Journal of the Korea Society of
Tobacco Science Vol. 22, No. 2, 184~189(2000)
Printed in Republic of Korea

Statistical approach for development of objective evaluation method on tobacco smoke

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(Received December 5, 2000)

ABSTRACT : This study was conducted to develop the objective evaluation method for tobacco smoke. The evaluation was carried out by using the data of cut or blended tobacco components, smoke components, electric nose system(ENS), and sensory test. By using the statistical methods, such as cluster analysis, discriminant analysis, factor analysis, correlation analysis, and multiple regression analysis, the relationship among the data of tobacco, smoke, ENS, and sensory evaluation was studied. By the results of cluster analysis, the data from smoke analysis by GC and ENS were able to select the difference of tobacco leaf characteristics. As the results of discriminant analysis, grouping by the components of tobacco leaves and smoke was possible and the results of GC analysis of smoke could be used for discrimination of tobacco leaves. In the results of factor analysis, nicotine, tar, CO, puff No and pH in the smoke were the factors effecting on the tobacco leaf characteristics. From the correlation analysis, aroma, taste, irritation, and smoke volume of sensory test had high relation to tar, p-cresol threonolatone, levoglucosane, and quinic acid-γ-lactone of smoke. The ENS data showed high efficiency for discriminant analysis and cluster analysis, but it was not good for factor analysis, and correlation analysis. It was possible to estimate tobacco leaves and their blending characteristics by the analytical data of tobacco leaves, smoke, ENS, and sensory test results. By the multiple regression analysis, some correlation among selected chemical components and sensory evaluation were found. This study strongly indicated that the some chemical analysis data was available for the objective evaluation of tobacco sensory attributes.

Key words : tobacco smoke, sensory evaluation, statistical treatment

Characterization of the tobacco smoke is complex task. Traditionally, each company had in its own method to evaluate tobacco smoke characteristics. It is necessary to carried out smoke sensory evaluation in order to judge the quality of tobacco smoke. This procedure is less objective and the results are difficult to use in a quantitative manner to estimate quality. Some sensory aspects of smoke and various chemical classes to the aroma of cigarette smoke reported previously by a number of publications(Cain, 1980 ; Sakuma, 1980; Dravnieks, 1975; Patrianakos, 1979). Sensory attributes are not easily characterized by classical chemical analysis, because they are often complicated mixtures of many different compounds. In addition, the human perception is frequently a non-linear response to the concentrations and ratios of the compounds in the mixture. In many cases the trace quantities of these compounds may not even be measurable by standard chemical means

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(Stone, 1998 ; Tso, 1982 ; Hasebe, 1999 ; Gordin, 1987). To investigate the possibility of chemical analysis as a replacement for the sensory evaluation of tobacco smoke, we analyzed the leaf and blended tobacco components, smoke compounds, odor characteristics by electronic nose system (ENS), and sensory evaluation in the different types of cigarette and then examined the relationship among chemical composition, odor characteristics, and sensory evaluation by statistical analysis.

MATERIALS AND METHODS

Thirty-seven different kinds of cut or blended tobaccos were manufactured into cigarettes of 84 mm length and 24 mm circumference with non perforated tipping paper. Several selected characteristics of the experimental cigarettes were listed in Table 1.

Table 1. Selected characteristics of the experimental cigarettes

Flue-cured		Burley		Oriental & Others		Blended
Korea	4	Korea	4	Greece	1	15 kinds
USA	2	USA	1	Turkey	1	(Mixed 2 or
		Toasted	5	Recon. Tobacco	2	more types of
				Expanded tobacco	2	tobaccos)

Chemical components of cut or blended tobaccos were analyzed using KGTRI established methods. Cigarette samples were selected by the pressure drop and weight of cigarette for smoke analysis and then conditioned and smoked by the standard ISO method.

After cigarette samples were smoked by 20 chennel smoking machine, cambridge pads were extracted and analyzed for smoke components. Other smoke components were analyzed based on KGTRI established method and CORESTA recommended method. In total, 50 components including smoke tar and nicotine were analyzed in this study. Analyses were repeated three times for each sample. The average value of the three analyses was used in the study. Electronic nose system has its ability to discriminate between odors that easily be classified as different by the human nose. By using electronic nose system (Neurotics Scientific Co., e-Nose 4,000), odor characters of mainstream smoke were analyzed by the response of 12 different sensors. Sensory evaluation of tobacco smoke for 8 attributes were scored on a nine-point scale by an expert panel trained to estimate smoking quality quantitatively. The eight attributes estimated were aroma, taste, offensive aroma, offensive taste, irritation, hotness, smoothness, and smoke volume. The data from chemical analysis, ENS, sensory evaluation was transferred to the computer system for statitical analysis using the Statistical Analysis System (SAS). Cluster analysis, discriminant analysis, factor analysis, correlation analysis, and multiple regression analysis were performed on this system in order to estimate the smoking quality.

