Beiträge zur Tabakforschung International · *Contributions to Tobacco Research* Volume 18 · No. 4 · April 1999

DOI: 10.2478/cttr-2013-0679

Internal Standard-based Analytical Method for Tobacco Smoke Vapor Phase Components*

by

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SUMMARY

We developed an internal standard-based method to analyze the vapor phase components of mainstream smoke. This method collects vapor phase components from sample cigarettes, which are smoked by a linear automatic smoking machine in a sampling bag. An internal standard gas was introduced to the bag. A 6-port valve with a 2-ml sampling loop was placed between the vapor phase smoke outlet of the smoking machine and the bag to regulate the volume of the internal standard. The mixed gas sample was then introduced, by an automatic injection device developed in-house, to a gas chromatograph (GC) for ten successive analyses. The sample in the bag was analyzed every two hours to assess the time serial changes of vapor phase smoke components as well as of the internal standard. After 18 hours, in the tenth analysis, the amounts of 37 vapor phase components decreased by less than 5 % from those in the first analysis. The repeatability of the sample analysis was assessed and 45 vapor phase components had coefficients of variation of less than 5 %. The overall reproducibility of this method including tobacco samples and instruments was also assessed using five other sampling bags and achieved coefficients of variation of less than 6 % for 42 vapor phase components. The advantages of this method include capability to handle 10 tobacco samples in a serial manner, capability to collect both the vapor phase and semivolatile components, and precise, easy and continuous component analyses.

We also present the results of multivariate analyses for the vapor phase and semivolatile components from 59 sample cigarettes. [Beitr. Tabakforsch. Int. 18 (1999) 131– 146]

ZUSAMMENFASSUNG

Eine Methode mit internem Standard zur Analyse der Gasphasenbestandteile im Cigarettenhauptstromrauch wurde entwickelt. Bei dieser Methode werden Gasphasenbestandteile aus Testcigaretten, die mit einer linearen, automatisierten Rauchmaschine abgeraucht wurden, in einem Probenbeutel gesammelt. Ein internes Standardgas wurde dem Sammelbeutel zugeführt. Ein sechswegiges Ventil mit einer 2-ml Probenschleife wurde zwischen den Gasphasenaustritt der Rauchmaschine und den Auffangbeutel geschaltet, um das Volumen des internen Standards zu regulieren. Die Gasprobenmischung wurde dann mit Hilfe einer automatischen Einspritzvorrichtung, die im Haus entwickelt wurde, einem Gaschromatographen für 10 aufeinanderfolgende Analysen zugeführt. Die Probe in dem Sammelbeutel wurde alle zwei Stunden analysiert, um sowohl zeitliche Veränderungen der Gasphasenbestandteile des Cigarettenhauptstromrauchs als auch Veränderungen des internen Standards zu messen. Nach 18 Stunden, während der zehnten Analyse, waren die Mengen von 37 Gasphasenbestandteilen um weniger als 5 % niedriger als bei der ersten Analyse. Die Wiederholbarkeit der Probenanalyse wurde berechnet und bei 45 Gasphasenbestandteilen waren die Variationskoeffizienten unter 5 %. Die Reproduzierbarkeit der

*Received: 5th May 1998 – accepted: 9th February 1999

Gesamtmethode einschließlich der verwendeten Tabakproben und Instrumente wurde ebenfalls bestimmt, indem fünf weitere Auffangbeutel installiert wurden. Hierbei waren die Variationskoeffizienten von 42 Gasphasenbestandteilen niedriger als 6 %. Die Vorteile dieser Methode bestehen darin, dass 10 Tabakproben in Serie untersucht werden können, dass sowohl Gasphasenbestandteile als auch semivolatile Komponenten aufgefangen werden können und dass eine präzise, einfache und kontinuierliche Analyse der Bestandteile des Hauptstromrauchs möglich ist.
Die Resultate der multivariaten Analyse von Gasphasenbestandteilen und semivolatilen Bestandteilen von 56 Tabakproben werden ebenfalls beschrieben. [Beitr. Tabakforsch. Int. 18 (1999) 131–146]

RESUME

Une méthode permettant d'introduire un étalon interne pour doser les composants de la phase gazeuse du courant principale de cigarettes a été développé. Ce système recueille dans un sac d'échantillons les composants de la phase gazeuse de cigarettes d'essais qui sont fumées avec une machine à fumer automatique linéaire. Le sac a été chargé d'un étalon interne. Une valve à six canaux avec une boucle d'échantillons de 2-ml était installée entre l'orifice d'émission de la phase gazeuse sur la machine à fumer et le sac d'échantillonnage à chaque canal pour régler le volume de l'étalon interne. L'échantillon du mélange de gaz a été ajouté dans le système GC à l'aide d'un dispositif d'injection de fabrication ‚maison' pour dix analyses consécutives. L'échantillon recueilli dans le sac de gaz a été analysé toutes les deux heures pour déterminer les changements en fonction du temps des composants de la phase gazeuse de la fumée et de l'étalon interne. Après 18 heures, au cours de la dixième analyse, les rendements de 37 composants de la phase gazeuse avaient diminués de moins de 5 % comparée aux résultats obtenus après la première analyse. La réproductibilité globale de cette méthode incluant les échantillons de tabacs et les instruments était également calculée à l'aide de cinq autres sacs d'échantillonnage et le coefficient de variation du système résultant était inférieur à 6 % pour 42 composants de la phase gazeuse. L'avantage de cette méthode comprend la capacité de manoeuvrer 10 échantillons de tabacs consécutivement, la possibilité de recueillir simultanément la phase gazeuse et les composants semi-volatiles et d'effectuer l'analyse en composante d'une manière précise, simple et continue.
Nous présentons également les résultats d'analyses multivariables appliquées aux composants analysés de la phase gazeuse et semi-volatile de 59 échantillons. [Beitr. Tabakforsch. Int. 18 (1999) 131–146]

INTRODUCTION

Scientists have actively developed a variety of analytical methods to determine the composition of mainstream and sidestream smoke more precisely, efficiently and simply. The composition of cigarette smoke depends on the types of tobacco leaf, cigarette paper and filter as well as the flavoring agents to be added. One report gives an indication of the composition of cigarette mainstream smoke (1). According to the report, gas phase components, mainly atmospheric nitrogen and oxygen, account for over 80 % (weight ratio) of mainstream smoke. The remaining less than 20 % is comprised of vapor phase components of which about 80 % is accounted for by CO_2, about 10 % by water, and the rest by hydrocarbons, carbonyls and furanes. Although particulate matter, trapped on the Cambridge filter, accounts for only a few percent of total mainstream smoke, over 90 % of the smoke components so far reported belong to particulate matter. Together with nicotine, the levels of these particulate matter components and their proportion heavily affect the taste and aroma of a particular cigarette whereas vapor phase components contribute to irritation (2, 3).

