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Multivariate Analysis among Leaf/Smoke Components and Sensory Properties about Tobacco Leaves Blending Ratio

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ABSTRACT: This study focused on the relationships among leaf and smoke components and sensory properties following tobacco leaf blending. A completely randomized experimental design was used to evaluate components of leaf and smoke and sensory properties for sample cigarettes with four mixtures of flue cured and burley tobacco (40:60, 60:40, 80:20 and 100:0). Eleven leaf components, six smoke components, and eight sensory properties of smoking taste were analyzed. A sensory evaluation method known as quantitative descriptive analysis was used to evaluate perceptual strength on a fifteen score scale. Raw data from ten trained panelists were obtained and statistically analyzed. Based on the MANOVA, clustering analysis, correlation matrix and partial least square (PLS) method were applied to find out which smoke component most affected sensory properties. The PLS method was used to remove the influence between explanatory variables in the leaf, smoke components derived from the results. High correlations ($p<0.01$) were found among ten specific leaf and smoke components and sensory attributes. Total nitrogen, ammonia, total volatile base, and nitrate in the leaf were significantly correlated ($p<0.05$) with impact, bitterness, tobacco taste, irritation, smoke volume, and smoke pungency. From the results of PLS analysis, influence variables are used to explain about the correlation. In terms of bitterness, with only two explanatory variables, Leaf NO_3 and Leaf crude fiber were enough for guessing their correlation. In the distance weighted least square fitting analysis, carbon monoxide highly influenced bitterness, hay like taste, and smoke volume.

***Key words*: quantitative descriptive analysis, correlation, PLS analysis**

An idea of close connection among leaf, smoke components and sensory properties has been studied by a number of researchers(BAT documents, 1986, 1992, 1994; B&W, 1992; Chemosensory Meeting, 1986; Chemosensory Research, 1990 1992; Kim, C.S. et al., 1995; Griffith, R.B. et al., 1965; Na, H.H. et al., 1984; Kim, J.O. et al., 1979; Honeycutt, R.H. et al., 1986; R.J.K. et al., 1997; Oh, S.Y. et al., 1983; Park. T.M. et al., 1988; Sun woo, Y.I. et al., 1980; Lee, Y.T. et al., 1992). Though many researchers tried to find out their connections, few results have been showed up clearly until now. In advance, various results about correlation between leaf or smoke components and sensory properties were reviewed. Literature review was conducted in order to cross check for our study. Bruckner(1936), Coulson(1958) and BAT(1990 1992) remarked as the intensity of taste, sharpness, harsh taste, irritation, mouth dryness and impact in respectively. Besides, B&W(1986) found out correlation between carbon dioxide and

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various sensory properties. Moreover, influence between smoke particle size and sensory attributes was discussed. And, KT&G's data(Hwang, K.J. et al., 2000) was showed that lactic acid; cresol and quinic acid have a significant correlation to smoke volume and irritation. This study was focused on the relationship within leaf, smoke components and sensory properties following tobacco leaf blending. We got two points about this study. One is verification of the correlation among leaf/smoke components and sensory properties. The other is derivation and selection of the major four influencing variables, such as leaf nitrates, leaf ammonia, leaf TVB, and smoke carbon monoxide. On the previous literature review, ammonia and TVB were found out influencing variables on the sensory properties by Coulson and BAT documents. This supports our insistence that this common theory make sense as for the cigarette made of the pure Korean tobacco leaves.

MATERIALS AND METHODS

Sample preparation

Sample cigarette was made of only two types of tobacco leaves, Flue cured and Burley without blending the others. And, which are all typical Korean tobacco leaves. Flue cured consisted of C2L and B2O, and burley consisted of C2W and B2T as the same amount. These four kinds of leaves are known as common in Korea. We set the standard of four types by blending ratio. On the basis of flue cured ratio of 40%, 60%, 80% and 100% were prepared.

