Quality assessment and design of alcoholic beverages based on grain distillates

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Abstract. The article presents data on the method of quality assessment and the design of beverage recipes with the use of extracts of plant raw materials: oak, cherry and plum wood. The method includes establishing a correlation between physical-chemical and organoleptic indices of beverages and consumer properties with mathematical processing of experimental data and determining the optimal quantitative ratio of oak, plum and cherry wood extracts in blends, at which the beverage will have the maximum values of quality, organoleptic evaluation and "psychological price". The optimal mix of extracts is 0-7% of oak wood extract, 70-100% plum wood extract, 0-25% cherry extract. The "Consumer quality" indicator was over 0.9, organoleptic evaluation was over 9.25, "psychological price" was over 500 rubles/l.

1. Introduction
For the design of beverages based on grain distillates with a long stage of aging with oak wood it is appropriate to use extracts of processed wood of cherry and plums trees. Those extracts are characterized by stability of the composition [1, 6]. Wood extracts have several advantages, such as accessibility of natural raw materials and the low cost of industrial production [1, 8].

The method of designing alcoholic beverages started with the collection and analysis of consumer properties (organoleptic characteristics, safety and accessibility of beverages) [1, 4]. For beverages, ten physical and chemical characteristics (PCC) were chosen. For design we used physical-chemical and organoleptic characteristics of 13 alcoholic beverages, presented on the market, and beverages based on vegetative raw materials without blending [1].

2. Materials and Methods
The content of micro impurities in the distillate samples was controlled by gas chromatography according to GOST R 51762-2001, GOST 30536-2013, GOST 32039-2013. The identification of aromatic aldehydes and phenolic acids was carried out by the HPLC method, the device for sample introduction, the spectrophotometric detector (with variable wavelength) according to GOST 32195-2013. For the analysis of gallic acid and vanillin derivatives in water-alcohol extracts and beverages, the method of microcolumn HPLC was used [4]. The analysis was performed on Milichrome4 chromatograph with µ-Bondapak C18 column (2×120 mm), the particle size of ten microns. The total content of tannins in wood extracts was controlled by the permanganometry method. To determine the content of tannins containing phenolic -OH groups in the ortho-position, in terms of quercetin, the conductometric method was used [1, 4].
Sensor evaluation of the samples on the point scale was conducted under the requirements of GOST R 55313-2012.

Correlation analysis is performed using the STATISTICA 10 software.

3. Results and Discussion

We have found out that each of the samples was similar to the market analogs in its set of characteristics (Tables 1, 2). To get blends of alcoholic beverages with original organoleptic properties, which include the main characteristics of different types of wood (saturation, softness of taste, fruity, spicy tones with shades of vanilla), we make blends of cherry, plum and oak extracts. The number of extracts from different types of wood varied in blends.

Component concentrations were determined based on: 1. consumer requirements for the quality of the beverage; 2. predicted organoleptic evaluation of the beverage; 3. predicted "psychological" price of the beverage.

Table 1. Physico-chemical characteristics, organoleptic assessments and the cost of similar alcoholic beverages on the market