Analyzing both semivolatile and vapor phase components will not only provide basic scientific knowledge, but also have a practical benefit of clarifying the type of substances that consumers take in through direct or indirect smoking of cigarette products. Unlike the analyses of semivolatile components, vapor phase components analyses have failed to provide authentic data due to their poor precision and low efficiency.

More recent methods for vapor phase component analysis are divided into four major types according to their trapping approaches: direct injection (4, 5); cryogenic trap (6–12); adsorbent trap (13–16); and the sampling bag method (17). The direct injection method has an advantage of measuring fresh cigarette smoke and minimizing component degradation with time and reactions among components. Because of the limited volume that can be introduced into GC, only one puff of vapor phase components or a part of it may be measured, resulting in a sharp fluctuation in measurements which makes quantitative analysis difficult. The procedure is also complex. Cryogenic trapping has the advantages of easy addition of internal standards to vapor phase components and minimized component degradation with time because it handles them at very low temperatures. Because of these advantages, this method is often used to collect certain vapor phase components. However, the procedure involved is very complex and the method requires that component solubility and volatility

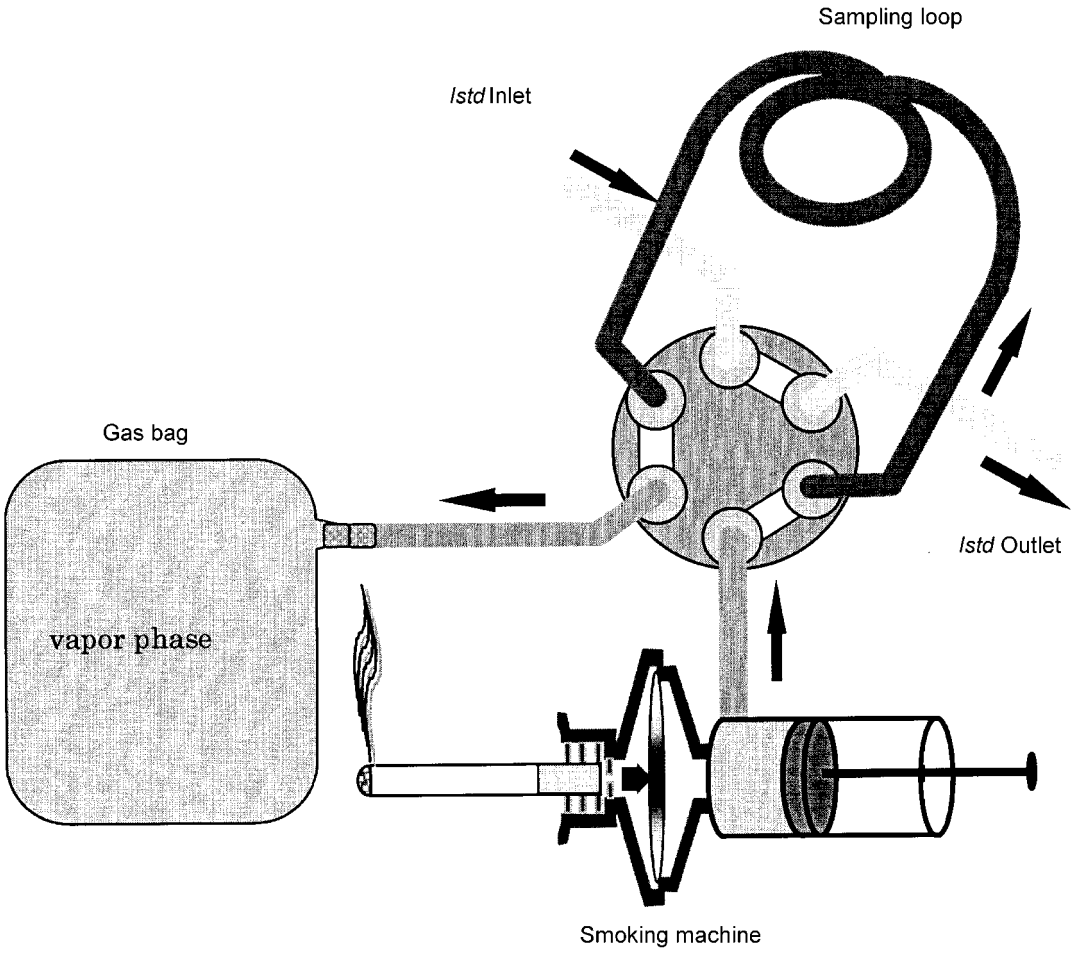

Figure 1.
Collection of mainstream smoke. One of 10 valves is shown.

to be taken into account. Thus, it is not always the best option to analyze all vapor phase components. Absorbent trapping can concentrate vapor phase components present at extremely low concentrations and thus it is widely used to collect air components (18). However, adsorption and desorption by the adsorbent used must be considered for each component, making it unsuitable for collecting all vapor phase components. While the sampling bag method can collect all vapor phase components, the collected components can degrade in the bag at room temperature. Since our study aims to analyze all vapor phase components, the sampling bag method was selected. An internal standard was used for quantitative analysis.

Previously, in the first phase of our study, we reported the automatic injection device we developed for use with GC (19) and, in the second phase, the use of the internal standard to analyze a wider array of vapor phase components (20). In the present report, we describe our analytical method in detail and present more data from the vapor phase component analysis to substantiate its usefulness.

EXPERIMENTAL METHOD

Cigarette samples

Commercially available cigarette samples from the Japanese market with 17 mg tar and a filter, were conditioned at 22 °C and 60 % RH for over 2 days.

Collection method

In accordance with the Tobacco Institute of Japan (TIOJ) puffing regimen (21) (puff volume: 35 mL, puff duration: 2 s, puff interval: 60 s), three sample cigarettes were smoked on a 20-port automatic linear smoking machine to collect their mainstream smoke components. The mainstream smoke was fractionated using a 26 mm Cambridge filter. We defined the components that passed the filter as vapor phase components and those that were trapped by the filter as semivolatile and nonvolatile components; however, only the vapor phase and semivolatile fractions were analyzed. The automatic smoking machine was modified to minimize the dead volume between the cylinder and the vapor phase component outlet.