Statistics

Raw data from ten trained panelists were obtained and statistically analyzed. The experimental conditions were designed two way layout for completely randomized design with two factors as follows; one is the sample cigarettes of four type by flue cured mixed with burley (40:60, 60:40, 80:20 and 100:0) and the other is three characteristics including sensory properties, leaf components and smoke components. In detail, sensory properties for smoking tastes were 8 attributes, that is, impact, irritations, bitterness, hay like, tobacco taste, smoke volume, smoke pungent and mouth clean. The six smoke components were total particulate matters, nicotine, tar, carbon monoxide, puff number and nicotine to tar ratio. And, leaf components were eleven the same as, nicotine, total sugar, total nitrogen, chloride, pH, ammonia, ether extract, total volatile base, nitrate, crude fiber and crude ash etc. The three variables, leaf/ smoke analytical components and sensory evaluation attributes individually conducted. On the statistics, based on the multivariate analysis, such as cluster analysis, partial least square method and distance weighted least square fitting analysis was conducted and significance level was five percent.

Panel selection

All panelists conducted about discriminative test for sensory properties including tobacco taste. Degree of difference test with seven category scale and quantitative descriptive analysis was conducted for panel selection. Empirical logic drawing example of sequential approach by same difference test and quantitative descriptive analysis method was used. Panel was separated from three groups, expert, trained panel and trainee as their performance. Every expert panelist in our research institute has been monitored

Table 1. Types of tobacco leaves and sample cigarettes by blending ratio

▣ Types of tobacco leaves	Flue cured(C2L 50% + B3O 50%) Burley(C2W 50% + B2T 50%)
▣ Sample cigarettes by blending ratio	F.C. 40% + Br. 60% F.C. 60% + Br. 40% F.C. 80% + Br. 20% F.C. 100%

and tracked regarding as sensitivity, reproducibility, agreement and cross over. Ultimately selected superior ten panelists considering over these four categories are all male panelists.

Sensory evaluation

Sensory evaluation method, known as quantitative descriptive analysis, was used to evaluate the perceptual strength with fifteen score scale by samples respectively in regard to all attributes. In terms of sensory evaluation, eight attributes such as, impact, bitterness, irritation, hay like, tobacco taste, smoke volume, smoke pungent and cleanness by ten trained panelists was done. Besides, panel setup was accomplished by use of quantitative descriptive analysis method over twelve times.

RESULTS AND DISCUSSION

Table 2 shows the correlation matrix between sensory properties and leaf/smoke components. In the correlation matrix, we found out high correlation between six sensory properties(dotted circle) and four leaf components(dotted rectangle) each other under the five percent significance level.

Fig. 1 and Table 3 show the result of single linkage method in cluster analysis. Cluster analysis was applied and two different analytical methods were used in order to analyze the result. One is "Single Linkage method," and the other is "Ward's method." Fig. 1 illustrates clustering state between variables. On the figure, the width of column is meaningless but, the height of col-

Table 2. Correlation matrix between sensory properties and leaf/smoke components

Variable	Correlation Marix_rawdata-Full Data Marked correlations are significant at p< .05000 N=264(Casewise deletion of missing data)							
	sensory-*IMP	sensory-BIT	sensory-HAY	sensory-TAS	sensory-IRR	sensory-SMV	sensory-SMP	sensory-CLN
Leaf-Nicotine	0.28	0.18	0.05	0.24	0.22	0.40	0.11	0.08
Leaf-Total Sugar	0.03	-0.10	-0.01	0.01	-0.09	0.07	-0.08	0.10
Leaf-Total nitrogen	0.20	0.22	0.04	0.08	0.25	0.27	0.13	-0.01
Leaf-Chloride	0.05	0.15	0.02	0.06	0.17	0.07	0.11	-0.08
Leaf-pH	-0.19	-0.14	-0.01	-0.14	-0.18	-0.27	-0.06	-0.03
Leaf-NH_3	0.17	0.18	0.05	0.16	0.21	0.23	0.14	-0.01
Leaf-Ether	0.20	0.16	0.01	0.17	0.17	0.26	0.06	0.03
Leaf-TVB	0.17	0.20	0.05	0.17	0.24	0.25	0.14	-0.01
Leaf-NO_3	0.16	0.20	0.04	0.15	0.22	0.21	0.14	-0.03
Leaf-Crude Fiber	-0.13	-0.00	-0.04	-0.13	0.01	-0.20	-0.00	-0.13
Leaf-Ceude Ash	-0.23	-0.08	-0.03	-0.19	0.11	-0.34	-0.02	-0.12
smoke-TPM	0.05	0.00	-0.04	0.03	-0.11	0.08	-0.06	0.02
smoke-Nicotine	0.22	0.09	0.02	0.20	-0.01	0.33	0.00	0.13
smoke-Tar	0.07	-0.04	-0.02	0.06	0.08	0.09	-0.08	0.08
smoke-CO	0.13	0.01	0.03	0.09	-0.07	0.13	0.01	0.10
smoke-Puff No.	0.25	0.12	0.02	0.21	-0.02	0.36	0.03	0.10
smoke-Nic./Tar	0.22	0.16	0.05	0.21	0.13	0.33	0.09	0.08

