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Grey Dominance Evaluation of Neutral Fragrance Components and Sensory Quality in Flue-Cured Tobacco

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In order to discuss the relative importance of neutral fragrance components in the evaluation system of tobacco leaf quality, 140 samples of aging flue-cured tobacco leaf from the tobacco growing areas in southwest China produced in 2006 were selected for study. The furfural, furancarbinol, 2-furyl methyl ketone, 5-methyl-furfural, benzaldehyde, 6-methyl-5-heptene-2 ketone, benzyl alcohol, phenyl acetaldehyde, 2-acetyl pyrrole, linalool, phenethyl alcohol, indole, solanone, β-damascone, dihydro damascenone, β-ionone, geranyl acetone, dihydroactinidiolide, megastigmatrienone neophytadiene and farnesyl acetone and sensory quality of all samples were tested in the paper. Then we use grey dominance evaluation method to assess the relative importance of each index of neutral fragrance components from the aspect of aroma characteristics and taste characteristics of neutral fragrance components and sensory characteristics and the results showed that: substances imposing a relatively great impact on the aroma characteristics of the sensory quality were respectively geranyl acetone, dihydroactinidiolide, megastigmatrien-one and furancarbinol, *etc.*, which constituted major factors that affected this characteristics. As for substances imposing a relatively great impact on the taste characteristics of the sensory quality were respectively geranyl acetone, dihydroactinidiolide, indole and megastigmatrienone *etc.*, as major factors that affected this characteristics. Neophytadiene has a relatively weak impact on two characteristics of the sensory quality, as a secondary factor affecting the aroma and taste characteristics of the sensory quality. The use of grey dominance evaluation is effective to identify the neutral fragrance components indicators, which can be then brought in the tobacco leaf quality evaluation index system.

Key Words: Neutral fragrance components, Grey dominance evaluation, Aroma characteristics, Taste characteristics, Quality evaluation.

INTRODUCTION

The chemical components of tobacco directly impose impact on its quality. In combination with the physiological structure of flue-cured tobacco, the chemical components affects the sensory characteristics, physiological effect, appearance, economy of production and impact on health. Commercial production of cigarettes requires maintenance of a stable formula and improvement of quality. Therefore, the relationship between the chemical components and tobacco quality needs to be clearly defined[1]. However, chemical components in tobacco leaf are so complex that according to Roberts, the total number of chemical components in tobacco leaf and smoke is 5,868, including 1,872 kinds of tobacco-specific components, as well as 1,172 kinds of shared components of tobacco leaf and smoke[2]. At present, there are dozens of neutral fragrance components indexes in tobacco leaf study, presenting a complexly interrelated and mutually opposite relationship. Thus, it is difficult to grasp all the information among them.

The sample sizes in grey system analysis are typically small and there is a high level of uncertainty in the information available for the samples. Systems like these are difficult to solve with probability statistics and fuzzy mathematics. Grey systems analysis seeks to find realistic rules for these systems by sequence generation from the information that is available. Consequently, grey systems analysis typically involves modeling with little information. Grey system theory is different from fuzzy mathematics because it focuses on systems where the extended application is clear but information required for the calculation is not. As a scientific method to solve uncertain and semi-complex problems, grey system theory provides a different approach to probability statistics and fuzzy mathematics. The application of grey system theory to tobacco quality assessment is valuable because a lot of the information required for accurate determination of tobacco quality is unknown[3].

Massive indicators not only increase the difficulty of tobacco quality analysis and comprehensive quality assessment, but also hinder the determination of suitable areas for chemical components of tobacco as well as the selection of raw materials of tobacco leaf recipes. Previous studies evaluated the relative importance of chemical components with grey statistical analysis approach and grey correlation cluster approach respectively. Thus, determining indicators with relatively great significance while simplifying the number of the chemical components indicators[4,5]. But none of the studies conducted evaluation of the importance of each indicator of the neutral fragrance components from the aspects of the relationship between neutral fragrance components and the aroma and taste characteristics of sensory quality. With the use of grey dominance evaluation approach, the paper studied the relationship between neutral fragrance components and the aroma and flavour taste characteristics of sensory quality and probed into the relative importance of each indicator of neutral fragrance components in cured tobacco from the perspective of sensory quality and aimed at establishing a tobacco quality evaluation index system.

