Chemical Composition Characteristics and Usability Evaluation of Flue-cured Tobacco Leaves – A Case Study of Tobacco-producing Areas in Chongqing Municipality, China

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Abstract—The market of Chongqing flue-cured tobacco always lacks a relatively perfect evaluation of its quality objective system. In order to solve the mentioned problem, this paper will carry on the appraisal to the chemical of flue-cured tobacco and availability. There are nine main tobacco-producing districts in Chongqing municipality, China. We divided them into three type regions due to the geographic features; 234 flue-cured tobacco samples of Yunyan87 (including B2F, C3F, X2F) had been collected in 2014 to test the content of total sugar, reducing sugar, nicotine, total nitrogen, potassium and chlorine. Besides, its feature was evaluated at the same time. The results showed that:(1) The contents of total sugar and reducing sugar and the ratio of nitrogen/alkali of Yunyan 87 in the samples were relatively higher, while the potassium and chorine were relatively lower, the ratio of potassium/chorine was higher with larger variation, however, the other chemical compositions and ratios were all within proper ranges.(2) The contents and ratios of chemical compositions differed significantly between the samples from different classes and geological landforms.(3) The class indexes of chemical compositions from high grade to low gradewear: C3F, B2F, X2F; and the usability indexes of chemical compositions in different geology and landformwere: the northeast area of Chongqing, the southeast area of Chongqing, the central area of Chongqing. Therefore, the characteristics of chemical compositions and usability of flue-cured tobacco differed from different geological and landforms in Chongqing tobacco planting areas.

Keywords—flue-cured tobacco; Yunyan87; chemical composition; geology and landform; usability

I. INTRODUCTION

Nowadays, the individualities of tobacco materials are strongly a market demand, especially for the stability, the homogeneity and compositeness of the raw material. In the course of acquisitions, the main good evidences of the leaf tobacco are the appearances and physical properties. Therefore, in this study we need to analyze on internal quality of tobacco leaves in different districts to ensure the characteristics orientation of quality style and to guarantee the similarity of external and internal quality, which has a vital significance to satisfy with the development of cigarette brand and to promote by the supply of tobacco and improve the characteristics of tobacco leaf quality [1, 2].

The evaluation of tobacco quality is, traditionally, identified by testing the sample [3]. But the data is not clear. Furthermore, in some extent, it is easily influenced by assessors. While the quality of tobacco leaves is decided for the content of chemical compositions, which are seriously influenced by the appearance quality of flue-cured tobacco leaves and so on [4]. The usability of flue-cured tobacco is directly decided by the process of making tobaccos, and the value of flue-cured tobacco is also depending on the classification of sample quality evaluation [5, 6]. The existed researches [7, 8] have studied the climate of tobacco area and the soil factors, but there are hardly researches about the classification of geological features in Chongqing tobacco areas and analyses on the chemical composition of tobacco in Chongqing. Therefore, in this paper the quality of chemical composition of Yunyan87 in Chongqing tobacco...
areas will be studied. In order to get quantified and comply with the industrial availability indexes, these will become comprehensive evaluation of chemical compositions of tobacco leaf in different geological features.

II. MATERIALS AND METHODS

A. Studies regions

Chongqing is located in the upper reaches of the Yangtze River, the southeast of Sichuan. The tobacco planting areas are mainly distributed in the eastern area where have less pollution in the Wuling Mountain and in the Three Gorges Reservoir Area. Its position is longitude 106°23′-110°11′degree east, and locate in latitude 28°09′-31°44′ degrees north. In 2014, pilot studies were selected in the nine major tobacco planting districts of Chongqing. According to the geological features in the 9 districts, there would be divided into 3 areas. The northeast area of Chongqing, including Wushan and Wuxi, have more terrains, and in the Karst landforms there are stone forest, Karst valley, funnels and the stoneholes in the geography. The southeast area of Chongqing, including Pengshui, Qianjiang and Youyang, are mainly distributed along the river to the II terraces which are preserved well. Also, the II terrace has a small slope at the ground and is higher than the surface of the river. But the II terrace is not preserved well because of the erosion. The central area of Chongqing, including Nanchuan, Wulong, Fengdu and Shizhu, are the hilly terrain with narrow valley. The geographical position is shown in Figure 1.