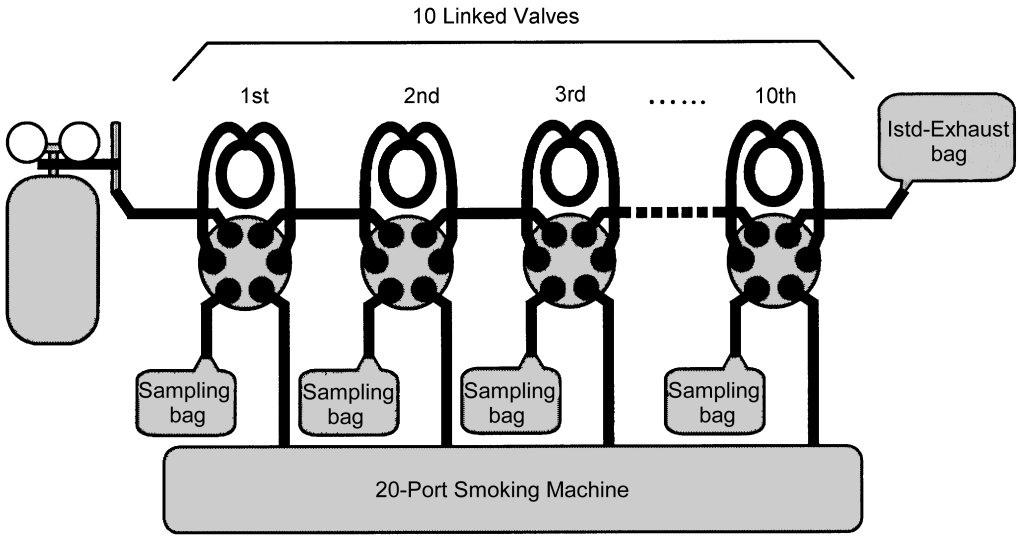

Figure 2.
Linked six-port valves. Step 1: Internal standard gas is fed to 10 sampling loops; step 2: Istd-exhaust bag is fitted to the 10th valve; step 3: internal standard gas is stopped to be fed; step 4: each valve is turned to connect the smoking machine, a sampling loop and a sampling bag; step 5: internal standard gas is introduced into the sampling bag by blank puff; step 6: each valve is turned back to connect the smoking machine and a sampling bag without a sampling loop; step 7: the cigarette is smoked to collect vapor phase and semivolatile components.

Collection of vapor phase components

A 6-port valve with a 2 mL sampling loop was placed between the smoking machine and a 4-layer aluminum bag. All the vapor phase components from the first puff to the last puff from three cigarettes were collected in the bag through the valve (Figure 1).

Internal standard gas

One percent 1,1,1,2-tetrafluoroethane balanced with helium was prepared in a gas cylinder to be used as the internal standard. The flow of the internal standard from the gas cylinder was regulated by a control valve to feed the gas at 100 mL per minute into the sampling loop on

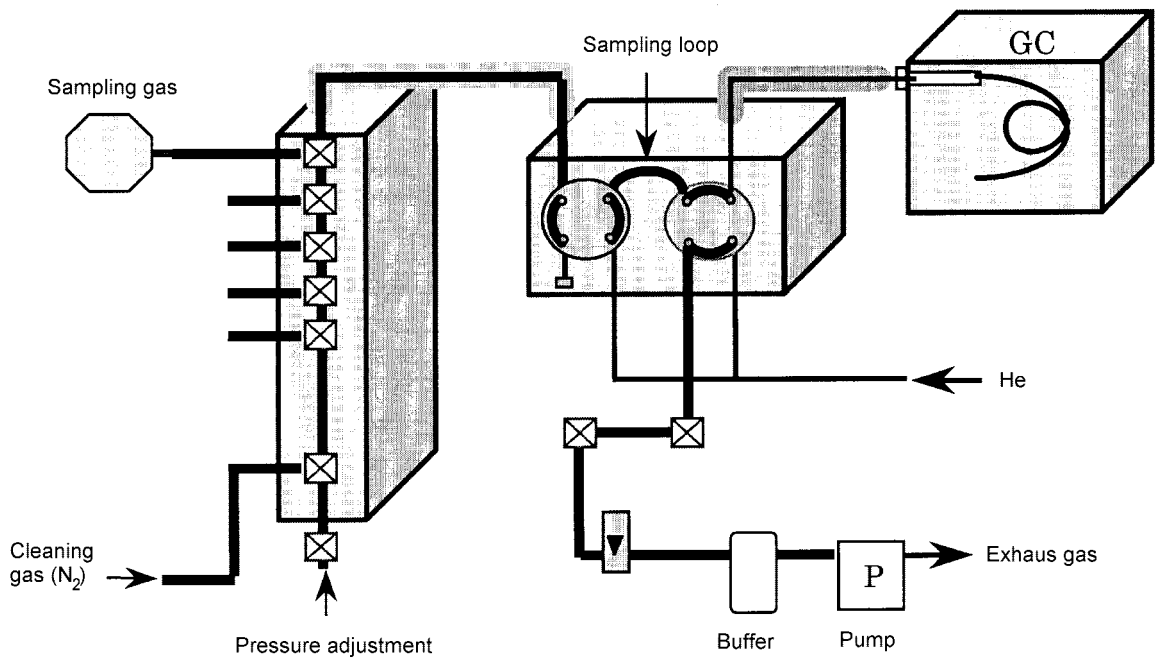

Figure 3.
Vapor phase component analytical system.

Table 1.
Vapor phase components.

Peak	Name	Peak	Name
V2	Methane	V32	Isoprene
V3	Ethylene & Acetylene	V35	unknown
V4	Ethane	V36	Propionitrile
V5	Propene	V38	unknown
V6	Propane	V39	unknown
V9	unknown	V40	Methylvinylketone
V10	Methylacetylene	V41	2-Methylfuran
V11	Methanol	V42	Diacethyl
V12	Acetaldehyde	V43	Methylethylketone
V14	Isobutane	V44	Methylacrylate
V16	1-Butene	V45	Isobutyronitrile
V17	1,3-Butadiene	V46	Crotonaldehyde
V18	*n*-Butane	V48	unknown
V19	*trans*-2-Butene	V50	Benzene
V20	*cis*-2-Butene	V51	Butyronitrile
V21	unknown	V52	unknown
V22	Acetonitrile	V53	Dimethylfurane
V23	Acroleine	V54	unknown
V24	Furan	V55	unknown
V25	Propionaldehyde	V56	*n*-Heptane
V26	Acetone	V57	Toluene
V27	Acryronitrile	V60	unknown
V30	Methylacetate	V61	unknown
V31	Cyclopentadiene		

the six-port valve. In order to analyze ten vapor phase component samples at a time, ten six-port valves were connected serially with the internal standard outlet of the first valve connected to the internal standard inlet on the next valve. Once the pressure in each sampling loop of the six-port valves is in equilibrium, then the sampling loop on each six-port valve mechanically holds that pressure. This means that each sampling loop on the six-port valves has the same amount of the internal standard gas (Figure 2). After the gas was fed to ten sampling loops for two minutes, the exhaust bag was fitted to the internal standard outlet of the 10th valve and supplied with gas for one more minute. Thirty seconds after the valve of the gas cylinder was closed, each six-port valve was turned to connect the smoking machine, a sampling loop and a sampling bag. The internal standard gas in the sampling loop was forced into the sampling bag by a blank puff of the smoking machine. This procedure was followed by the collecting of the cigarette smoke, and the mixture of the internal standard and vapor phase components were collected in ten bags in a single step.