*IMP: Impact, BIT: Bitterness, HAY: Hay like, TAS: Tobacco tas0.19te, IRR: Irritation, SMV: Smoke volume, SMP: Smoke pungent, CLN: Cleanness/Mouth clean umn has the meaning. The height means linkage distance. In cluster analysis, Euclidean distances express correlation. Namely, if the correlation is high, the distance becomes closer. On the contrary, in case of correlation is low, the distance become keep apart. Through the figure and table, we found out that degree of correlation between smoke pungent and bitterness is higher than that of tobacco taste and impact. The linkage distance expressed in the Fig. 1 was showed to the numerical value as table 3. Table 4 is demonstrating the stepwise forming stage of clustering state. For example, 'bitterness' and 'smoke pungent' was bound to the first similar group. And then, this group and 'hay like' was bound to the second similar group. The next, previous group and 'cleanness' was bound to the third adjacent group.

Continuously, a little different grouping pattern is shown in the following diagram. In the Fig. 2 and Table 5, Ward's method is being displayed. This method shows correlation diagram into distance form of the sum of square of variables. A different calculation result was obtained because of different calculating method. But, the same result indicated in the Fig. 2. In general, ward's

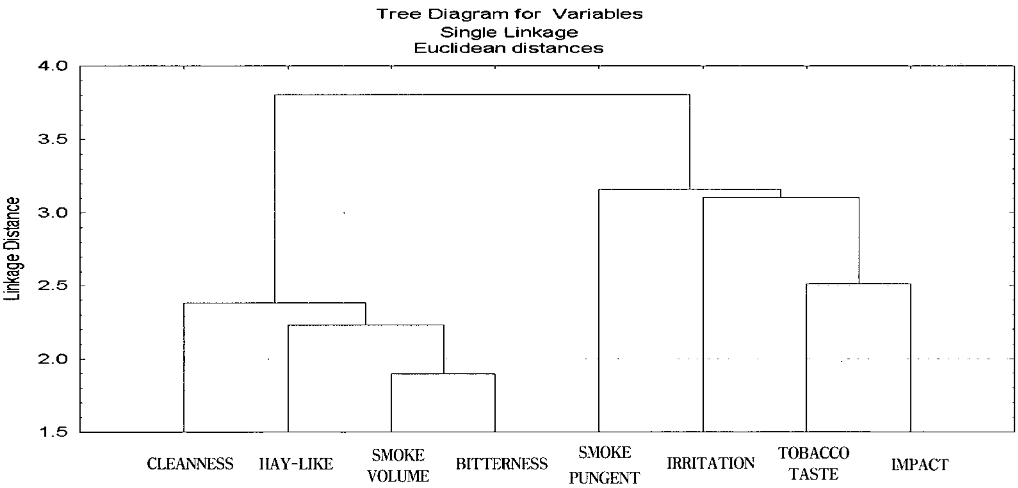

Fig. 1. Result of single linkage method in cluster analysis.