B. Samples

The variety of trial in Chongqing tobacco planting areas mainly are Yunyan87. Selected in the tobacco fields where contain fecund soil. In order to guarantee representation of the samples, grading would be used by the sampling method. A total of 234 flue-cured tobacco samples were collected, divided into 3 categories. In the Southeast area of Chongqing includes 44 flue-cured tobacco samples which have 14 samples of B2F, 16 samples of C3F and 14 samples of X2F. In the northeast area of Chongqing includes 118 flue-cured tobacco samples which have 37 samples of B2F, 44 samples of C3F and 37 samples of X2F. In the central area of Chongqing includes 72 flue-cured tobacco samples which have 27 samples of B2F, 19 samples of C3F and 26 samples of X2F. The mentioned above measures have passed 85% in qualification rate. Each portion weighed 3.0kg to analyze on main chemical compositions.

C. Experimental Methods

1) Index Test

After the samples were exposed to mini cyclone, it would be scanned by infrared spectroscopy in the Near Infrared of the MPA (Bruker, Germany). It is using Near Infrared Prediction Model to calculate the quantitative data regarding the content of total sugar, reducing sugar, nicotine, total nitrogen, potassium and chlorine [9]. Then, it also can be calculated in the ratio of nitrogen/nicotine, the ratio of total sugar/nicotine and the ratio of potassium/chlorine of Yunyan87 in the samples. The Descriptive Statistics, Membership Function [10] and Principal Components [11,12] are used to analyze on participating indicators and to calculate the Chemical compositions Usability Index (CCUI) of flue-cured tobacco in order to confirm a comprehensive evaluation on chemical compositions of flue-cured tobacco.
2) Statistics methods

SPSS 17.0 [13] and EXCEL would be used to test results, and Multiple Comparisons are analyzed for Duncan’s New Multiple Range method.

III. RESULTS AND DISCUSSION

A. Descriptive statistics analysis of chemical compositions

It’s widely acknowledged that suitable content range of chemical compositions of flue-cured tobacco is about 18% and 22% for total sugar, 16% and 20% for reducing sugar, 1.5% and 3.5% for nicotine and total nitrogen, 0.3% and 0.8% for chlorine, more than 2% for potassium, 8 and 12 regarding the ratio of total sugar/nicotine, approximately 1 for the ratio of nitrogen/alkali, more than 4 for the ratio of potassium/chlorine [2, 14]. According to Table I, chemical composition variation coefficients of the general trend are chlorine, potassium, nicotine, total sugar, reducing sugar, total nitrogen. On the table of the narrative, Yunyan87 of tobacco are all in the range of requirement, including total nitrogen, nicotine, the ratio of total sugar/nicotine, the potassium/chlorine. While, the total sugar, reducing sugar and the ratio of nitrogen/alkali is slightly higher than the requirement of the flue-cured tobacco. And the chlorine ion and potassium ion is slightly lower than the average value. Among them, the variation of chlorine ion, the ratio of total sugar to nicotine and the potassium ion are considered. What’s more, it also shows that different tobacco planting areas of Chongqing at the ratio of potassium/chlorine varies greatly, which the coefficient of variation is greater than 1. From the coefficient of skewness, some of them are negative skewed peaks which the coefficient are less than 0 including total sugar, reducing sugar and the ratio of nitrogen/nicotine. Others are the positive skewed peaks. From the coefficient of kurtosis, concentration with chlorine, the ratio of total sugar/nicotine and the ratio of potassium/chlorine have longer tail than normal distributions.