Gas chromatographic analysis of vapor phase components

For simple and stable determination of vapor phase components collected in the sampling bag, our team developed an automatic injection device (19). This injection device (Figure 3) has a sampling loop that dispenses 5 ml of vapor phase components at a time from up to ten sampling bags to be supplied to the GC for

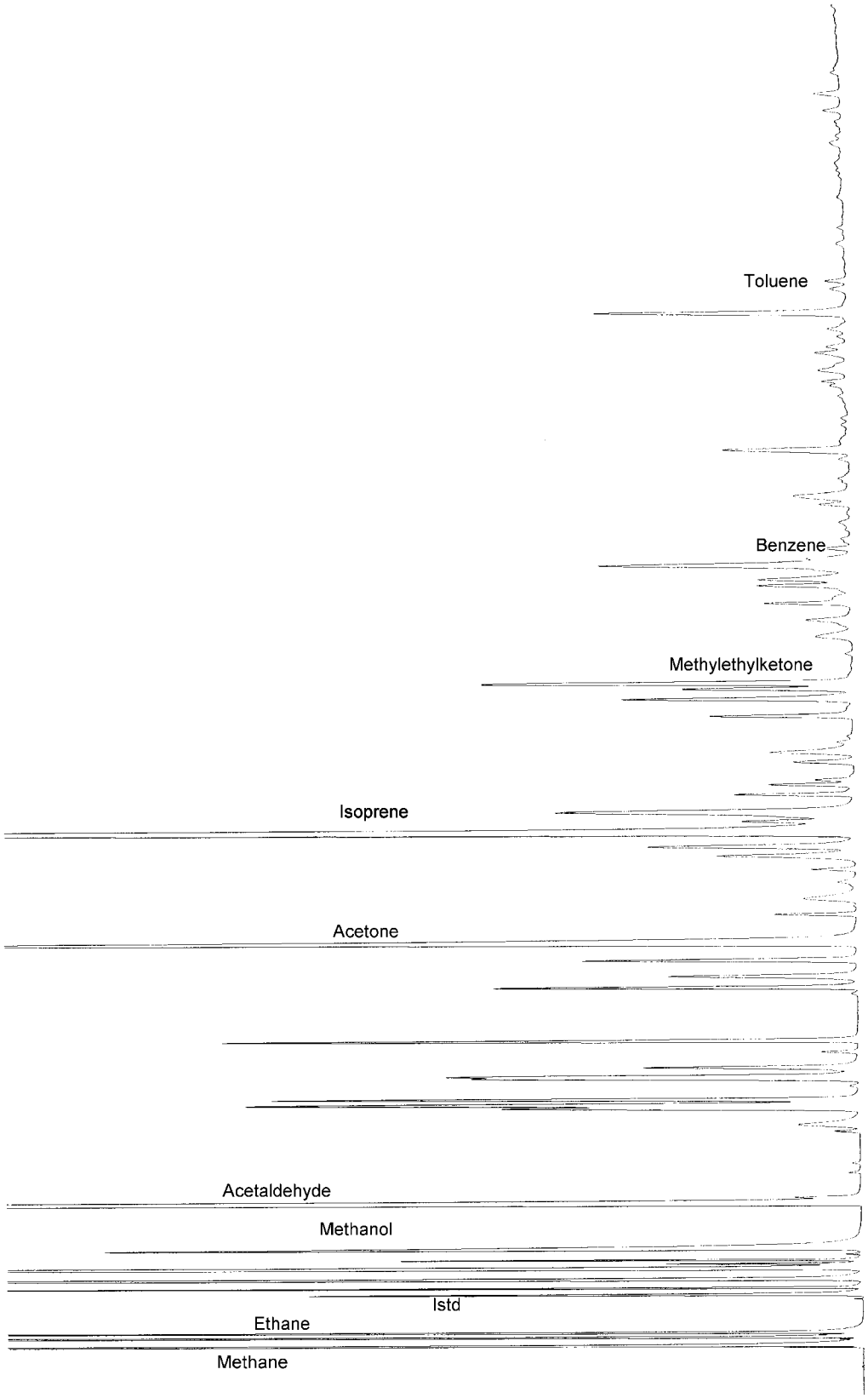

Figure 4.
Chromatogram of vapor phase components.

automatic analysis. A valve switching system changes the sample flow line to direct the sample in the loop to the GC. The sample is carried by He which is controlled by an electronic pressure controller (EPC). A Hewlett-Packard HP 5890 Series II GC-FID system was used. Vapor phase components were fed, by He carrier gas with

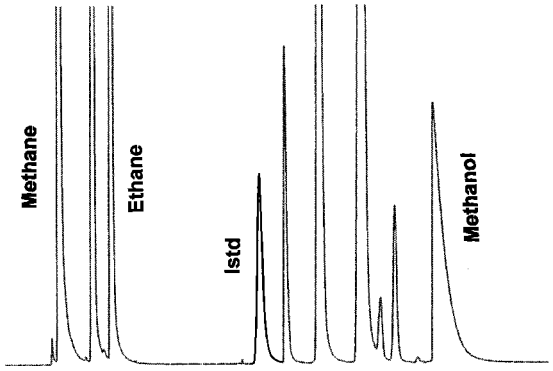

Figure 5.
Peak of Istd.

elevated temperature was held for 10 minutes. The analyzed vapor phase components and their chromatogram are shown in Table 1 and Figures 4 and 5. Each component was identified by GC-MS and its retention time.

Semivolatile components analysis

The semivolatile components, trapped on the Cambridge filter, were extracted with 0.75 mL of dichloromethane and methanol (4:1) containing ethyl phenyl acetate (0.45 mg) as an internal standard, followed by GC analysis. A Hewlett-Packard HP 5890 Series II GC-FID system was used. Semivolatile components were fed, by He carrier gas with a head pressure of 13.9 p.s.i.g. (constant

Table 2.
Semivolatile components.