Table 3. Euclidean distances value among sensory attributes

	Euclidean distances_Correlation-rawdata-16del_del_survivor							
	sensory-IMP	sensory-BIT	sensory-HAY	sensory-TAS	sensory-IRR	sensory-SMV	sensory-SMP	sensory-CLN
sensory-IMP	0.00	6.71	5.56	2.51	3.10	3.15	6.32	5.17
sensory-BIT	6.71	0.00	2.95	7.30	4.65	4.96	1.89	4.62
sensory-HAY	5.56	2.95	1.00	5.92	4.83	4.03	2.23	4.62
sensory-TAS	2.51	7.30	5.92	0.00	4.43	3.54	6.86	4.75
sensory-IRR	3.10	4.65	4.83	4.43	0.00	3.17	4.64	5.33
sensory-SMV	3.15	4.96	4.03	3.54	3.17	0.00	4.31	3.80
sensory-SMP	6.32	1.89	2.23	6.86	4.64	4.31	0.00	3.70
sensory-CLN	5.17	4.62	2.38	4.75	5.33	3.80	3.70	0.00

Table 4. Stepwise forming stage of clustering state by single linkage method

linkage distance	Amalgamation Schedule_Correlation-rawdata-16del_del_survivor Sigdie Linkage_Euclidean distances							
	Obj. No. 1	Obj. No. 2	Obj. No. 3	Obj. No. 4	Obj. No. 5	Obj. No. 6	Obj. No. 7	Obj. No. 8
1.889444	sensory-BIT	sensory-SMP						
2.227106	sensory-BIT	sensory-SMP	sensory-HAY					
2.376973	sensory-BIT	sensory-SMP	sensory-HAY	sensory-CLN				
2.507987	sensory-IMP	sensory-TAS						
3.098387	sensory-IMP	sensory-TAS	sensory-IRR					
3.254362	sensory-IMP	sensory-TAS	sensory-IRR	sensory-SMV				
3.801316	sensory-IMP	sensory-TAS	sensory-IRR	sensory-SMV	sensory-BIT	sensory-SMP	sensory-HAY	sensory-CLN

method is known as the more effective method than single linkage method. In the result, the single linkage method was used for cross checking.

Generally, regression analysis has the risk for giving a meaningless model in case of the correlation between independent variables exists. So the partial least square method(PLS) was applied to find out which component has more influence on the sensory properties. This method removes influencing power between explanatory variables and improves analytical power. To explain "haylike," nine explanatory variables are needed to explain above ninety percent for independent variables such as, leaf nitrates, smoke carbon monoxide, leaf crude fiber, ammonia, sugar, chloride, ether, Smoke puff and TPM. We could certainly find out above nine influencing variables by using regression coefficient table, regression trend line and distance weighted least square fitting analysis.

For example, in case of 'Hay-like', nine explanatory variables are needed until above ninety percent of influencing power. According to the distance weighted least square fitting analysis, influencing power is in proportion as the height of the bar in the Fig. 3. Table 7 illustrates the distance value about different component parallel

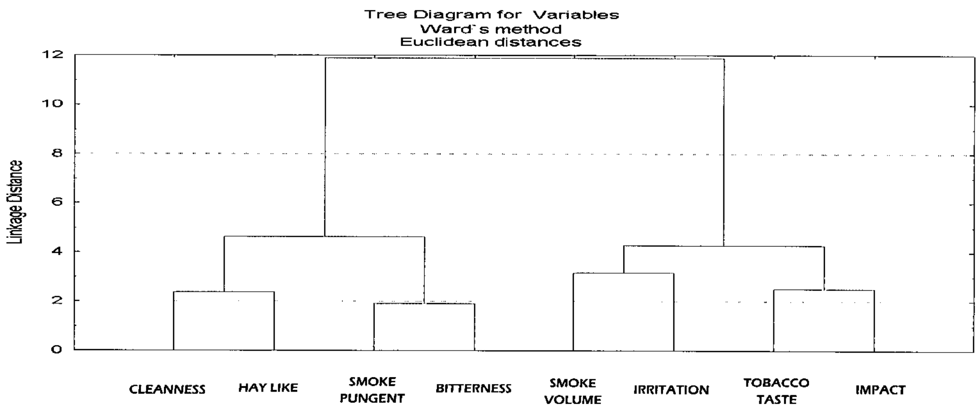

Fig. 2. Result of Ward's method in cluster analysis.

