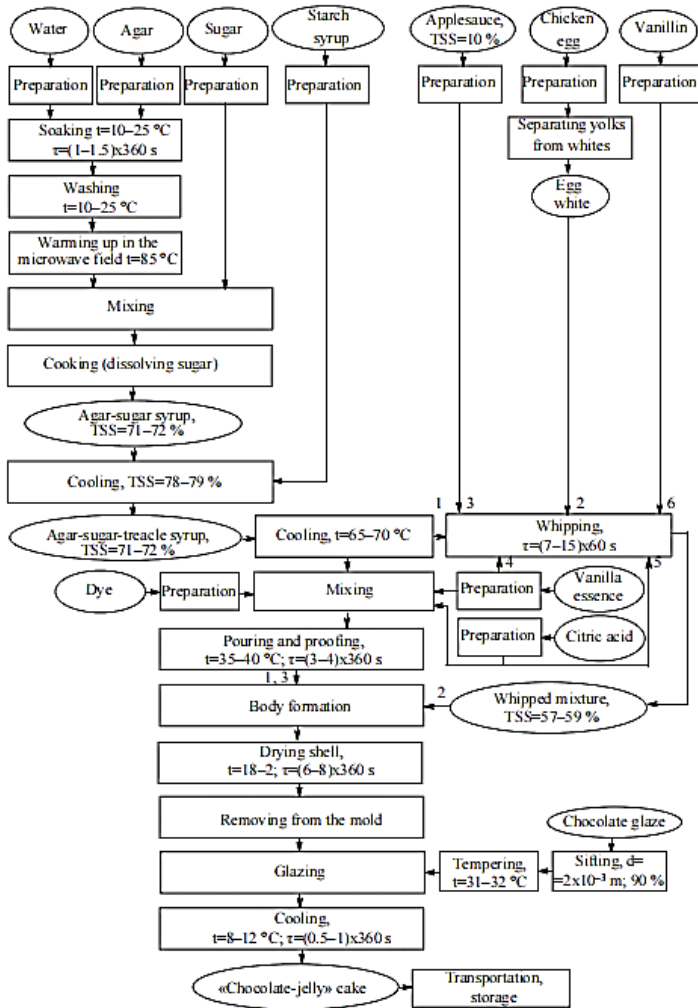
Fig. 3.2.1. Technological scheme for the production of the "Chocolate-marshmallow" cake based on a complex gelling agent

CONCLUSIONS

It has been proven that scientific substantiation, development and implementation of scientific and applied methods of adjusting the gelatinization process through the influence of various low-molecular additives, combining gelatinizers and the action of external electromagnetic

fields, allows to effectively use the resource and technological potential of structure formers of various origins, to create new innovative and competitive technologies of jelly products, enriched with physiologically functional ingredients, of improved quality with high consumption properties and extended shelf life.

The theoretical modeling of hydrogen bonds inside the spirals of the structure-former and between macromolecules of different structure-formers determined the mechanism of stabilization of molecules in an aqueous solution, which consists in the formation of stable hydrogen bonds between -NH groups of chains of one molecule and oxygen atoms of another. Quantum chemical calculations revealed the formation of two types of hydrogen bonds: strong (H…NH, OH…H) and weak (CH-OH), which makes the main contribution to the high dynamic stability of aggregates in aqueous solutions.

The molecular dynamic modeling of the process of formation of structures in aqueous solutions of gelatin and polysaccharides is substantiated. The potentials of the active groups of macromolecules were chosen, which made it possible to fully reproduce the structure of force interactions in solutions. It has been proven that the stability of molecules in the appropriate solution is achieved through the formation of up to 20 strong and 20…30 weak hydrogen bonds for every 9 nm of macromolecule length.

It was found that the treatment of solutions of structure-formers with an ultra-high frequency field leads to the strengthening of the structure of red seaweed polysaccharides. Defined processing modes that lead to the best structuring effect. A method of increasing the strength of sulfated polysaccharide gels and a method of producing a jelly cake with a 40 % reduction in the consumption of a structure former was developed.

The dependences of the strength of agar, furcellaran, and agaroid gels at different mass concentrations of sodium alginate and calcium chloride were established. It was determined that the combination of mass fractions of these components can vary the strength of gels within the range of 360…1020 g, depending on the purpose. For practical use, nomograms of the strength of gels made from red seaweed polysaccharides have been compiled, which serve as a basis for the development of jelly product technologies.

SUMMARY

The goal of our research was scientific substantiation of resource-saving technologies of jelly products, through the development and analysis of theoretical and empirical models of gel formation processes by structure-forming agents of various origin, under the influence of additives and external force fields.

In order to achieve this goal, we solved the following tasks:

– the properties of solutions and gels of red seaweed polysaccharides were studied, as well as the influence of various chemical additives and physical fields on the change of these properties;

– using the molecular dynamic modeling methods, a theoretical model of the process of structure formation in aqueous solutions of gel-forming agents of various origins was obtained;

– the influence of the ultra-high frequency field on the solutions of structure formers was studied with the aim of further targeted influence on the functional properties of jelly products (such as increasing the rate of structure formation, increasing strength and melting temperature, changing viscosity, etc.);

– technological conditions for the use of complex structure-formers for the purpose of obtaining jelly products with previously known properties are justified and experimentally confirmed;

– the new technologies for production of jelly products which allow to reduce the consumption of structure-forming agents of various origins are developed and scientifically substantiated.

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