Peak	Name	Peak	Name
S2	2,3-Butandione	S25	Solanone
S3	1-Pentene-3-one	S26	unknown
S4	Toluene	S27	Nicotine
S5	*m*-Xylene	S28	3-Ethyl-2-hydroxy-cyclopenten-1-one
S6	Cyclopentanone	S29	Neophytadiene
S7	Pyridine	S30	Phenol & *o*-Cresol
S8	Limonene	S31	2-Pyrrolidone
S11	3-Methylpyridine	S32	2,5-Dimethyl-4-hydroxy-3(2*H*)-furanone
S12	2-Cyclopentene-1-one	S33	*p*-Cresol
S13	2-Methyl-2-cyclopentene-1-one	S35	*m*-Cresol
S14	3-Ethylpyridine	S37	2,3-Dihydro-3,5-dihydroxy-6-methyl-4*H*-pyran-4-one
S15	Acetic acid	S38	Glycerol
S16	3-Vinylpyridine	S39	4-Vinylphenol
S17	3-Methyl-2-cyclopentene-1-one	S40	3-Hydroxypyridine
S18	Pyrrole	S41	Indole
S19	2,3-Dimethyl-2-cyclopentene-1-one	S43	5-Hydroxymethyl-2-furaldehyde
S20	5-Methyl-2-furfuran	S47	Hexadecanoic acid
S21	unknown	S48	1,4-Benzenediol
S24	Furfurylalcohol	S49	Hentriacontane

a head pressure of 27.5 p.s.i.g. (constant flow mode), to a PoraPLOT Q™ (25 mm × 0.32 mm i.d., 10 μm film thickness) fused-silica capillary column for separation. The temperature of the injection port was 225 °C in the split mode (split, 40:1) and that of the detector was 225 °C. The GC oven was held at 60 °C for 16 minutes, followed by heating at 2 °C/min to 230 °C and the flow mode), to a DBTM-WAX (30 mm × 0.25 mm i.d., 0.25 μm film thickness) fused-silica capillary column for separation. The temperature for the injection port was 250 °C in the split mode (split, 22.5:1) and that for the detector was 250 °C. The GC oven was held at 50 °C for 7 minutes, followed by heating at 2 °C/min to 240 °C

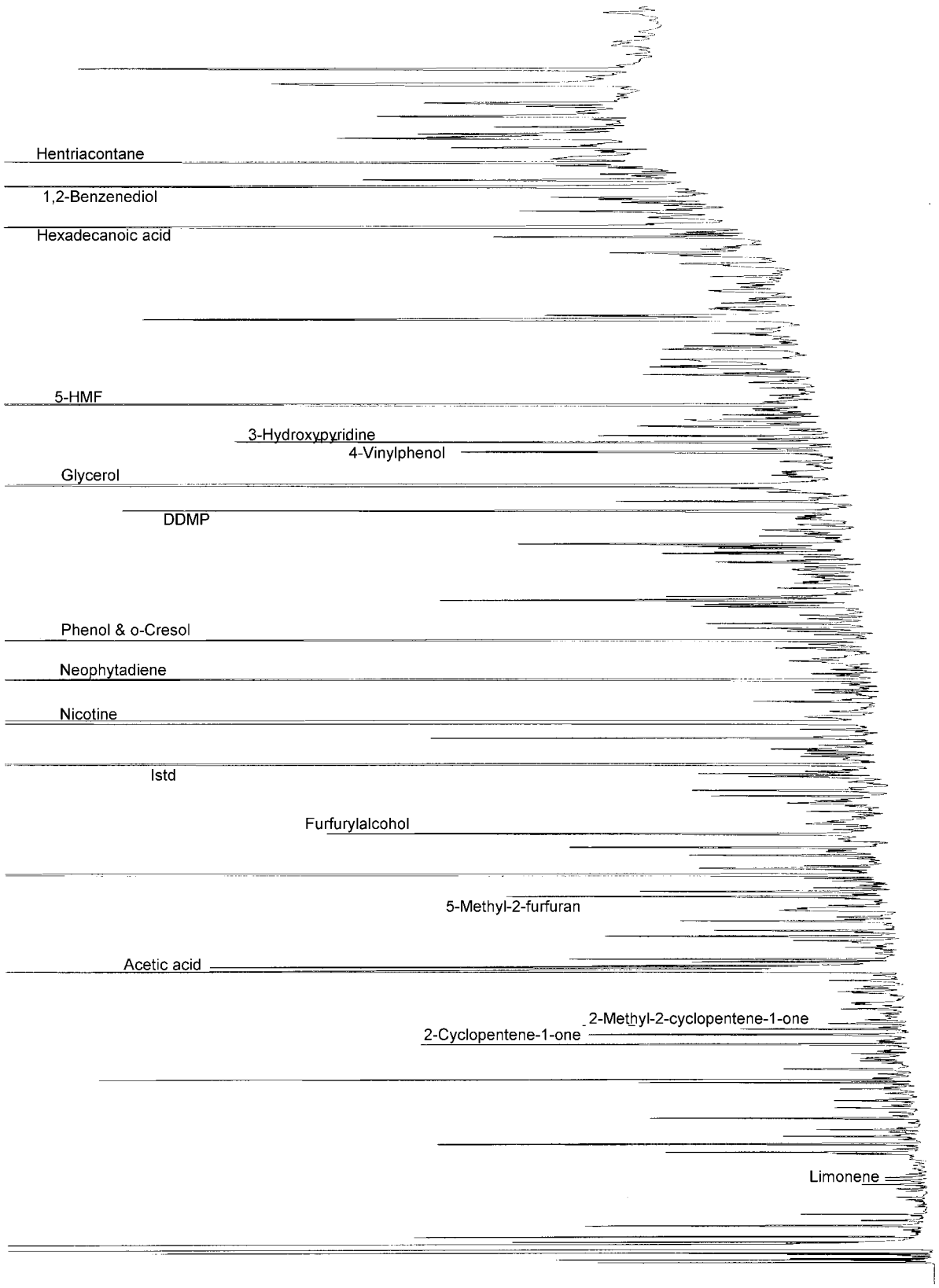

Figure 6.
Chromatogram of semivolatile components.

and the elevated temperature was held for 50 minutes. The analyzed semivolatile components and their chromatogram are shown in Table 2 and Figure 6. Each component was identified by GC-MS and its retention time.

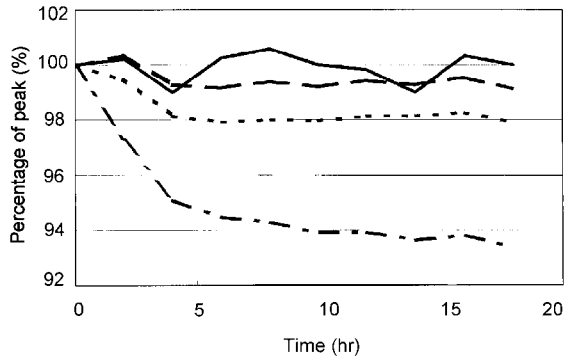

Figure 7.
Time serial changes of vapor phase components.
The same sampling bag was analyzed 10 times at two-hour intervals. (— — —: Acetone; ———: Benzene; - — - : Acrolein; - - - : Acetaldehyde).