Table 5. Stepwise forming stage of clustering state by Ward's method

linkage distance	Amalgamation Schedule_Correlation-rawdata-16del_del_survivor Ward's method_Euclidean distances							
	Obj. No. 1	Obj. No. 2	Obj. No. 3	Obj. No. 4	Obj. No. 5	Obj. No. 6	Obj. No. 7	Obj. No. 8
1.889444	sensory-BIT	sensory-SMP						
2.376973	sensory-HAY	sensory-CLN						
2.507987	sensory-IMP	sensory-TAS						
3.167017	sensory-IRR	sensory-SMV						
4.274753	sensory-IMP	sensory-TAS	sensory-IRR	sensory-SMV				
4.616010	sensory-BIT	sensory-SMP	sensory-HAY	sensory-CLN				
11.86804	sensory-IMP	sensory-TAS	sensory-IRR	sensory-SMV	sensory-BIT	sensory-SMP	sensory-HAY	sensory-CLN

Table 6. Regression coefficient about Hay-like based on correlation among raw data by PLS

	Summary of PLS_Correlation-rawdata-16del Responses: sensory-HAY options: no intrecept auto scale			
	Increase R^2 of Y	Average R^2 of Y	Increase R^2 of X	Average R^2 of X
Comp* 1	0.149558	0.149558	0.330341	0.330341
Comp 2	0.310082	0.459640	0.109634	0.439975
Comp 3	0.012568	0.472208	0.396306	0.836280
Comp 4	0.096397	0.568605	0.071685	0.907965
Comp 5	0.123558	0.692163	0.048624	0956588
Comp 6	0.158282	0.850445	0.009719	0.966307
Comp 7	0.019449	0.869894	0.023605	0.989913
Comp 8	0.028254	0.898148	0.004260	0.994173
Comp 9	0.021088	0.919236	0.003403	0.997576
Comp 10	0.056348	0.975583	0.001007	0.998583
Comp 11	0.024417	1.000000	0.001417	1.000000

*Comp1: Leaf_NO_3, Comp2: Smoke_CO, Comp3: Leaf_Crude F., Comp4: Leaf_NH_3, Comp5:Leaf_Sugar, Comp6: Leaf_Chloride, Comp7: Leaf_Ether, Comp8: Smoke_puff no., Comp9: Smoke_TPM

in Fig. 3 by showing order.

Cumulated average r squared value of regression model equation over the table 6 is expressed in Fig. 3 as the regression trend line. It means that we input first explanatory variable into model then R Square is 0.149 and input second explanatory variable into model then R Square is 0.459. To do so, we find out minimum number of explanatory variable for find out model which is best describing data In the Fig. 4, the circled line says that how many components are needed to arrive at ninety percent of r squared value.