RESUITS AND DISCUSSION

Chemical analyses are usually based on the established principle of a proportional response to the concentration of a single chemical or a group of related chemicals. We have attempted to establish a objective method for tobacco smoke by using chemical analysis data treating statistical approaches. We found significant differences among the analytical methods as well as among the chemical components. Each chemical analysis data was plotted on the Table 2 grouping from the cluster analysis.

Bright, burley, and oriental tobacco samples were separated from others by different analytical method. In the cluster analysis, chemical analysis data of cut tobacco was not clearly separated the difference of cigarette samples, comparing with GC analysis data or ENS data. This may be related to the fact that wet analytical data has higher variation than that of instrumentally analytical data. From this result, chemical analysis data of cut or blended tobacco did not show significant differences among selected cigarette samples, and not able to use for separating the characteristics of tobaccos.

Same as the results of cluster analysis, discr-

Table 2. Results of cluster analysis under different analytical methods

Analytical Method	Components	Results of Cluster Analysis		
		Cluster No. 1	Cluster No. 2	Cluster No. 3
Mainstream smoke	Nicotine, TAR, CO, Puff No	B6, B7, B8, B10, H4, H6	B1, B2, B3, B5, H1, H2, H3, H5, N1, N2	B4, B9, N3, N4, N5
Cut tobacco	Sugar, Nitrogen, Ammonia, etc.	N2, N4, H1, H3, H5, H6	B6, B7, B8, B9, B10, H2, H4, N1, N3, N5	B1, B2, B3, B4, B5
Sidestream smoke	Sidestream Components	B8, B10, H3, H4, H5, N3	B1, B2, B3, B4, B5, B9, H1, H6, N4, N5	B6, B7, H2, N1, N2
GC Anal. for TPM	16 components such as Glycolic acid	H1, H2, H3, H5, H6, N1, N2	B1, B2, B3, B4, B5, H4, N3, N4	B6, B7, B8, B9, B10, N5
ENS	12 values from Sensor	H1, H2, H3, H4, H5, H6	B1, B2, B3, B4, B5	

