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Impact of Dispersion Medium on Functional Properties of The Proteins.

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ABSTRACT

Possibility of directional regulation of the functional and processing properties of proteins and food mixtures on their basis has been shown based upon the results of molecular modeling and experimental research. It has been established that interaction between gelatins molecule and catholyte as compared with drinking water results in arrangement of structures at jellification, improvement in quality and structural-mechanical properties of the jells.

Keywords: molecular modeling, gelatin, jellification, the electrochemically activated water, catholyte.

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INTRODUCTION

In the modern food industry, the most widely presented biopolymers are the proteins, which, thanks to unique character of their molecular structures and functional properties, can fulfil a lot of necessary functions in production processes under development.

Functions that are specific to a polymeric nature of the proteins include their textural function which is characterized by ability of the biopolymers to various conformational changes, complex formation, adsorption at phase boundaries [1, 2, 3].

Previously, using the molecular modeling techniques, we determined a positive impact of the catholyte on hydratation and emulsifying capacity of α_{s1}-casein, the higher efficiency of using the dry milk protein products hydrated by electrochemically activated water as the emulsifiers and water-binding components was confirmed experimentally [4].

The purpose of the work was a further research of impact of the electrochemically activated water (catholyte) on functional properties of the proteins by means of molecular modeling, quantum-chemical calculations, and analysis of experimental results.

MATERIALS AND METHODS

Subject of research was a gelatin as one of the common food biopolymers, and "Aspik fest" complex dietary supplement on its basis from Frutarom Savory Solutions GmbH (Germany) designed to produce jellified foodstuffs.

Molecular modeling of intra- and intermolecular interactions in protein with dispersion aquatic medium during its jellification was conducting with Langevin dynamics method realized within HyperChem program [5, 6].

Critical gelation concentration was determining based on the results of evaluating a jell yield value (kPa). It was prepared a series of ten dispersions of the "Aspik fest" dietary supplement in distilled water and catholyte with concentration interval of 1%. Dispersions were mixed thoroughly and transferred to glass vials with volume of 10 ml. The vials were placed into heating block and allowed to stand for 30 minutes at 70-75°C, cooled with cold water down to room temperature, placed into refrigerator and allowed to stand for 1 hour at 4-6°C. Then the lead balls were placed at the jell surface. For critical gelation concentration at 4-6°C it was taken a concentration of dietary supplement which corresponds to a sample where there was no jell destruction under lead ball's pressure.

RESULTS AND DISCUSSION

At present it is found that in aqueous solutions the gelatin molecules when coming close are positioned relative each other in such a way that their oppositely charged centers coincide. The gelatin obtains a structure that reminds the collagen fibers [7, 8, 9] which is founded and becomes stable as a result of formation of the intersegment hydrogen bonds.

Therefore, one of the directions to improve quality of resultant jell, its structural and strength characteristics is using such external influences and media which will provide for qualitative increase of hydrogen bonds in the structure.

As a result of molecular modeling, it was found that in the gelatin molecule fragment under examination [10], the areas with high electron density are localized in end sections of amino-acid residues (Fig. 1). The highest electron density is typical for the end sections with oxygen atoms of glutamine acid with charge value of (-0.625), glycine (-0.420), hydroxyproline (-0.395) and arginine (-0.393). The amino-acid residues with high electro density form hydration shells at the expense of ion-dipole interaction with water dipoles [11].

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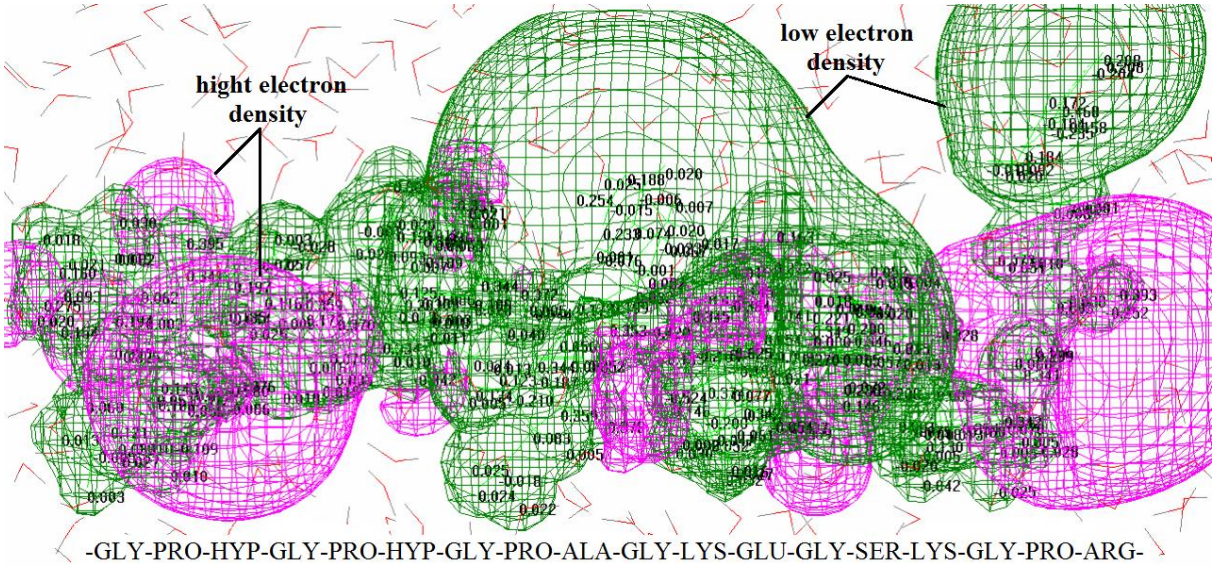