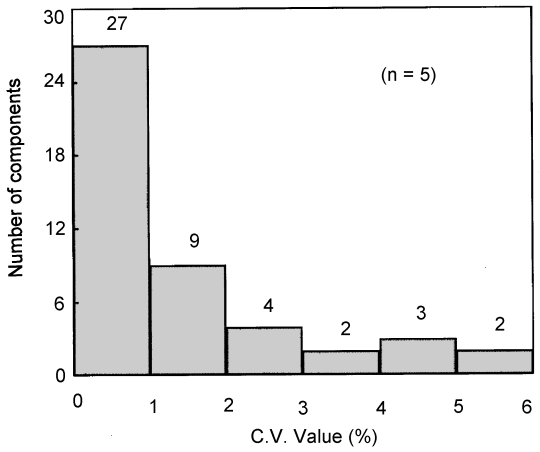

Figure 8.
Repeatability of vapor phase components analysis.

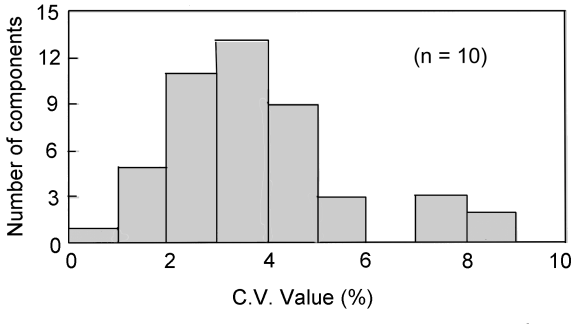

Figure 9.
Reproducibility of vapor phase components analysis.

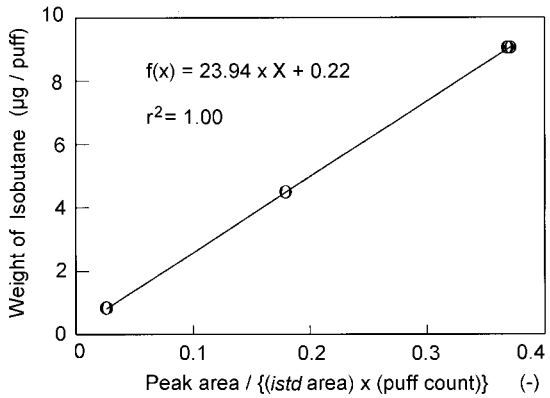

Figure 10.
Example of a calibration curve.

Quantitative analysis of vapor phase components

One percent isobutane, 1-butene, 1,3-butadiene, benzene, toluene, methanol, *cis*-2-butene and *n*-heptane balanced with helium was prepared in each gas cylinder as the reference gas. Each sample gas was diluted with helium and mixed with 2 ml of the internal standard gas on the automatic smoking machine.

RESULT

Selection of internal standard

In order to determine the optimum internal standard, we examined halides, especially fluorides, which are not present in the vapor phase components. Most internal standard candidates other than the controlled ozone-depleting substances overlapped with the collected vapor phase components on the chromatogram. The only substance that separated distinctively from collected vapor phase components was 1,1,1,2-tetrafluoroethane (Figure 5).

Time-serial changes in collected vapor phase components

Our system automatically analyzes 10 samples in a successive manner and it takes approximately 18 hours to complete the serial analysis of all the 10 samples. In order to evaluate the effect of time elapses during the serial analysis on the stability of the vapor phase components collected in the sampling bag, a sample in the same bag was analyzed under the same conditions every 2 hours for 18 hours. During this 18-hour period, the measured values of 24 out of 47 vapor phase component samples decreased only by less than 1 % and 13 out of 47 decreased by 1–5 %. The time-serial changes of four representative components are shown in Figure 7. When

Table 3.
Tobacco samples.

Variety	Origin	Number of samples
Flue-cured	Japan	8
	USA	6
Burley	Japan	8
	USA	7
Oriental		10
Total		39

these measurements are presented as the results of repeated analyses of the same samples in the same bag, 45 out of 47 components have a coefficient of variation (CV) of less than 5 %. These CV are sufficiently low and thus the series of analyses may be considered to have sufficiently good repeatability (Figure 8).

Reproducibility of vapor phase components analysis

The precision of our analytical system was also evaluated by repeating the analysis 5 times. The procedures involved smoking the sample cigarettes and analyzing their vapor phase components on GC. Forty-two out of 47 vapor phase components analyzed had a CV of less than 6 % (Figure 9).

Quantitative analysis of vapor phase components

For isobutane, the linearity of the system response was determined ($r^2 = 1$) within the expected range of concentration from the calibration plots of the reference gas (Figure 10). Response linearity was also confirmed for other vapor phase components. Based on these calibration curves, 39 tobacco samples (Table 3) were analyzed and the average quantitative values of different types and origins of tobacco leaves are shown as the average weight of the entire puff in Table 4.

APPLICATION

The possibilities of classifying cigarettes by tobacco variety, by country of origin and by stalk position based on the vapor phase and semivolatile component data, were evaluated. The data from 59 different tobacco samples (Table 5) were analyzed using principal component analysis (PCA), a kind of multivariate analysis. We already confirmed and reported that the data from the extracts of tobacco leaves were useful to classify the varieties of total tobacco leaves, the counties of origin and the stalk positions of both flue-cured and Burley tobacco samples (22, 23).

Table 4.
Average weight of vapor phase components (µg/puff).

Components	Flue-cured		Burley		Oriental
	Japan (SD)	USA (SD)	Japan (SD)	USA (SD)	(SD)
Isobutane	1.35 (0.15)	1.53 (0.14)	1.33 (0.16)	1.69 (0.10)	1.59 (0.15)
1-Butene	5.29 (0.20)	6.02 (0.49)	5.09 (0.43)	5.54 (0.37)	5.38 (0.40)
1,3-Butadiene	4.73 (0.40)	5.87 (0.73)	4.84 (0.53)	3.66 (0.93)	4.47 (0.40)
Benzene	5.84 (0.25)	5.77 (0.20)	5.65 (0.52)	6.29 (0.62)	5.53 (0.49)
Toluene	7.21 (0.85)	7.66 (0.71)	6.75 (1.13)	7.30 (0.95)	6.56 (0.46)
Methanol	15.49 (3.62)	39.58 (5.37)	27.74 (7.53)	14.29 (1.05)	15.04 (5.44)
cis-2-Butene	2.56 (0.09)	2.83 (0.20)	2.7 (0.33)	2.77 (0.16)	2.55 (0.20)
n-Heptane	0.60 (0.06)	0.71 (0.40)	0.82 (0.21)	1.10 (0.18)	0.59 (0.08)

Table 5.
Tobacco samples.

