Innovative approaches to modeling the gerontological beverages composition

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Abstract. The article presents the results of the formulating gerontological beverages with high antioxidant activity. To determine the antioxidant activity a potentiometric method was used using the K3 [Fe (CN) 6] / K4 [Fe (CN) 6] mediator system. Drinks were prepared on the basis of whey with the addition of sea buckthorn, carrot juice, green tea extract, curcumin in water-soluble form in the composition of the compound stevioside-curcumin, aspartame, vitamin premix, yeast extract, natural flavor and milk whey. By mathematical simulation using the method of multicriteria optimization, a drink was chosen that has the best set of particular optimization parameters: 1.83 ± 0.03 mmol-eq / l, which is 10 times higher than the antioxidant activity of a drink without curcumin, the content of vitamin C is 40.3 ± 0.9 mg / 100 ml, acidity - 2.0 ± 0.1 cm3 1 M NaOH solution per 100 cm3.

1. Introduction
Aging is an important issue for humanity. The number of people is expected in the age of 60 and over to be more than double from 901 million in 2015 to more than 2.1 billion by 2050 [1, 2]. However, the risk of occurring diseases increases, working capacity decreases, so it requires the developing measures aimed at health promotion. One of the main factors affecting health is nutrition. Therefore, research on the development of food products intended for older people is particularly relevant [3]. According to the free radical theory of aging proposed by D. Harman, one of the main causes of age-related changes in the cells of the body is the accumulation of damage caused by free radicals [4, 5]. With age, the antioxidant system of the body loses its activity leading to an increase in the share of free radicals and increased oxidative damage to protein molecules, DNA, lipids [6, 7]. Therefore, it is advisable to include antioxidants and other ingredients that are rich in antioxidants and enhance their action in the gerontological formulation of food products.

On this basis, the purpose of this study is to develop formulations of beverages with high antioxidant properties and to conduct an assessment of the quality of the developed beverages using the generalized Harrington advisability function.

2. Experimental procedure

2.1 Equipment
Potentiometric measurements were carried out using a TA-Ion multifunctional pH meter / ionomer (NPP Tomianalit, Russia) using a two-electrode electrochemical cell (ECN), in which the silver chloride Ag |
AgCl | 3.5 M KCl type served as a reference electrode EVL-1M3.1 (GZIP, Belarus), and the indicator - a platinum screen-printed electrode (NSAID "IVA", Russia).

2.2 Modeling the beverage composition

Modeling recipes to determine the qualitative beverage composition, an analysis of the ingredients was carried out, taking into account their organoleptic comparability, functional orientation, solubility, and economic efficiency. The following components were included in the simulated beverage composition: sea buckthorn, carrot juices, green tea extract, water-soluble curcumin in the compound stevioside-curcumin, obtained according to [8], cottage cheese whey, vitamin premix 730/4 (Valetek, Russia), yeast extract “Pronadisa”, natural flavoring “Sea buckthorn” [9].

2.3 Determination of antioxidant activity

A potentiometric method was used, in which the source of information on the concentration of antioxidants is the shift of the potential of the platinum electrode, observed in the process of introducing a sample into the solution of the K3 [Fe (CN) 6] / K4 [Fe (CN) 6] mediator system, as a result of a chemical reaction between the antioxidants the sample and the oxidized form of the mediator system according to formula 1 [9]:

$$a \cdot [Fe(CN)_6]^{3-} + b \cdot AO = a \cdot [Fe(CN)_6]^{4+} + b \cdot AO_{ox}$$  

(1)

where AO is the antioxidant (s), AOox is the oxidation product (s) of the antioxidant (s). Antioxidant activity was calculated by the formulas (2–3):

$$AOA = \frac{C_{ox} - \alpha C_{Red}}{1 + \alpha}$$  

(2)

$$\alpha = \frac{C_{Red}}{C_{ox}} \cdot 10^{\frac{E1 - E}{nFRT}}$$  

(3)

where E is the initial potential of the mediator system, mV; E1 - the potential of the mediator system, established after the introduction of the sample, mV; n is the number of electrons in the electrode reaction (n = 1); F is the Faraday constant (96485,333 C / mol); R is the universal gas constant (8.314 J / mol • K); T - temperature in Kelvin, K.

The analysis algorithm was the following: 1) 3 ml of K-Na phosphate buffer solution with a pH of 7.2, containing the K3 [Fe (CN) 6] / K4 [Fe (CN) 6] mediator system, were introduced into the electrochemical cell; 01: 0.0001 M; 2) the working electrode and the reference electrode were immersed in the cell; 3) measured the initial potential of the mediator system (E1); 4) add the test sample; 5) measured the potential of the mediator system with the sample (E2); 6) carried out the calculation of antioxidant activity in accordance with formulas (2) - (3).