Figure 1: 3D map of electrostatic potential distribution of gelatin molecule fragment in drinking water (modeling by Langevin dynamics method)

Analysis of 3D map of electrostatic potential distribution on the surface of gelatin molecule fragment in drinking water as a result of system modeling by Langevin dynamics has shown (Fig. 1) that the most powerful centers of high electronic density are formed at -GLY-PRO- and -GLY-PRO-ARG- sections.

It was found that in comparison with the results of modeling performed using the drinking water, in catholyte the negatively charged area of electrostatic potential of molecule fragment decreases, and positively charged one increases substantially. The 3D map of electrostatic potential distribution as compared with counterpart for drinking water has more compact rod-like form of surface and more symmetric distribution of positive and negative charges (Fig. 2).

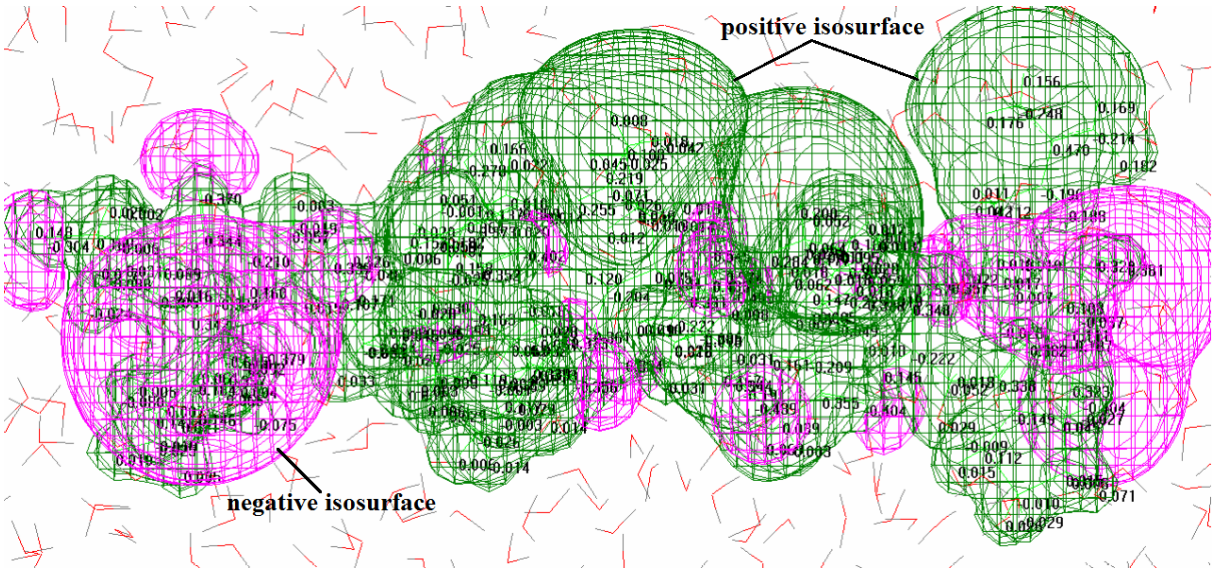

Figure 2: 3D map of electrostatic potential distribution of gelatin molecule fragment in catholyte (modeling by Langevin dynamics method)

Conducted modeling has shown that when forming the jell based on catholyte, a number of hydrogen bonds between investigated gelatin molecule fragment and water molecules increases by 1.3 times as compared with the results of modeling the jell on the basis of drinking water, and by 1.2 times in comparison

with initial state of gelatin-catholyte system. A number of intramolecular hydrogen bonds of gelatin in jell on the basis of catholyte increases by 1.4 times as compared with the jell based on drinking water.