| Sample | Aldehydes, mg/l | Tannins, mg/l | Gallic acid, mg/l | Carbohydrates, mg/l | Furfurol, mg/l | Higher alcohols, mg/l | Ether, Aldehydes, mg/l | Organoleptic Score | Price per unit volume (ml), RUB |
|--------|----------------|---------------|------------------|---------------------|---------------|----------------------|-----------------------|------------------|----------------------|
| 1      | 10.12          | 1.01          | 0.110            | 0.180               | 12.0          | 1375                 | 234                   | 28.0             | 9.10                 | 320                  |
| 2      | 9.76           | 1.72          | 0.105            | 0.172               | 13.0          | 1420                 | 310                   | 28.0             | 9.10                 | 554                  |
| 3      | 14.00          | 1.95          | 0.150            | 0.163               | 12.0          | 1277                 | 276                   | 36.0             | 9.90                 | 620                  |
| 4      | 11.45          | 1.82          | 0.150            | 0.152               | 12.0          | 1304                 | 280                   | 31.5             | 9.45                 | 558                  |
| 5      | 9.75           | 1.22          | 0.130            | 0.158               | 5.0           | 1355                 | 254                   | 40.0             | 8.90                 | 326                  |
| 6      | 10.21          | 1.62          | 0.140            | 0.164               | 13.0          | 1606                 | 298                   | 39.0             | 9.30                 | 510                  |
| 7      | 13.10          | 1.36          | 0.140            | 0.168               | 12.0          | 1186                 | 213                   | 47.0             | 9.40                 | 500                  |
| 8      | 12.60          | 1.76          | 0.130            | 0.175               | 12.0          | 1432                 | 254                   | 43.6             | 9.40                 | 542                  |
| 9      | 11.20          | 2.4           | 0.110            | 0.163               | 14.0          | 2306                 | 272                   | 45.4             | 9.00                 | 294                  |
| 10     | 9.68           | 1.43          | 0.140            | 0.170               | 12.0          | 1514                 | 261                   | 52.2             | 8.61                 | 234                  |
| 11     | 13.00          | 1.80          | 0.150            | 0.180               | 16.3          | 1307                 | 278                   | 46.0             | 9.05                 | 298                  |
| 12     | 13.00          | 1.80          | 0.150            | 0.187               | 8.0           | 1220                 | 252                   | 43.3             | 9.00                 | 258                  |
| 13     | 14.00          | 1.93          | 0.150            | 0.210               | 3.1           | 1189                 | 244                   | 52.4             | 10.00                | 680                  |

Table 2. PCC and organoleptic score of oak, cherry and plum wood extracts

| Wood Extract | Aldehydes, mg/l | Tannins, mg/l | Gallic acid, mg/l | Carbohydrates, mg/l | Furfurol, mg/l | Higher alcohols, mg/l | Ether, mg/l | Aldehydes, mg/l | Organoleptic Score |
|--------------|----------------|---------------|------------------|---------------------|---------------|----------------------|------------|----------------|------------------|
| oak          | 31.6           | 3.10          | 0.42             | 0.42                | 16.7          | 1984                 | 136.3      | 12.3           | 8.95             |
| plum         | 22.8           | 2.53          | 0.24             | 0.39                | 12.6          | 1962                 | 127.2      | 13.9           | 10.00            |
| cherry       | 28.3           | 2.4           | 0.34             | 0.29                | 13.4          | 1971                 | 114.1      | 16.9           | 7.25             |

The source data for the correlation analysis are presented in Table 1. Pearson's correlation coefficients calculated by the formula were used to analyze the correlation between the characteristics of beverages:

\[ r_{xy} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{(n-1) \cdot \sigma_x \cdot \sigma_y}. \]
Here $r_{xy}$ is the correlation coefficient (the abbreviation $r$ is used); $n$ – amount of market analogs (in this case 13 samples); $x_i$ and $y_i$ – values of indicators between which the correlation is determined; $\bar{x}$ and $\bar{y}$ – average values of indicators; $\sigma_x$ and $\sigma_y$ – standard deviations of indicators.

Correlation coefficients $r$ for the investigated characteristics have been calculated. The closer the value of the correlation coefficient to a unit is, the stronger the two connected corresponding characteristics are [2, 3].

The analysis of the eight most significant correlations leads to the following conclusions. To improve the organoleptic evaluation and increase the price of the beverage it is necessary to increase the content of aldehydes ($r = 0.70$) and tannins ($r = 0.57$, $r = 0.56$). Therefore, the market analogs increase the content of aldehydes of tannins and gallic acid (correlation coefficients 0.63, 0.62, 0.59). We compared tables 1 and 2 and noted that beverages based on extracts of oak, plum and cherry have higher content of tannins and gallic acid than all analyzed market analogs. Therefore, beverages based on mix of the extracts will receive high organoleptic grades and have a higher "psychological price".

The content of higher alcohols ($r = -0.48$, $r = -0.27$) has a negative impact on organoleptic evaluation and the price of the beverage. As the content of higher alcohols increases, the content of aromatic aldehydes decreases ($r = -0.71$), which improves organoleptic evaluation and increases the cost of the beverage. As the content of higher alcohols increases, the content of esters increases either ($r = 0.53$), which increases the "psychological price" of the beverage ($r = 0.15$). The offered beverages based on extracts of oak, plums and cherries are inferior to market analogs in content of higher alcohols, aromatic aldehydes and esters.