For the bitterness, as the same manner, leaf

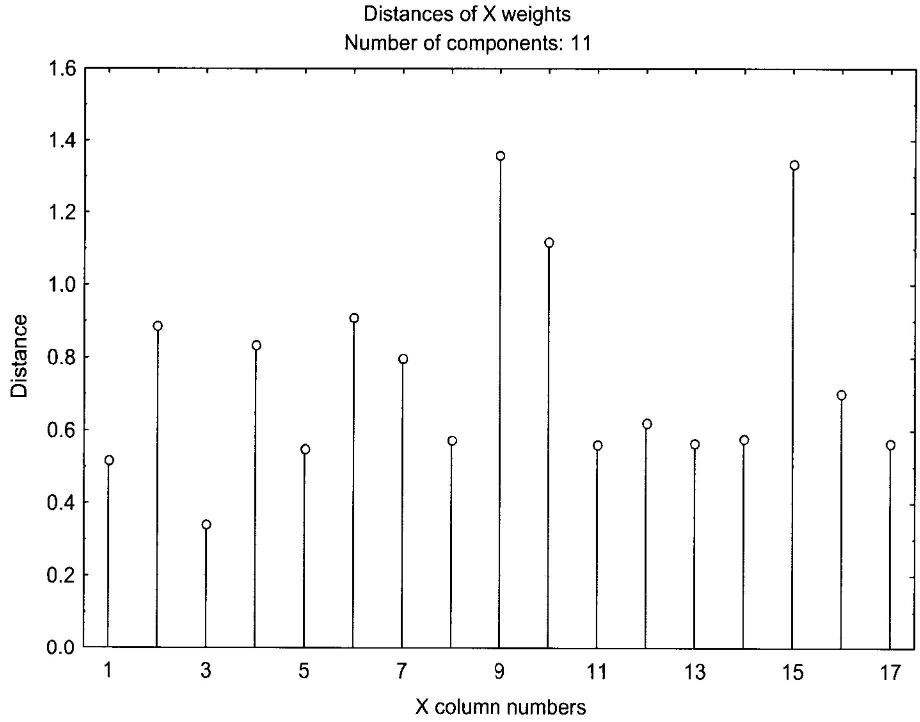

Fig. 3. Graph of the distance weighted least square fitting analysis about Hay-like by PLS.

Table 7. Distance weight value in various components about Hay-like by PLS

	Distances of X weights_Correlation_rawdata_16del_del survivor Responses: sensoryHAY/ options: no intercept auto scale										
Leaf Components	**Leaf** _Nic.	_total sugar	_total nitrogen	_chloride	_pH	$\_NH_3$	_ether	_TVB	$\_NO_3$	_crude fiber	_crudeash
Distances	0.516327	0.886852	0.339308	0.833937	0.550822	0.909284	0.798207	0.573302	1.357868	1.117693	0.560352

	Distances of X weights_Correlation_rawdata_16del_del survivor Responses: sensoryHAY/ options: no intercept auto scale					
Smoke Components	**Smoke** _TPM	_Nic.	_Tar	_CO	_puff No.	_Nic./Tar
Distances	0.621762	0.563915	0.575651	1.334609	0.703688	0.566525

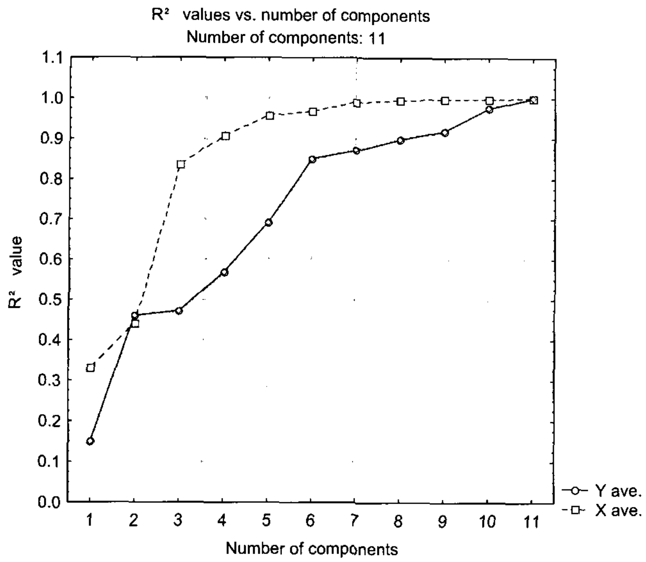

Fig. 4. Regression trend line about Hay like by PLS.

Table 8. *Regression coefficient about Bitterness by PLS*

	Summary of PLS_Correlation-rawdata-16del_del survivon Responses: sensory-BIT/Options: no intercept auto scale			
	Increase R^2 of Y	Average R^2 of Y	Increase R^2 of X	Average R^2 of X
Comp* 1	0.880801	0.880801	0.427112	0.427112
Comp 2	0.045319	0.926120	0.084731	0.511843
Comp 3	0.007288	0.933409	0.334248	0.846127
Comp 4	0.018208	0.951617	0.069638	0.915765
Comp 5	0.033268	0.984885	0.036484	0.952250
Comp 6	0.007310	0.992195	0.023259	0.975509
Comp 7	0.004580	0.996775	0.009528	0.985037
Comp 8	0.001086	0.997861	0.010594	0.995631
Comp 9	0.000882	0.998743	0.002017	0.997648
Comp 10	0.000339	0.999081	0.001942	0.999590
Comp 11	0.000919	1.000000	0.000410	1.000000

*Comp1 : Leaf_NO_3, Comp2 : Leaf_Crude F.