The found results of increase in number of hydrogen bonds are consistent with the results of work [12].

Value of dipole moment of gelatin molecule fragment in catholyte (33.49 D) is by 1.5 times lover than in drinking water (50.35 D). In such a way, solubility of gelatin in catholyte is higher than in drinking water, and a structure of jell spatial grid is formed to the better energetic state.

The detected changes of main conformational characteristics of gelatin molecule fragment confirm its geometric restructuring which results in formation of more stable jells.

Data of conducted quantum-chemical researches have confirmed by the results of field experiments. Based on the preliminary studies, it was found that the gelatin product "Aspik fest" has higher gelling ability and forms strong jells at 1:10 hydration by drinking water. When concentration of gelling food additive hydrated in drinking water decreases, it was found a decreasing strength of resultant jells.

Results of determination of critical gelling concentration on gelling product under research (Fig. 3) have shown a decrease of this index for study sample by 1.2 times as compared with jells based on drinking water which is consistent with the results of molecular modeling.

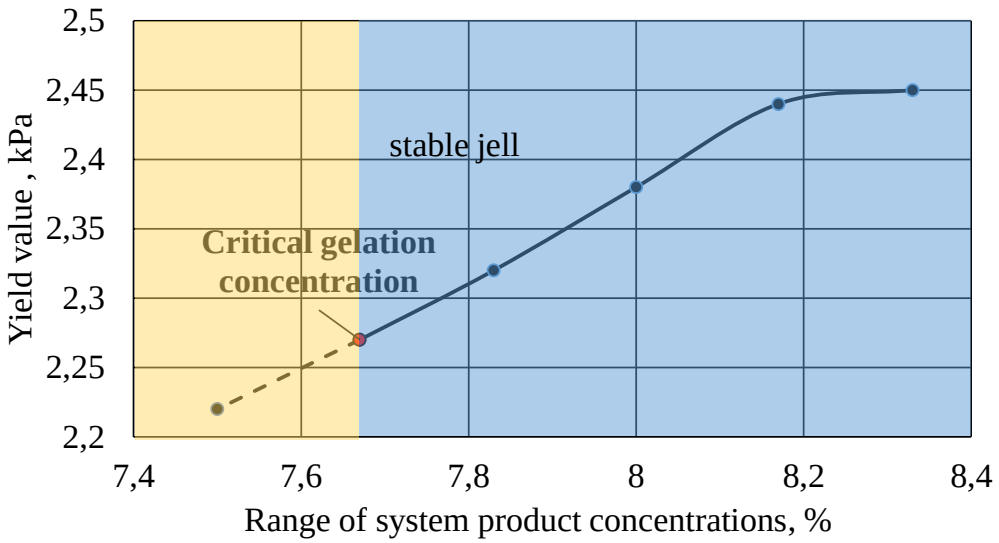

Figure 3: Critical concentration of gelling food additive "Aspik fest" in catholyte

A range of system product concentrations, at which jell breakdown under pressure of the lead ball was observed is indicated by dashed line on diagram (Fig. 3). Increase of "Aspik fest" concentration by more than 7.67% results in strengthening the system with formation of required consistency.

It was found that strength jells are formed at hydration of "Aspik fest" with catholyte in the ratio of 1:12. Thus, the results of experimental research confirm the conclusions resulted from molecular modeling about positive influence of catholyte on gelling of its protein-bearing systems.

CONCLUSION

Resulting from conducted computer modeling, it was found the existence of more clear division between areas with positive and negative potential on the surface of gelatin molecule using the catholyte and increase of uniformity in electronic density distribution as compared with using the drinking water, that results in arrangement of structures during gelling.

The obtained molecular modeling results allow to argue that realignment of gelatin molecules during catholyte-based jell structuring is characterized by specific distribution of charges and electrostatic potential. Stabilization of the structure under formation takes place in consequence of increase of number of intramolecular hydrogen bonds by 1.4 times.

The experimental research results have shown decrease of critical gelling concentration for gelatin-based food additive by 1.2 times as compared with the jells based on drinking water. So, to improve structural and mechanical properties of gelatinous jells, it can be recommended to use catholyte as a solvent.

Thus, complex of conducted researches which are presented in this article and have been earlier conducted [4] allows to recommend using the electrochemically activated water (catholyte) for directional regulation of functional and processing properties of the proteins and food mixture on their basis.

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