The advantages of the designed beverages are increased content of carbohydrates (in comparison with market analogs) and the reduced content of aldehydes, which increases the "psychological price" of the beverage ($r = 0.12$ and $r = -0.20$), and increases organoleptic evaluation ($r = 0.39$ and $r = -0.05$). Organoleptic evaluation correlation coefficient with the beverage price – 0.89. The value of the correlation coefficient is close to 1, therefore the price of a beverage is almost proportional to the organoleptic evaluation. This means that the cost of alcoholic beverages on the market is determined not by the brand, but by the organoleptic qualities of the beverage.

Let's look at the method of testing the quality of beverages. According to the QFD method, the quality criterion is calculated based on comparison of consumer properties and PCC of the product [2]. Here, the criterion is built based on the concept of proximity of the PCC of the designed beverage to the average values of its market analogs:

$$Q(c_o, c_p, c_c) = \sum_{j=1}^{N_{PCC}} \left[ \frac{P_j(c_o, c_p, c_c) - P_{jP}}{P_{jP} - P_j} \right] \alpha_j m_j. \quad (2)$$

Here $Q$ is an intermediate quality criterion (the less $Q$, the better the product); $N_{PCC}$ - number of PCC; $i$ – number of consumer properties; $j$ – number of PCC; $P_j(C_o, C_p, C_c)$ – PCC for a beverage based on mix of extracts of oak, plum, cherry with concentrations of $C_o, C_p, C_c$; $P_{jP}$ – averaged PCC by analogs; $P_{jP}$ – averaged PCC by extracts; $N_{CP}$ – number of consumer properties; $\alpha_i$ – components of the matrix of relative importance of consumer properties; $m_{ij}$ – components of the matrix of coordination of consumer properties and PCC.

The characteristics of $P_{ij}$ for the designed beverage are defined as a linear combination of the corresponding characteristics of $P_{io}, P_{ip}, P_{ic}$ for oak, plum and cherry wood extracts:

$$P_{ij}(c_o, c_p, c_c) = c_o \cdot P_{io} + c_p \cdot P_{ip} + c_c \cdot P_{ic}. \quad (3)$$

The intermediate quality criterion is inconvenient for the analysis, therefore the quality criterion $Q$ is used:
\[ Q(C_o, C_p, C_c) = \max \frac{Q(C_o, C_p, C_c)}{Q(C_o, C_p, C_c)}. \]  

Here \( Q(C_o, C_p, C_c) \) is the maximum value of the intermediate quality criterion \( Q \).

Quality criterion it changes from 0 (at a considerable deviation of characteristics of a designed beverage from characteristics of market analogs) to 1 (at almost full coincidence of characteristics of a designed beverage and market analogs).

The design of beverages was carried out as a procedure for determining the optimal quantitative ratio of oak, cherry and cherry extracts in blends. Here, the beverage will have maximum values of \( Q \) quality, organoleptic evaluation \( OE \) and psychological price \( PP \) (Figure 1).

![Beverage design based on a combination of wood extracts](image)

**Figure 1.** Setting the task for the design of alcoholic beverages based on wood extracts

The design task can be presented as:

\[
\begin{align*}
Q(C_o, C_p, C_c) &\to \max; \\
OE(C_o, C_p, C_c) &\to \max; \\
PP(C_o, C_p, C_c) &\to \max.
\end{align*}
\]  

Calculation of the predicted \( OE \) for the combination of extracts was carried out based on known estimates for wood extracts of oak, plum, cherry:

\[ OE = c_o \cdot OE_o + c_p \cdot OE_p + c_c \cdot OE_c. \]  

Calculation of a beverage \( PP \) was carried out according to the following formula:

\[
PP = \frac{\sum_{j=1}^{N_{PP}} \beta_j \cdot PP_M[i \text{ if } |c_o - c_o, c_p - c_p, c_c - c_c| = \min]}{\sum_{j=1}^{N_{PP}} \beta_j}. 
\]  

Here \( \beta_j \) is an estimate of the PCC impact to the price of a beverage; \( PP_M \) is the price of a market analog. To reduce the number of parameters and to improve the validity, all weighting factors are assumed to be the same: \( \beta_j = 1/N_{PP} \).