2.4 Statistical analysis

The results of determining the content of vitamin C, acidity and antioxidant activity are presented as the average value of the determined value ± confidence interval for three independent measurements at a significance level of 0.05.

2.5 Calculate Harrington’s generalized desirability function

The following optimization parameters were chosen as private parameters: antioxidant activity (in mmol-eq / l), vitamin C content (in mg / 100 g of drink) and acidity (in cm3 of 1 M NaOH solution per 100 cm3 of drink). The generalized desirability function of Harrington D was calculated as the geometric mean of the advisability of individual optimization parameters using the formula 4:
\[
D = \sqrt[d_1 \cdot d_2 \cdots \cdot d_q]
\]

where \( d_1, d_2, \ldots, d_q \) is the desired level of the 1st, 2nd, etc. optimization parameters (vary from 0 to 1).

The following one-sided restrictions were imposed on the optimization parameters: \( y_1 \geq 0.18 \text{ mmol-eq / l} \); \( y_2 \geq 13.5 \text{ mg / 100 g} \); \( y_3 \geq 2.0 \text{ cm}^3 \text{ 1 M NaOH solution per 100 cm}^3 \).

3. Results and discussion

Model beverage samples were developed: sample No. 1 (control) — without plant extracts, sample No. 2 and sample No. 3 — with 25% and 50% curcumin content from the recommended daily intake rate, respectively. Local functions of desirability were obtained for beverages prepared looking like:

\[
\begin{align*}
 d_1 &= \exp\left[-\exp\left(0.53 - 2.98 \cdot y_1\right)\right] \\
 d_2 &= \exp\left[-\exp\left(1.71 - 0.13 \cdot y_2\right)\right] \\
 d_3 &= \exp\left[-\exp\left(0.53 - 2.98 \cdot y_1\right)\right]
\end{align*}
\]

The drink prepared without the addition of extracts (Sample No. 1), is characterized by the worst set of particular optimization parameters. The particular desirability functions for each optimization parameter are presented in table 2.

| Sample | Antioxidant activity, mmol-eq / l | Vitamin C content, mg/100 g | Acidity, cm$^3$ 1 M NaOH solution per 100 cm$^3$ |
|--------|-----------------------------------|-----------------------------|--------------------------------------------------|
|        | \( y_1 \) | \( d_1 \) | \( y_2 \) | \( d_2 \) | \( y_3 \) | \( d_3 \) |
| Sample No 1 (without extracts) | 0.18±0,02 | 0.37 | 34.9±1,1 | 0.94 | 2.0±0.1 | 0.98 |
| Sample No 2 (25% curcumin) | 1.32±0,02 | 0.96 | 40.3±0,9 | 0.97 | 2.2±0.1 | 0.98 |
| Sample No 3 (50% curcumin) | 1.83±0,03 | 0.98 | 40.2±0,9 | 0.97 | 2.1±0.1 | 0.97 |

According to the data given in table 1, the generalized function of the advisability of beverage samples was calculated by the formula (4):

\[
\begin{align*}
 D_1 &= (0.37 \cdot 0.94 \cdot 0.98)^{1/3} = 0.67 \\
 D_2 &= (0.96 \cdot 0.97 \cdot 0.98)^{1/3} = 0.91 \\
 D_3 &= (0.98 \cdot 0.97 \cdot 0.97)^{1/3} = 0.97
\end{align*}
\]

Samples No. 2 and No. 3 have the highest value of the generalized advisability function. As can be seen from table 1, Sample No. 1 without the addition of plant extracts had the lowest value of antioxidant activity — 0.18 ± 0.02 mmol-eq / l. It was found that Sample No. 3 with 50% curcumin content from the recommended daily intake rate gives an increase in antioxidant activity by 38.6% compared with Sample No. 2 with 25% curcumin content from the recommended daily intake rate - 1.83 ± 0.03 and 1.32 ± 0.02 mmol-eq / l, respectively. Therefore, for the further modeling of the beverage composition sample number 3 was selected.

4. Conclusion
Gerontological beverage formulations with high antioxidant activity have been developed. The following particular parameters of advisability were chosen: antioxidant activity, vitamin C content and acidity. As a result of calculating the generalized advisability functions of Harrington, Sample No. 3 was selected, which has the best set of optimization parameters. It is established that the antioxidant activity is \(1.83 \pm 0.03 \text{ mmol-eq/l,}\) which is 10 times higher than the antioxidant activity of a drink without curcumin, the content of vitamin C is \(40.3 \pm 0.9 \text{ mg/100 ml,}\) the acidity is \(2.0 \pm 0.1 \text{ cm3 of 1 M NaOH solution per 100 cm3.}\)

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