| Indexes           | Average | Maximum | Minimum | Standard Deviation | Coefficient of Variation | Coefficient of Skewness | Coefficient of Kurtosis |
|-------------------|---------|---------|---------|--------------------|--------------------------|-------------------------|-------------------------|
| Total Sugar/%     | 23.93   | 36.20   | 10.20   | 4.90               | 20.47                    | -0.36                   | -0.16                   |
| Reducing Sugar/%  | 21.80   | 31.60   | 9.88    | 4.41               | 20.23                    | -0.42                   | -0.02                   |
| Nicotine/%        | 3.06    | 5.88    | 0.72    | 0.91               | 29.74                    | 0.06                    | -0.20                   |
| Chlorine/%        | 0.12    | 0.75    | 0.00    | 0.10               | 83.33                    | 2.65                    | 9.63                    |
| Potassium/%       | 1.90    | 3.61    | 0.70    | 0.57               | 30.00                    | 0.28                    | -0.21                   |
| Nitrogen/%        | 2.13    | 3.42    | 1.25    | 0.36               | 16.90                    | 0.48                    | 0.27                    |
| Total Sugar/Nicotine | 9.02  | 39.17   | 2.24    | 5.00               | 55.43                    | 2.77                    | 12.56                   |
| Nitrogen/Nicotine | 1.43    | 2.23    | 0.39    | 0.33               | 23.08                    | -0.30                   | 0.37                    |
| Potassium/Chlorine| 33.12   | 294.00  | 1.73    | 42.50              | 128.32                   | 3.12                    | 11.42                   |

B. The difference between the levels of main chemical compositions

According to Table II, the differences among each grade are significant. The content of nicotine, the ratio of nitrogen/nicotine and chlorine from high to low is B2F, C3F, X2F, which is significantly different among grades. The grade of C3F and X2F in total nitrogen content is not significantly different, but these are significantly higher than B2F. Also, the content of total sugar from high to low is C3F, B2F, X2F, which is significantly different among grades. And the content of reducing sugar from high to low is C3F, B2F, X2F, which is significantly different among grades. Then, the grade of C3F and X2F in total sugar/nicotine is not significantly different, but these are all significantly higher than B2F. What’s more, the content of potassium from high to low is X2F, C3F, B2F, which is significantly different among grades. The grade of C3F and B2F in the ratio of potassium/chlorine...
is not significantly different, but these all are significantly lower than X2F.

**TABLE II. DIFFERENCE ANALYSIS OF MAIN CHEMICAL COMPOSITIONS OF FLUE-CURED TOBACCO IN DIFFERENT GRADES**

| Grade | Sample Size | Total Sugar/\% | Reducing Sugar/\% | Nicotine/\% | Chlorine/\% | Potassium/\% | Nitrogen/\% | Total Sugar/Nicotine | Nitrogen/Nicotine | Potassium/chlorine |
|-------|-------------|----------------|------------------|-------------|-------------|--------------|-------------|---------------------|-----------------|------------------|
| B2F   | 234         | 21.13Cc        | 19.51Bb         | 3.89Aa      | 0.15Aa      | 1.66Cc       | 2.37Aa      | 5.70Bb              | 1.65Aa          | 21.99Bb          |
| C3F   | 234         | 26.25Aa        | 23.71Aa         | 2.98Bb      | 0.10Bb      | 1.85Bb       | 2.06Bb      | 10.12Aa             | 1.45Bb          | 29.10Bb          |
| X2F   | 234         | 24.31Bb        | 22.08Cc         | 2.32Cc      | 2.32Cc      | 2.21Aa       | 1.96Bb      | 11.2Aa              | 1.19Cc          | 49.50Aa          |