Table 9. Distance weight value in various components about Bitterness by PLS

	Distances of X weights_Correlation-rawdata-16del_del_survivor Responses: sensory-BIT/Options: no intercept auto scale							
	Leaf-Nic	Leaf-total sugar	Leaf-total nitrogn	Leaf-chlorid	Leaf-pH	Leaf-NH_3	Leaf-Ether	Leaf-TVB
Distance	0.564422	0.733807	0.502780	0.832611	0.573463	0.960146	0.780901	0.772523

	Distances of X weights_Correlation-rawdata-16del_del_survivor Responses: sensory-BIT/Options: no intercept auto scale						
	Leaf-NO_3	Leaf-crude fiber	Leaf-crude	smoke-TPM	smoke-Nic.	smoke-Tar	smoke-CO
Distance	1.211356	1.030248	0.705859	0.846367	0.598896	0.810864	0.938310

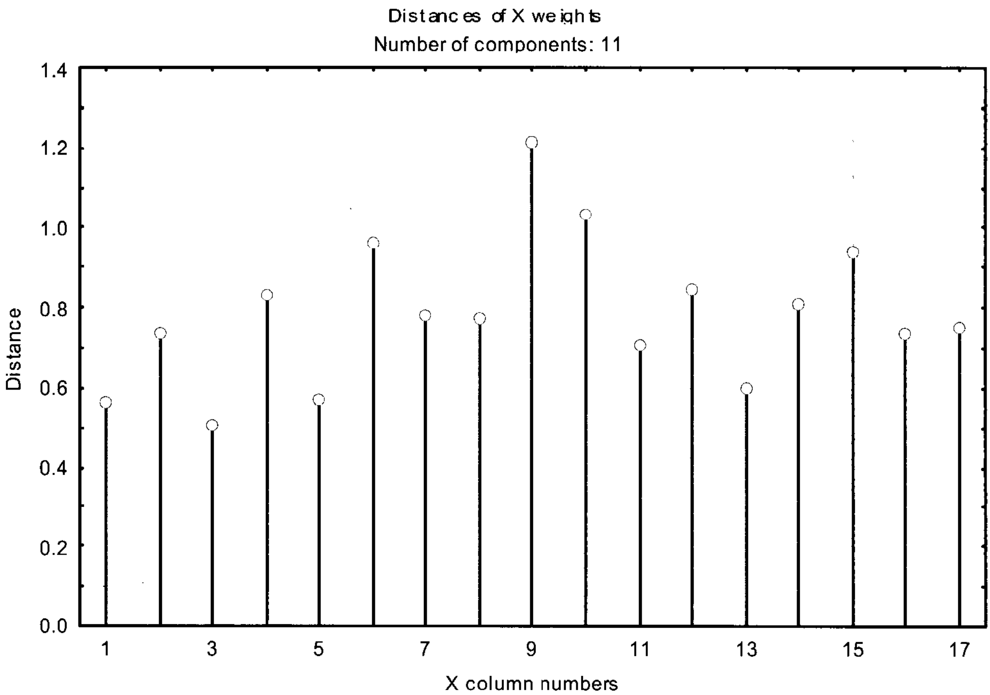

Fig. 5. Graph through the distance weighted least square fitting analysis about Bitterness by PLS.

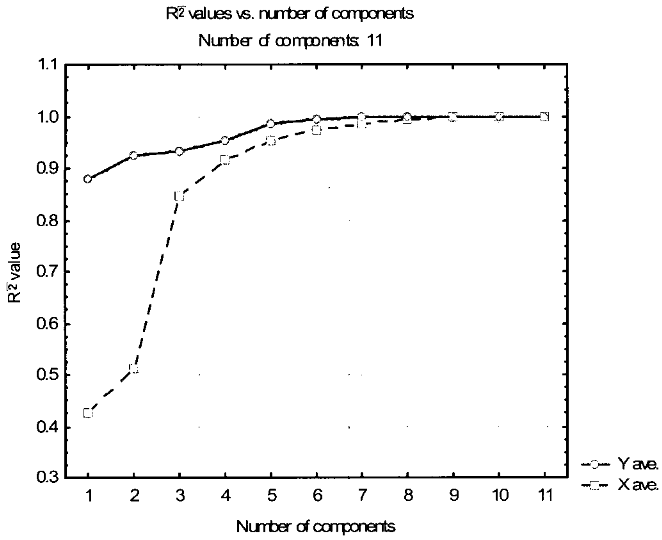

Fig. 6. Regression trend line about Bitterness by PLS.