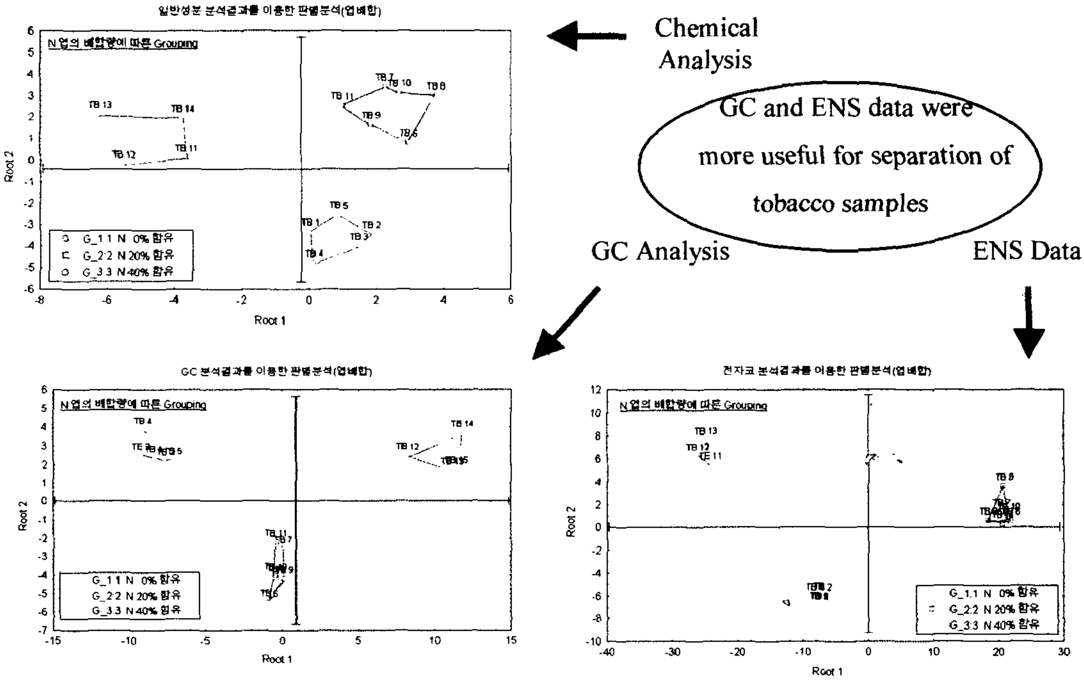


Fig. 1. Distribution of chemical, GC, and ENS data by discriminant analysis.

iminant analysis did show that the GC or ENS data were separated by the difference of cigarettes samples. The results of discriminant analysis represent in Figure 1.

The distribution of analytical data by each analysis method showed different pattern. When the ENS data appeared the most concentrated distribution, the chemical analysis data of cut tobacco showed the most scattered distribution. Those results indicated that GC analysis and ENS data were available to discriminate the different type of tobaccos or blended cigarettes successfully. Factor analysis have become widely available and applied to the reduction of large data sets. Table 3 listed the results of factor analysis among cut tobacco analysis, smoke analysis, and ENS data.

Table 3. Results of factor analysis by chemical, GC, and ENS data

Component	Factor 1	Factor 2	Component	Factor 1	Factor 2
Nicotine	-.923459 *	.058917	CO	-.046782	.583004
Tar	-.872668 *	.429938	CO2	-.804864 *	.234836
Puff No.	-.781065 *	.416326	Nitrogen	-.820065 *	-.160383
Sugar	.147249	.878067 *	Alkaloid	-.478735	-.811567 *
Protein	-.498642	.775731 *	Ammonia	.002458	-.515742
SS nicotine	-.900022 *	-.283157	Lactic acid	-.280628	.796079 *
SS CO	.109361	.286397	SS tar	-.883804 *	-.283566
HCN	-.072948	.442308	Furoic acid	-.20511	-.361466
Glycolic acid	.84005 *	.365495	pH	.39736	-.885153 *
Butyric acid	.94189 *	.298914	Levulinic acid	.84517 *	-.459580
Benzoic acid	.96607 *	-.116960	Phenylacetic acid	.44711	-.861050 *
Butanoic acid	.19603	-.823850 *	Palmitic acid	.35057	-.079580
Phenol	.83615 *	-.472533	Pyridine	.93552 *	-.309064
p-Cresol	.96581 *	-.061672	Xylenol	.84738 *	-.188773
Vinyl phenol	.87098 *	-.028038	Pyrocatechol	.88184 *	.444224
Methyl catechol	.97773 *	-.000387	Hydroquinone	.90967 *	.156528
Ethyl catechol	.86087 *	.484777	Vinyl catechol	.80430 *	.492317
Levoglucosan	.76773 *	.504967	Quinic acid	.74524 *	.646484
Quinic acid	.74524 *	.646484	Neophytadiene	.66338 *	-.597977
ENS sensor 1	.980537 *	-.022619	ENS sensor 2	.951230 *	-.160042
ENS sensor 3	.845949 *	-.357665	ENS sensor 4	.997733 *	-.018723
ENS sensor 5	.974902 *	.204622	ENS sensor 6	.967825 *	-.207112
ENS sensor 7	.858695 *	-.479730	ENS sensor 8	.207598	-.937621
ENS sensor 9	.952562 *	-.278937	ENS sensor 10	.974468 *	-.217653
ENS sensor 11	.933796 *	-.342441	ENS sensor 12	.942399 *	-.324323

* significant level : 0.05

Through factor analysis of each analytical data, GC data and ENS data were good marker to evaluate the quality of tobacco smoke. Each sample was plotted on the principal component scores calculated from the first and second factor. As the first factor separated smoke components and ENS data in that order, the second factor separated cut tobacco constitutes. This results represented the most important factors associated with the levels of sensory evaluation appeared to be smoke components and ENS data other than cut tobacco and sidestream smoke components. It also showed that GC analysis data and ENS data were useful factor to develop objective evaluation method on tobacco smoke.