For the analysis of the mathematical quality model, a software (Object Pascal) was created [5]. The developed software allows one to define the composition of a extracts mix, at which the maximum value of one criterion (quality, organoleptic evaluation or psychological price) is achieved, to get concentration dependencies of criteria in a double (Figures 3-5) and triple (Figures 6-7) combination of extracts.
First, the search for the best composition \((C_o, C_p, C_c)\) was carried out, where the quality criterion takes the maximum value. For this purpose, the program repeatedly (10,000,000 times) randomly generated the composition \((C_o, C_p, C_c)\) and calculated the criteria \(Q, OE\) and \(PP\). The option with the highest \(Q\) value was selected. Concentrations at the highest \(Q\) were: \(C_o = 9.02 \times 10^{-7}\); \(C_p = 0.597\); \(C_c = 0.403\). Other criteria had rather high values: \(OE = 8.89\); \(PP = 505\) RUB/l.

Thus, the maximum quality \((Q = 1)\) will have \((prediction)\) a beverage made from 59.7\% of plum wood extract and 40.3\% of cherry without oak wood extract.

Since oak wood extract is an important traditional component of alcoholic beverages, a mix of oak+plum extracts (Figure 2) and oak+cherry extracts (Figure 3) was analyzed.

![Figure 2. Impact of plum and oak wood extracts \((C_o = 100 - C_p; C_c = 0)\) on the qualitative and value indicators](image)

With the increasing content of plum wood extract in its combination with oak wood extract, the quality, organoleptic evaluation and "psychological price" of the beverage increase (Figure 2). Therefore, adding a plum to oak extract in any quantity leads to improved quality and value of the beverage. With a concentration of plum wood extract exceeding 85\%, very high indicators can be achieved: the consumer quality index exceeds 0.9, organoleptic evaluation exceeds 9.8 points, psychological price exceeds 500 RUB/l.

Analysis of the double combination of oak and cherry wood extracts led to the conclusion that such a combination, without plum wood extract, is not reasonable. The quality index exceeds 0.9 only in a narrow range of \(CB\) concentrations = 93-100\% (in a blend cherry extract, Figure 3, a). However, in this concentration range the organoleptic evaluation is too low (less than 7.5 points, Figure 3, b). Psychological price exceeds 500 RUB/l also for cherry wood extract only, without adding other extracts (Figure 3, c). Thus, the production of alcoholic beverages based on a double combination of oak and cherry wood extracts is not appropriate.

We analyzed the mix of plum and cherry wood extracts without oak wood extract. As the concentration of cherry wood extract increases, the organoleptic evaluation of the beverage increases (Figure 4, b), while the "psychological price" of the beverage does not change (Figure 4, c). The maximum quality of the beverage is achieved at \(C_p = 70\%\); \(C_c = 30\%\). The diagrams show concentration ranges, at which the quality criterion is not less than 0.9, organoleptic evaluation is not less than 9.25 points (average organoleptic evaluation of market analogs), price is not less than 500 RUB/l. The range of concentrations \(C_p = 73-100\%;\) \(C_o = 0-27\%\) corresponds to all these conditions.
Thus, a beverage based on cherry and plum wood extracts, with the content of plum wood extract over 73% of the beverage, will have (predicted) $Q$ over 0.9, $OE$ over 9.25, $PP$ over 500 RUB/l.

The triple combination of extracts was analyzed as well. Criteria for 21 variants of blends have been calculated, in which the concentrations of components changed with 10% step (Table 3). The maximum values of the criteria (cells are highlighted) are achieved at low concentration of oak wood extract (less than 10%), plum wood extract over 60–100% and cherry wood extract – 0–40%.