**TABLE III. CORRELATION ANALYSIS ON DIFFERENT GEOLOGICAL TYPES AND THE CHEMICAL INDEXES OF TOBACCO GRADES**

| Geologic Types | Grade | Sample Size | Total Sugar/\% | Reducing Sugar/\% | Nicotine/\% | Chlorine/\% | Potassium/\% | Nitrogen/\% | Total Sugar/Nicotine | Nitrogen/Nicotine | Potassium/chlorine |
|----------------|-------|-------------|----------------|------------------|-------------|-------------|--------------|-------------|---------------------|-----------------|------------------|
| I              | B2F   | 14          | 22.51Aa        | 19.96Aa          | 3.72Aa      | 0.16Aa      | 1.17Bb       | 2.18Bb      | 6.43Aa              | 1.72Aa          | 15.34Aa          |
| II             | B2F   | 37          | 20.36Aa        | 18.90Aa          | 4.03Aa      | 0.17Aa      | 1.85Aa       | 2.46Aa      | 5.24Aa              | 1.65Aa          | 23.64Aa          |
| III            | B2F   | 27          | 21.46Aa        | 20.13Aa          | 3.79Aa      | 0.13Aa      | 1.67Bb       | 2.35Aab     | 5.96Aa              | 1.62Aa          | 23.18Aa          |
| I              | C3F   | 16          | 26.36Aa        | 23.86Aa          | 2.36Bb      | 0.10Aa      | 1.72Bab      | 1.95Aa      | 14.90Aa             | 1.21Bb          | 21.51Aa          |
| II             | C3F   | 44          | 26.18Aa        | 23.60Aa          | 3.17Aa      | 0.10Aa      | 1.97Aa       | 2.12Aa      | 8.88Bb              | 1.50Aa          | 33.39Aa          |
| III            | C3F   | 19          | 26.32Aa        | 23.81Aa          | 3.06Aa      | 0.13Aa      | 1.67Bb       | 2.02Aa      | 8.97Bb              | 1.54Aa          | 26.01Aa          |
| I              | X2F   | 14          | 22.08Bb        | 20.36Bb          | 1.98Aa      | 0.15Aa      | 1.81Bb       | 1.98Aa      | 12.20Aa             | 1.03Aa          | 19.88Aa          |
| II             | X2F   | 37          | 24.06Bb        | 21.51Bb          | 2.42Aa      | 0.06Bb      | 2.36Aa       | 2.00Aa      | 10.44Aa             | 1.21Aa          | 68.16Aa          |
| III            | X2F   | 26          | 25.85Aa        | 23.81Aa          | 2.36Aa      | 0.10Aa      | 1.22Aa       | 1.90Aa      | 11.75Aa             | 1.25Aa          | 40.70AaBb        |

1 stands for the northeast area of Chongqing, 2 stands for the southeast area of Chongqing and 3] stands for the central area of Chongqing.

C. Differences of the main chemical composition in different regions

According to the geological types in the places of mainly planting tobacco areas in Chongqing of nine counties, these are divided into 3 regions. As is shown in Table III, the grade of B2F in potassium is not significant differences in the northeast area of Chongqing and the central area of Chongqing, but these all are significantly lower than the southeast area of Chongqing. The content of potassium from high to low is the southeast area of Chongqing, the central area of Chongqing, which is extremely significant difference among regions. The rest of chemical index were not significant.

In the grade of C3F, nicotine and nitrogen/nicotine are not significant differences in the southeast area of Chongqing and the central area of Chongqing, but these all are significantly higher than the northeast area of Chongqing. The content of potassium from high to low is the southeast area of Chongqing, the central area of Chongqing, the northeast area of Chongqing, which is significantly different among regions. The ratio of total sugar/nicotine is not significant differences in the southeast area of Chongqing and the central area of Chongqing, but these all are significantly higher than the northeast area of Chongqing. The rest of chemical index were not significant.

In addition, in the grade of X2F, the content of total sugar from high to low is the central area of Chongqing, the southeast area of Chongqing, the northeast area of Chongqing, which is significantly different in these regions. The reducing sugars are not significant difference in the southeast area of Chongqing and the northeast area of Chongqing, but the level of reducing sugar of both regions is significantly lower than the central area of
TABLE IV. THE INDEX SELECTION, THE INFECTION POINT AND THE WEIGHT VALUE OF THE USABILITY EVALUATION OF CHEMICAL COMPOSITIONS IN FLUE-CURED TOBACCO