Variety	Origin	Number of samples
Flue-cured	Japan	8
	USA	6
	Other	10
Burley	Japan	8
	USA	7
	Other	10
Oriental		10
Total		59

SPSS Ver. 6 computer software. The factor loadings and the principal component scores, generated by PCA, are shown in Figures 11 and 12. In the chart of the principal component scores, the combination of the first and second principal components successfully identified the variety of total tobacco leaves. However, the plots are not particularly distinctive for counties of origin for both flue-cured and Burley tobaccos. From the chart of factor loadings, it is shown that propane (V6), crotonaldehyde (V46), 1-butene (V16) and benzene (V50) contribute most to the first principal components, whereas methyl acetate (V30) and furan (V24) contribute most to the second principal components. Because hydrocarbons, carboxylic acids, esters, ketones and aldehydes were distributed intricately throughout the scattered plots of factor loadings, the relation between tobacco leaves and vapor phase components could not be identified.

Table 6.
PCA of vapor phase components.

Factor	Eigenvalue	Proportion	Cumulative proportion
1	6.59	0.412	0.412
2	4.32	0.270	0.681
3	2.05	0.128	0.809
4	1.07	0.067	0.876

Table 7.
PCA of semivolatile components.

Factor	Eigenvalue	Proportion	Cumulative proportion
1	5.15	0.396	0.396
2	2.80	0.215	0.612
3	1.55	0.119	0.731
4	1.23	0.095	0.825

Principal component analysis using vapor phase components data

The data on 41 vapor phase components were analyzed using PCA (Table 6). The PCA was performed using

Principal component analysis using semivolatile component data

The data on 38 semivolatile components were analyzed using PCA (Table 7, Figures 13 and 14). In the chart of

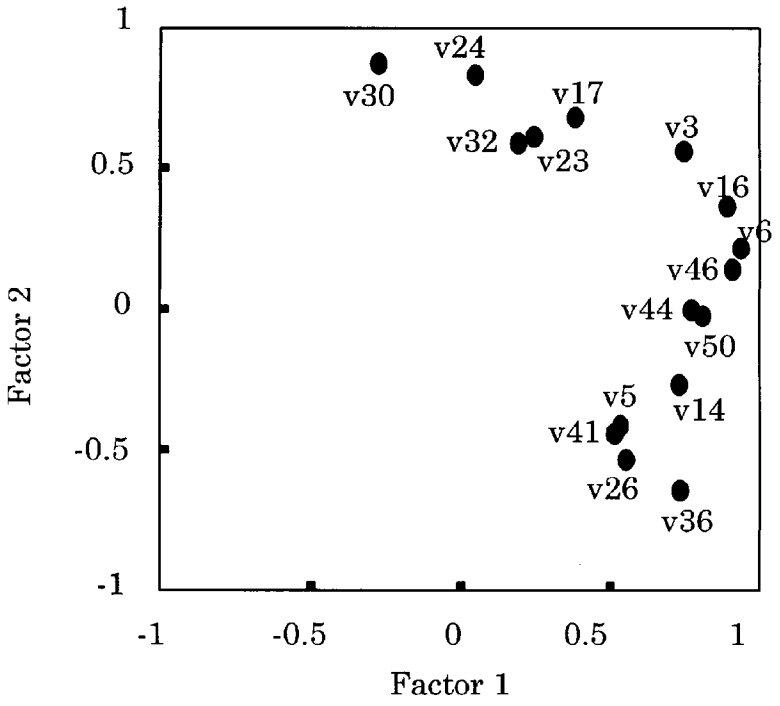

Figure 11.
Factor loadings (● vapor phase components).

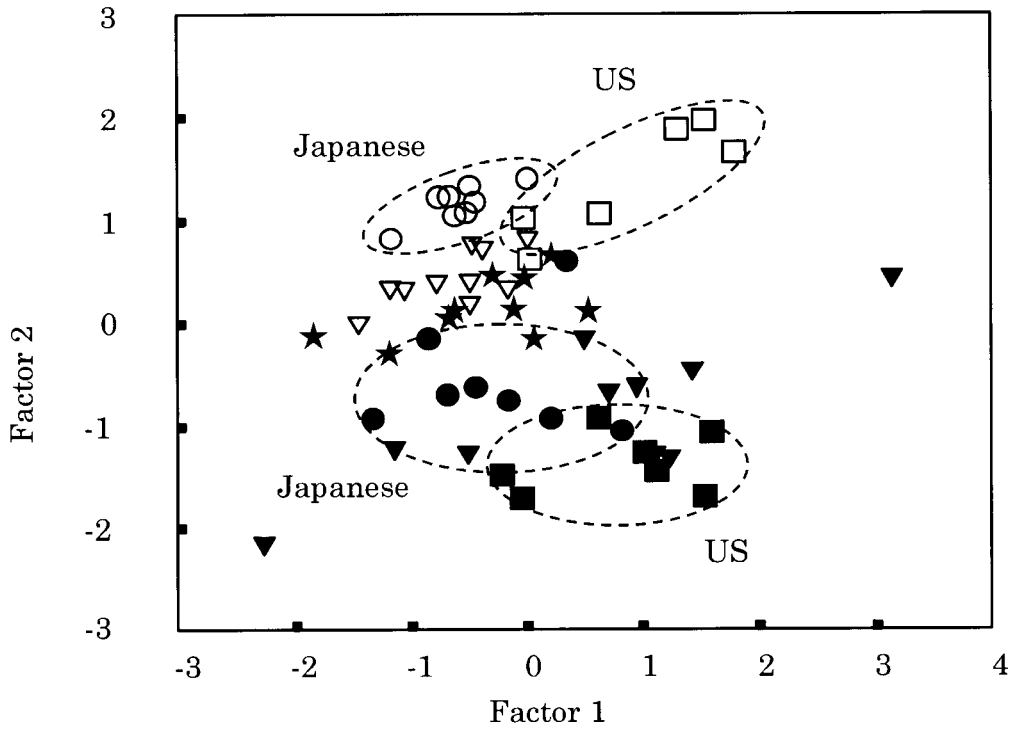

Figure 12.
Principal component scores (vapor phase components).
(★: Oriental; □ : flue-cured USA; ○ : flue-cured Japan; ▽ : flue-cured other countries; ■ : Burley USA; ● : Burley Japan; ▼ : Burley other countries)

principal component scores, the combination of the first and second principal components successfully identified the variety of total tobacco leaves more clearly than that of vapor phase components. As far as flue-cured tobacco