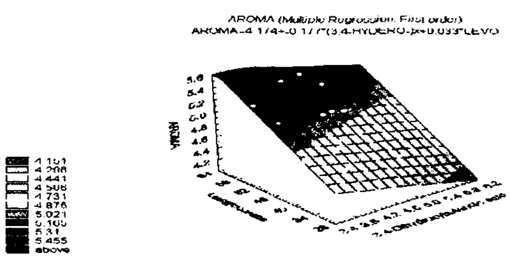
To know the relation between analytical data and sensory evaluation data, we treated the data on correlation analysis. Some correlation among selected chemical components and sensory evaluation were listed in Table 4. Variables such as lactic acid, p-cresol, threonolatone, quinic acid, and NFDPM were positively correlated with irritation. Also, smoke volume was positively correlated with lactic acid, glycolic acid, p-cresol, threonolatone,

Table 4. Correlation analysis between sensory evaluation and chemical analysis data.

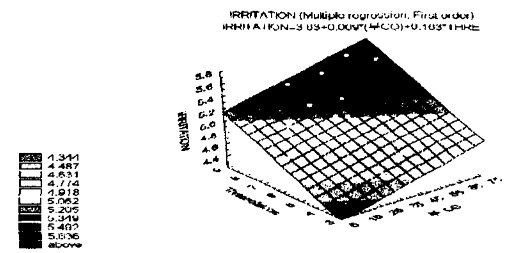
Variable	Lactic acid	Glycolic acid	p-Cresol	Threono-latone	Butanoic acid	Levogluco san	Quinic acid	Tar	CO
Aroma	.36	.45	.48	.28	-.21	.73 *	.31		
Taste	.26	.18	.27	.43	-.21	.54 *	.06		
Off-aroma	.25	-.12	-.02	.04	-.28	-.06	-.08		
Off-taste	.26	-.08	-.06	.10	-.24	.07	-.10		
Irritation	.53 *	.39	.56 *	.64 *	.24	.47	.52 *	.52*	.42
Hotness	-.29	-.27	-.13	.31	.62 *	-.16	-.08		
Smoothness	.32	.19	.14	.08	-.20	.22	.25	.14	.58*
Smoke volume	.69 *	.53 *	.59 *	.58 *	.06	.61 *	.62*	.62*	.38

* Significant level : 0.05

Regression Summary
For **Aroma**
R = .78764735
R^2 = .62038834
F(2,12) = 9.8056
P < .00299
Standard error of estimate : .22759



Regression Summary
For **Irritation**
R = .77443781
R^2 = .59975392
F(2,12) = 8.9908
P < .00441
Standard error of estimate : .25236



Regression Summary
For **Smoke Volume**
R = .77086853
R^2 = .59423830
F(2,12) = 8.7870
P < .00446
Standard error of estimate : .32425

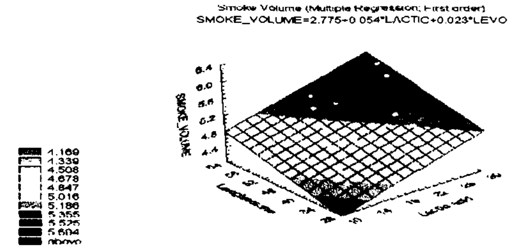


Fig. 2. Results of multiple regression among sensory evaluation and smoke analysis data

levoglucosan, qumic acid, and NFDPM. Levoglucosan appeared to be positively correlated with aroma and taste, but the correlation value were not high, although they showed statistical significance. These correlations can serve as indicators for the chemical mature of smoke constituents and can suggest smoke quality. This study strongly indicates that the some smoke components increase with increasing sensory evaluation score. It was also demonstrated that increased NFDPM levels accelerate irritation and smoke volume of cigarettes. On the basis of the simple correlation data, we had selected several important variables for computation of multiple regression. The results of multiple regression represented in Figure 2.

We can predict the level of certain sensory attributes of smoke when a few smoke components were known. When only 3,4-dihydroxybutanoic acid and levoglucosan were used, estimated aroma score = 4.174 + 0.177(3,4-dihydrobutanoic acid) + 0.033 (levoglucosane). When tar and threonolatone were used, estimated irritation score = 3.83 + 0.009(NFDPM) + 0.183(threonolactone). When lactic acid and levoglucosane were used, estimated smoke volume = 2.775 + 0.054(lactic acid) + 0.023(levoglucosane). In essence this procedure determines how much of the sensory data can be reconstructed from the chemical data, and which parts of the chemical data are used in this reconstruction. Statistical approach for tobacco smoke quality which theoretically has promise, but in practice much difficulty, for evaluation cigarette differences.

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