EXPERIMENTAL

One hundred and forty samples of the flue-cured tobacco that had been produced in 2006 and stored at Chuanyu Industrial Corporation (Chengdu, China) were analyzed. These samples were grown in a tobacco planting area in Southeast China.

For chemical components of neutral fragrance (furfural, furancarbinol, 2-furyl methyl ketone, 5-methyl furfural, benzaldehyde, 6-methyl-5-heptene-2 ketone, benzyl alcohol, phenyl acetaldehyde, 2-acetyl pyrrole, linalool, phenethyl alcohol, indole, solanone, β-damascone, dihydro damascenone, β-ionone, geranyl acetone, dihydroactinidiolide, megastigmatrienone, neophytadiene and farnesyl acetone), the detection was conducted according to the previous report[6]. Sensory sample test smoking was conducted. The sensory quality (aroma and taste characteristics) was evaluated according to the "nine sensory characteristics" for unblended cigarette test smoking. The nine sensory characteristics were evaluated on a scale of 1-9 as follows: aroma mass, 1 (= very bad) to 9 (= very good); amplitude, 1 (= rich) to 9 (= very thin); smoke strength, 1 (= very thick) to 9 (= very thin); irritancy, 1 (= very slight) to 9 (= very strong); offensive taste, 1 (= very slight) to 9 (= very heavy); impact, 1 (= very strong) to 9 (= very slight); aftertaste represent, 1 (= very good) to 9 (= very bad); ease of lighting, 1 (= very good) to 9 (= very bad); colour of ash, 1 (= white) to 9 (= black).

RESULTS AND DISCUSSION

We conducted neutral fragrance components detection of the flue-cured tobacco samples that had been stored at Chuanyu Industrial Corporation (Chengdu, China) and were grown in Southeast China in a tobacco planting area of the Chuanyu Industrial Corporation.

Absolute grey correlation matrix

Data Standardization: First, the original data (x_{ij}) were standardized according to:

$$x'_{ij} = \frac{x_{ij}}{\bar{x}_j}$$

where, x'_{ij} represents the data after standardization and $\bar{x}_j$ represents the mean of j indicators.

The annihilation operator of the initial point with respect to each index of the chemical composition was used to obtain S_i, (S_j) and $|S_j - S_i|$.

Suppose that there were n objects and m indices, the original data sequence was obtained:

$$\begin{cases} x_1 = (x_1^{(1)}, x_1^{(2)} \ldots, x_1^{(n)}) \\ x_2 = (x_2^{(1)}, x_2^{(2)}, \ldots, x_2^{(n)}) \\ \vdots \\ x_m = (x_m^{(1)}, x_m^{(2)}, \ldots, x_m^{(n)}) \end{cases}$$

The annihilation operator of the initial point with respect to the original data sequence was:

$$\begin{cases} x_1^0 = (x_1^0(1), x_1^0(2) \ldots, x_1^0(n)) \\ x_2^0 = (x_2^0(1), x_2^0(2), \ldots, x_2^0(n)) \\ \vdots \\ x_m^0 = (x_m^0(1), x_m^0(2), \ldots, x_m^0(n)) \end{cases}$$

where,

$$x_i^0(k) = x_i(k) - x_i(1)$$

resulted in,

$$|s_i| = \left| \sum_{k=2}^{n-1} x_i^0(k) + \frac{1}{2} x_i^0(n) \right|$$

$$|s_j| = \left| \sum_{k=2}^{n-1} x_j^0(k) + \frac{1}{2} x_j^0(n) \right|$$

$$|s_j - s_i| = \left| \sum_{k=2}^{n-1} (x_j^0(k) - x_i^0(k)) + \frac{1}{2}(x_j^0(n) - x_i^0(n)) \right|$$

Each chemical composition indicator of the targeted sample serves as a characteristic column and each chemical composition indicator of the potential substitute sample as a factor column. The grey absolute incidence degree between the targeted and substitute samples was calculated using:

$$r_{ij} = \frac{1 + |s_j| + |s_i|}{1 + |s_j| + |s_i| + |s_j - s_i|}$$

Sequencing was conducted on the basis of the grey absolute incidence degree to obtain the incidence sequence of all the evaluated samples and the targeted object. This was used to determine the similarities among the evaluated samples and the targeted sample.