| Indexes            | Function Types       | Lower Limit/ \( x_1 \) | Lower Limit of Optimal Value/ \( x_2 \) | Upper Limit of Optimal Value/ \( x_4 \) | Upper Limit/ \( x_3 \) | Weight Values/\% |
|--------------------|----------------------|-------------------------|------------------------------------------|------------------------------------------|-------------------------|------------------|
| Nitrogen           | 1.1                  | 2.0                     | 2.3                                      | 3.4                                      | 9.05                    |
| Nicotine           | 1.2                  | 2.1                     | 2.4                                      | 3.5                                      | 13.25                   |
| Total Sugar        | 10.0                 | 20.0                    | 28.0                                     | 35.0                                     | 10.75                   |
| Reducing Sugar     | 11.5                 | 19.0                    | 20.0                                     | 27.0                                     | 10.85                   |
| Weight Values/%    |                      |                         |                                          |                                          |                         |
| S-types membership function:                                          |                     |                         |                                          |                                          |                         |
| Nitrogen/Nicotine   | 0.55                 | 0.95                    | 1.05                                     | 1.45                                     | 9.52                    |
| Chloride           | 0.8                  | 0.3                     | 0.8                                      | 1.2                                      | 10.52                   |
| Potassium          | 0.8                  |                         | 2.5                                      | 13.75                                    |
| Chloride/Chlorine  | 0.8                  |                         | 8.0                                      | 9.94                                     |

Chongqing. The content of chlorine from high to low is the northeast area of Chongqing, the central area of Chongqing, and the southeast area of Chongqing, which is significantly different among regions. What’s more, the content of potassium are not significantly different between the southeast area of Chongqing and the central area of Chongqing, but they are significantly lower than the northeast area of Chongqing. The ratio of potassium/chlorine is not significant in the southeast area of Chongqing and the northeast area of Chongqing, but they are significantly higher than the central area of Chongqing. The rest of chemical index were not significant.

**D. The comprehensive evaluation of chemical composition in Chongqing tobacco planting areas of Yunyan87**

Due to the range of every index is not consistent, it is valuable to use the main chemical compositions indexes which are mentioned to flue-cured tobacco chemical compositions, regarding Chongqing tobacco planting areas of Yunyan87. In order to eliminate the influence of the dimension, it will use the theory of fuzzy mathematics to calculate the quality index figure, which could make the raw data of the evaluation index convert between 0.1 and 1. Hence, there are two types of membership function: S-types membership function and parabolic membership function. The formulas are:

S-types membership function:

\[ f(x) = \begin{cases} 
1.0 & x \geq x_2 \\
0.9(x - x_1)/(x_2 - x_1) & x_1 < x < x_2 \\
0.1 & x \leq x_1 
\end{cases} \]

Parabolic membership function:

\[ f(x) = \begin{cases} 
0.1 & x < x_1; x > x_2 \\
0.9(x - x_1)/(x_3 - x_1) & x_1 \leq x < x_3 \\
1.0 & x_3 \leq x \leq x_4 \\
1.0 - 0.9(x - x_4)/(x_2 - x_4) & x_4 < x \leq x_2 
\end{cases} \]

Thus, the membership values of each component indexes were calculated, which reflect the pros and cons on the chemical availability [15]. Its maximum is 1.0, which represents best condition of the chemical availability in flue-cured tobacco. The membership values reduce from 1 to 0.1 meaning the chemical compositions of state are getting worse. According to the practical production, the minimum value of membership is 0.1.

In the formula, the alphabet of \( x_1, x_2, x_3 \) and \( x_4 \), each separately represent lower limit, upper limit, lower limit of optimal value, upper limit of optimal value, and \( x \) represent for the actual content of the chemical composition. Based on the practical experience and the past researches [16, 17], it will locate the evaluation indexes and break point. At the same time, the 234 samples should be analyzed by the principal components analysis. Three principal components are supposed to extract total contribution which is more than 80%. Also,
the chemical compositions indexes will be calculated to get weight value [18] (Table IV).

E. The comparison of chemical compositions index

The chemical composition indexes can be calculated by the formula of \( CCUI = \sum_{i=1}^{n} Wi \cdot Bi \). In this formula, the \( Wi \) and \( Bi \) represent for the weights coefficient and membership value on the \( i \) chemical index, respectively. The values of \( CCUI \) range from 0 to 100. The higher the value, the better the usability of flue-cured chemical composition is.