Table 3. Results of beverage design based on combinations of oak, plum and cherry wood extracts

| $C_{pp}$, % | 0 | 20 | 40 | 60 | 80 | 100 |
|-------------|---|----|----|----|----|-----|
|             | $Q$ = 0.468 | $Q$ = 0.588 | $Q$ = 0.621 | $Q$ = 0.717 | $Q$ = 0.826 | $Q$ = 0.945 |
|             | $OE$ = 8.95  | $OE$ = 8.61  | $OE$ = 8.27  | $OE$ = 7.93  | $OE$ = 7.59  | $OE$ = 7.25  |
|             | $PP = 473$  | $PP = 473$  | $PP = 473$  | $PP = 473$  | $PP = 473$  | $PP = 505$  |
|             | $Q$ = 0.550  | $Q$ = 0.636  | $Q$ = 0.736  | $Q$ = 0.850  | $Q$ = 0.975  |               |
|             | $OE$ = 9.16  | $OE$ = 8.82  | $OE$ = 8.48  | $OE$ = 8.14  | $OE$ = 7.80  |               |
|             | $PP = 473$  | $PP = 473$  | $PP = 473$  | $PP = 473$  | $PP = 505$  |               |
|             | $Q$ = 0.646  | $Q$ = 0.749  | $Q$ = 0.866  | $Q$ = 0.994  |               |               |
|             | $OE$ = 9.37  | $OE$ = 9.03  | $OE$ = 8.69  | $OE$ = 8.35  |               |               |
|             | $PP = 473$  | $PP = 473$  | $PP = 473$  | $PP = 505$  |               |               |
|             | $Q$ = 0.754  | $Q$ = 0.871  |               | $Q = 1.000$  |               |               |
|             | $OE$ = 9.58  | $OE$ = 9.24  |               | $OE = 8.90$  |               |               |
|             | $PP = 472$  | $PP = 472$  |               | $PP = 505$  |               |               |
|             | $Q$ = 0.868  | $Q = 0.993$  |               |               |               |               |
|             | $OE$ = 9.79  | $OE = 9.45$  |               |               |               |               |
|             | $PP = 505$  | $PP = 505$  |               |               |               |               |
|             | $Q = 0.974$  |               |               |               |               |               |
|             | $OE = 10.00$ |               |               |               |               |               |
|             | $PP = 505$  |               |               |               |               |               |
From Table 3 analytical formulas for calculation of $Q$, $OE$ and $PP$:

$$
Q(C_p, C_c) = 9.271 \times 10^{-6} \cdot C_p^2 + 1.579 \times 10^{-5} \cdot C_c^2 + 3.905 \times 10^{-5} \cdot C_p \cdot C_c + 4.205 \times 10^{-3} \cdot C_p + 3.228 \times 10^{-3} \cdot C_c + 0.465 \quad (8)
$$

$$
PP(C_p, C_c) = 8.735 \times 10^{-3} \cdot C_p^2 + 9.539 \times 10^{-3} \cdot C_c^2 + 0.015 \cdot C_p \cdot C_c - 0.571 \cdot C_p - 0.726 \cdot C_c + 480. \quad (9)
$$

The surface plot for visual pattern is shown in Figure 5. For practical use, these dependencies have been rearranged in the form of flow charts (Figure 6). On the flow charts the highlighted areas are for higher criteria ($Q$ – over 0.9, $OE$ – over 9.25, $PP$ – over 500 RUB/l). In Figure 6, the intersection of optimum areas is shown, giving the overall optimum area. The optimal mix is $C_o = 0–7\%$; $C_p = 70–100\%$; $C_c = 0–25\%$.

![Figure 5. Surface plots of the triple combination of oak, plum, cherry wood extracts](image)

![Figure 6. Flow charts of triple combinations of oak, plum and cherry wood extracts](image)

The black color highlights the overall optimal area for the percentage of extracts. The optimal composition of the combination of extracts should be 0–7% of oak wood extract, 70–100% of plum wood extract, 0–25% of cherry extract. At the same time the beverage will have (predicted) $Q$ over 0.9, $OE$ over 9.25, $PP$ over 500 RUB/l.

4. Conclusion

A system for quality assessment of alcoholic beverages with the calculation of quality criteria has been developed. A method for designing alcoholic beverages based on wood extracts mix has been proposed. The flow charts are presented. The recommended ratios of extracts have been calculated: up to 7% of oak wood extract, 70–100% of plum wood extract, up to 25% of cherry wood extract. A software in Object Pascal language was compiled in the Borland Delphi 7. Software allows one to define the structure of the extracts mix. The maximum value of one criterion (quality, organoleptic evaluation or "psychological price") is observed in the blend.

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