Table 10. Explanatory variables for sensory properties IMP, BIT, HAY and TAS

Dependent Variable	IMPACT		BITTERNESS		HAY-LIKE		TOB. TASTE	
Explanatory Variable	Leaf	-TVB*	Leaf	$-NO_3$*	Leaf	$-NO_3$*	Leaf	$-NO_3$*
		$-NO_3$*		-Crude F.	Smoke	-CO*		$-NH_3$*
		$-NH_3$*			Leaf	-Crude F.	Smoke	-Nic.
		-Sugar				$-NH_3$	Leaf	-Ether
	Smoke	-CO*				-Sugar	Smoke	-TPM
	Leaf	-Ether				-Chloride	Leaf	-pH
		-Crude F.				-Ether		-Sugar
		-pH			Smoke	-Puff No.		-Nic.
	Smoke	-N/T				-TPM		-Crude F.
								-Crude A.

Table 11. Explanatory variables for sensory properties IRR, SMV, SMP and CLN

Dependent Variable	IRRITATION		SMOKE VOLUME		SMOKE PUNGENT		CLEANNESS	
Explanatory Variable	Leaf	$-NO_3$*	Leaf	$-NO_3$*	Leaf	$-NO_3$*	Leaf	$-NO_3$*
		$-NH_3$*		-TVB*		$-NH_3$*	Smoke	-Puff No.
		-TVB*	Smoke	-CO*	Leaf	-Crude A.	Leaf	$-NH_3$*
	Smoke	-Puff No.	Leaf	-Crude F.		-TVB*		-TVB*
		-N/T		-Crude A.		-Crude F.		-Crude F.
								-ether
								-sugar

Table 12. Acquired explanatory variables and related sensory properties

Explanatory Variables	Related Sensory Properties
▣ Major ◦ Leaf nitrate, ammonia, TVB ◦ Smoke carbon monoxide	▣ Present Tobacco taste, Mouth dryness, Harsh taste Sharpness, Irritation, Impact etc.
▣ Minor ◦ Leaf crude fiber, total sugar ◦ Smoke nicotine, nicotine/tar	▣ Findings ◦ Hay-like, Smoke volume ◦ Smoke pungent, Cleanness

nitrates and leaf crude fiber was enough to explain. Table 8, 9, Fig. 5, and 6 demonstrate the fact.
According to statistical results, we obtained the table 10 and 11 about explanatory variables.
Associated explanatory variables about sensory properties were developed such as, impact, bitterness, hay like, tobacco taste, irritation, smoke volume, smoke pungent and cleanness in separately. The enumerated components are followed by the number of components and an example of sufficient variable for explaining above ninety percent. The asterisked character means derived common major variables by our research. In addition, explanatory variables and related sensory properties were shown in table 12 ultimately.

CONCLUSION

This study could be summarized in two points. One is verification of the correlation among leaf/smoke components and sensory properties. The other is derivation and selection of the major four influencing variables, such as leaf nitrates, leaf ammonia, leaf TVB, and smoke carbon monoxide. In addition, we verified the minor four explanatory variables, namely, leaf crude fiber, total sugar, smoke nicotine and nicotine to tar ratio. New related four sensory attributes such as hay like, smoke volume, smoke pungent and cleanness with smoke/leaves components were developed. And we got a prospective point like feasibility for quality function deployment by selected main variables, and possibility for product guidance by all selected explicable compo nents was that. In the same ways, sensory properties with related to these influencing variables were taken about irritations, smoke volume, smoke pungent and cleanness. We developed four common major explicable variables.

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