The sensory quality was taken as the characteristic set and various chemical compositions of other objects were taken as factor column. According to $r_{ij} = \frac{1 + |s_j| + |s_i|}{1 + |s_j| + |s_i| + |s_j - s_i|}$, the absolute grey correlation analysis of the target object and other objects were calculated.

The sensory quality (aroma mass, amplitude, offensive taste, after taste and irritancy) were listed as the characteristic set and as the chemical compositions of the neutral fragrance were taken as factor set. According to the above formula, the absolute gray correlation of sensory quality and various indexes of chemical compositions of neutral fragrance could be calculated, generating the absolute grey correlation matrix. The results were shown in Table-1.

TABLE-1
ABSOLUTE GRAY CORRELATION MATRIX OF SENSORY QUALITY AND NEUTRAL FRAGRANCE COMPOSITIONS

Neutral fragrance compositions	Aroma mass	Amplitude	Offensive taste	After taste	Irritancy
Furfural	0.5467	0.5702	0.5275	0.5492	0.5543
Furancarbinol	0.8248	0.9887	0.6916	0.8423	0.8780
2-Furyl methyl ketone	0.6272	0.5845	0.7156	0.6207	0.6093
5-Methyl furfural	0.8652	0.7428	0.9038	0.8466	0.8139
Benzaldehyde	0.5999	0.5664	0.6693	0.5948	0.5858
6-Methyl-5-heptene-2 ketone	0.6134	0.5754	0.6922	0.6076	0.5974
Benzyl alcohol	0.6241	0.6868	0.5732	0.6308	0.6444
Phenylacetaldehyde	0.7925	0.9401	0.6726	0.8082	0.8404
2-Acetyl pyrrole	0.5340	0.5226	0.5576	0.5323	0.5292
Linalool	0.6982	0.6317	0.8359	0.6881	0.6703
Phenylethanol	0.7553	0.8841	0.6506	0.769	0.7971
Indole	0.9421	0.7939	0.8336	0.9196	0.8799
Solanone	0.5416	0.5626	0.5245	0.5438	0.5484
β-damascone	0.5782	0.6176	0.5461	0.5824	0.5910
Dihydro damascenone	0.7242	0.8373	0.6323	0.7362	0.7609
β–ionone	0.6036	0.5689	0.6756	0.5983	0.5890
Geranyl acetone	0.9718	0.8522	0.7783	0.9971	0.9554
Dihydroactinidiolide	0.9464	0.8722	0.7634	0.9704	0.9813
Megastigmatrienone	0.8983	0.9172	0.7350	0.9197	0.9635
Neophytadiene	0.5037	0.5056	0.5022	0.5039	0.5043
Farnesyl acetone	0.5585	0.5881	0.5345	0.5617	0.5681

Grey eominance evaluation: Set $Y_i(i = 1,2,...,s)$ as system characteristic behaviour series, $X_j(j = 1,2,...,m)$ as a sequence of related factors,

$$\Gamma = (\gamma_{ij}) = \begin{bmatrix} \gamma_{11} & \gamma_{12} & \cdots & \gamma_{1m} \\ \gamma_{21} & \gamma_{22} & \cdots & \gamma_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ \gamma_{s1} & \gamma_{s2} & \cdots & \gamma_{sm} \end{bmatrix}$$

as absolute grey correlation matrix; if $l,j \in \{1,2,...,m\}$ exists and $\gamma_{il} \geq \gamma_{ij}, i = 1,2,..., s$ was met, X_t was regarded as system factors, prior to X_j, denoted as $X_l \succ X_j$. If $\forall j = 1,2,..., m, j \neq l$, it always has $X_l \succ X_j$ and X_l was called the optimal factor; if $l \in \{1,2,...,m\}$ exists, make $\forall j = 1,2,..., m, j \neq l$, it is subject to $X_l \succeq X_j$ and X_l was regarded as a quais-priority factor.

Based on the absolute grey correlation matrix, dominance factors of aroma (aroma mass, amplitude and offensive taste) and taste (after taste and irritancy) characteristics in sensory quality affected by various indicator systems of neutral fragrance compositions were calculated in accordance with the above-mentioned grey dominance evaluation formula. Results were presented in Table-2.