1) The usability indexes of flue-cured chemical compositions in different grades

According to Table V, the grade of C3F has the highest usability index figure which is on average of 71.65. The grade of B2F is the second usability and the grade of X2F is the third usability. The standard deviation of these three of grades is less than 6%. It proves the difference among the values is small. And the variation coefficient of grades is less than 10%, it becomes relatively close to all values.

| Grades | Average | Variations | Standard Deviation | Variation Coefficients/% |
|--------|---------|------------|-------------------|--------------------------|
| B2F    | 68.42   | 63.43–74.27| 5.45              | 7.96                     |
| C3F    | 71.65   | 65.77–77.42| 5.34              | 7.45                     |
| X2F    | 67.05   | 61.06–72.38| 5.96              | 8.90                     |

2) The usability indexes of flue-cured chemical composition in different geological areas

According to the Figure 2, regarding the grade of B2F and C3F, the usability index in the northeast area of Chongqing is highest, which is 71.68 and 75.42, respectively. The lowest grade in the central area of Chongqing.
Chongqing is 65.49 and 66.30, respectively. In the grade of X2F, the highest and the lowest grade are 70.68 in the central area of Chongqing and is 62.32 in the southeast area of Chongqing, respectively. In summary, the northeast area of Chongqing highest usability of chemical composition and the central area of Chongqing provide lowest usability of chemical composition.

IV. Conclusions

The Yunyan87 tobacco leaves have good chemical composition usability. It has high total sugar, reducing sugar, the nitrogen, nicotine, the ratio of potassium/chlorine and moderate total sugar/nicotine. Also, low potassium and chlorine levels have been associated with the tobacco leaves. Potash fertilizer is one of the important fertilizers in the production of tobacco. Therefore, the efficiency of fertilizing in the planting process can improve the quality and production [19]. Moreover, fertilization can improve the fragrance of Yunyan87. As mentioned above, to improve the content of potassium, it can be fulfilled by increasing the usage of potash fertilizer and by increasing the utilization rate of potash fertilizer. In addition, if the content of chlorine in flue-cured tobaccos too high or too low, it will reduce the yield and quality of Yunyan87 [20]. So, chloride fertilizer should be applied appropriately in Chongqing tobacco area. But overall, in the future Chongqing regions should improve genetic part of flue-cured tobacco, promote the environmental-friendly tobacco corps and increase the maturity of tobacco leaves on the field. Furthermore, carbon and nitrogen metabolism could be increased, and carbohydrate of tobacco leaves should be regulated to the appropriate level [21]. Beyond these, the chemical composition is different among grades.

Also geography difference influences the chemical composition of Yunyan87.

Membership values are used to measure the quality status of chemical availability. This method has certain guidance for comprehensive evaluation analysis on the usability of chemical compositions in flue-cured tobacco, which can be calculated by the comparison of chemical composition directly to get availability indexes. According to the analysis on the usability indexes of chemical compositions in different grades of flue-cured tobacco, it is easy to find the usability indexes. In different regions, the analysis on the usability indexes of chemical compositions indicates significant differences. The results of the usability indexes of chemical composition in each grade get the highest figure of 71.65 with C3F and the lowest figure of 67.05 with X2F. According to the analysis of the usability indexes of chemical composition in different Chongqing regions, it shows that the northeast area of Chongqing has the highest usability indexes and the central area of Chongqing has the lowest index.

At a matter of fact, the qualities of flue-cured tobacco include appearance, chemical, physical, smoking, safe factors and etc., but this study only evaluate on the content of chemical composition and its ratio to the usability of flue-cured quality. Therefore, in the future we can study on these combine with chemical composition. The impact on the quality of tobaccos not only the chemical composition of tobacco leaves, but the effect of chemical composition on the quality of tobacco leaves which is quite complex. Different cigarettes companies have different requirements to the tobacco leaves. Because of the special landscape of Chongqing tobacco areas, how to cope with the requirements of individuation in different regions are the key, which are connected with the local styles and the raw material. There should be further research to establish the comprehensive evaluation indexes of flue-cured tobacco in Chongqing.

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