The degree of the dominance values of various indicators in Table-2 indicates the influential degree of different compositions on aroma and taste characteristics. According to the size and sequence of the dominance values of various indicators, the significance degree of the impact from individual indicator on sensory quality can be analyzed.

TABLE-2
DOMINANCE FACTORS IN VARIOUS INDEX SYSTEMS OF NEUTRAL FRAGRANCE COMPOSITIONS THAT AFFECT THE SENSORY QUALITY

Aroma characteristics		Taste characteristics	
Dominance Indicators	Dominance Value	Dominance Indicators	Dominance Value
Geranyl acetone	1.8240	Geranyl acetone	2.7308
Dihydroactinidiolide	1.8186	Dihydroactinidiolide	2.7150
Megastigmatrienone	1.8155	Indole	2.6331
Furancarbinol	1.8135	Megastigmatrienone	2.6182
Indole	1.7360	5-Methyl furfural	2.5643
Phenylacetaldehyde	1.7326	Furancarbinol	2.4118
Phenylethanol	1.6394	Phenylacetaldehyde	2.3211
5-Methyl furfural	1.6080	Phenylethanol	2.2167
Dihydro damascenone	1.5615	Linalool	2.1942
Linalool	1.3299	Dihydro damascenone	2.1294
Benzyl alcohol	1.3109	2-Furyl methyl ketone	1.9456
2-Furyl methyl ketone	1.2117	6-Methyl-5-heptene-2 ketone	1.8972
β-Damascone	1.1958	β-Ionone	1.8629
6-Methyl-5-heptene-2 ketone	1.1887	Benzaldehyde	1.8499
β-Ionone	1.1724	Benzyl alcohol	1.8485
Benzaldehyde	1.1663	β-Damascone	1.7195
Farnesyl acetone	1.1466	Farnesyl acetone	1.6643
Furfural	1.1169	Furfural	1.6310
Solanone	1.1041	2-Acetyl pyrrole	1.6191
2-Acetyl pyrrole	1.0566	Solanone	1.6167
Neophytadiene	1.0093	Neophytadiene	1.5104

From the significance of the tobacco chemistry, tobacco carbonyl compounds were one essential component of tobacco oil. Carbonyl groups in aldehydes and ketones are the aroma groups and most are important aroma components[6]. Geranyl acetone belongs to unsaturated carbonyl compounds in tobacco structure and can give smoke aroma and enhance the aroma density of smoke. Megastigmatrienone is one of the major components that generate the aroma of tobacco essential oils[7]. Dihydroactinidiolide is azalides material of tobacco, sending out stronger aroma than acid and alcohol and serving the role of eliminating the stimulation in tobacco. Furancarbinol is the alcoholic compound of tobacco, endowing the smoke with the aroma of grain and oil, thus enhancing the density of smoke aroma. Indole is the fused nitrogen-containing fused ring compound by benzene ring and pyrrole ring, sending out elegant fragrance of a flower. From the results of dominnance analysis of neutral fragrance components in Table-2, materials with relative great impact on the aroma characteristics of sensory quality are respectively geranyl acetone, dihydroactinidiolide, megastigmatri-enone and furancarbinol and so on; materials with relative great impact on the taste characteristics of sensory quality are respectively geranyl acetone, dihydroactinidiolide, indole and megastiigmatrienone *etc*. Neophytadiene has a relatively small impact on the aroma and taste characteristics of sensory quality, thus serving as a secondary factor. The size of dominance value is consistent with analysis of tobacco chemical significance of these components.

Conclusion

Purely from the perspective of tobacco chemistry, some indicators were found to have greater impact on sensory quality of tobacco. Yet, according to the analysis of this paper, relatively small dominance evaluation values were found, which may be related to the limitations of experiments in the study. As samples were taken from Chuanyu Industrial Corporation (Chengdu, China) grown in Southeast China in a tobacco planting area of the Chuanyu Industrial Corporation., this may made an inconsistence with compositions of samples from large growing bases and other growing areas. Yet, with the means of the dominance analysis approach, as well as the integration with the actual samples of the tobacco base of our Company, factors with important impact on the sensory quality of tobacco leaves can be selected and indicators selected can be included in the quality evaluation index system.

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