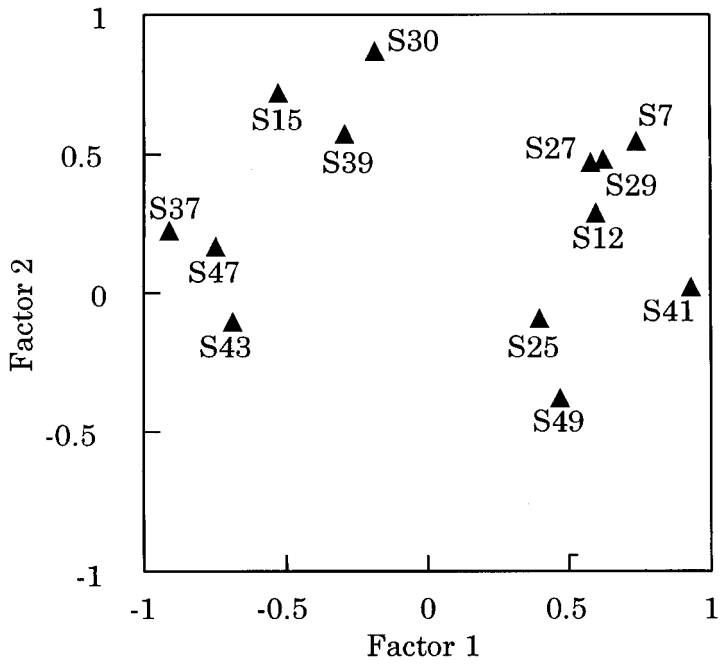

Figure 13.
Factor loadings (▲ : semivolatile components).

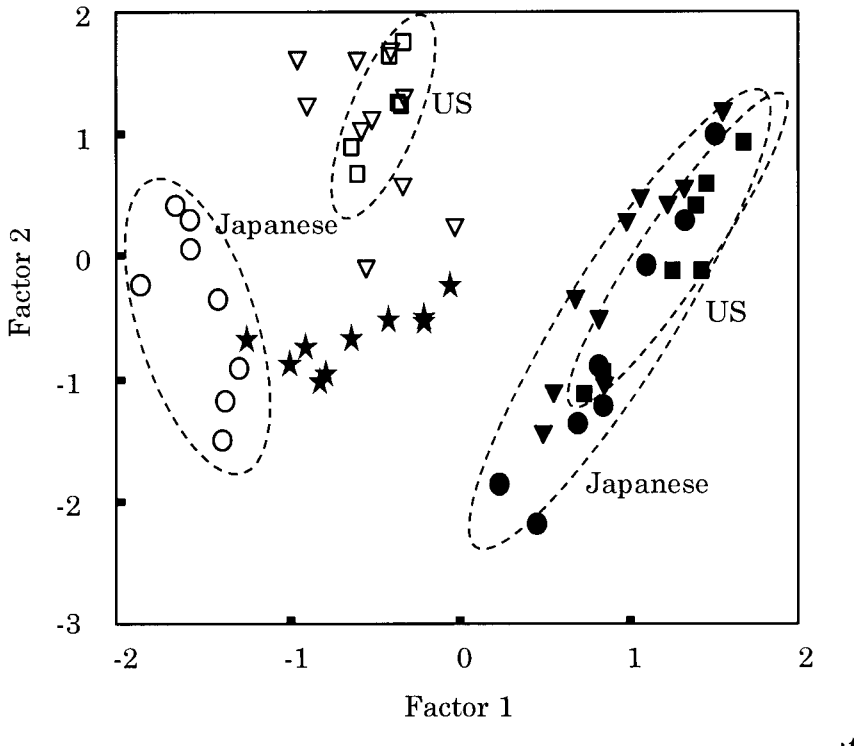

Figure 14.
Principal component scores (semivolatile components).
(★: Oriental; □ : flue-cured USA; ○ : flue-cured Japan; ▽ : flue-cured other countries; ■ : Burley USA; ● : Burley Japan; ▼ : Burley other countries)

is concerned, semivolatile component data successfully divided the plots into two distinctive groups each

representing different country of origin more clearly than the vapor phase component data. It seems that the same data did not have sufficient information to classify Burley tobacco by county of origin. On the chart of factor loadings, the scatter plots might be divided into three groups: (1) oxygen-containing components, which seem to be derived from sugar pyrolysates; (2) phenols; and (3) nitrogen-containing components. The proportions of oxygen and nitrogen-containing components differentiate flue-cured and Burley tobacco. It seems that the Japanese flue-cured tobacco contains more oxygen-containing components and US flue-cured contains morephenols and acetic acid.

Principal component analysis using both vapor phase and semivolatile component data

The combined vapor phase and semivolatile component data were analyzed using PCA (Table 8, Figures 15 and 16). In the chart of principal component scores, the combination of the first and second principal components

Table 8.
PCA of combined data.

Factor	Eigenvalue	Proportion	Cumulative proportion
1	9.92	0.342	0.342
2	6.95	0.240	0.582
3	3.53	0.122	0.704
4	2.02	0.070	0.774
5	1.87	0.064	0.838
6	1.37	0.047	0.885

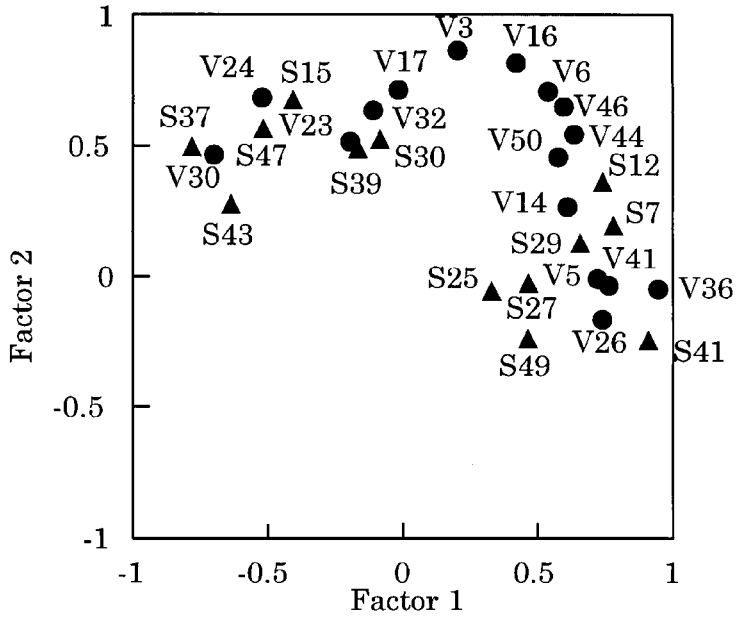

Figure 15.
Factor loadings. (● : vapor phase components; ▼ : semivolatile components).

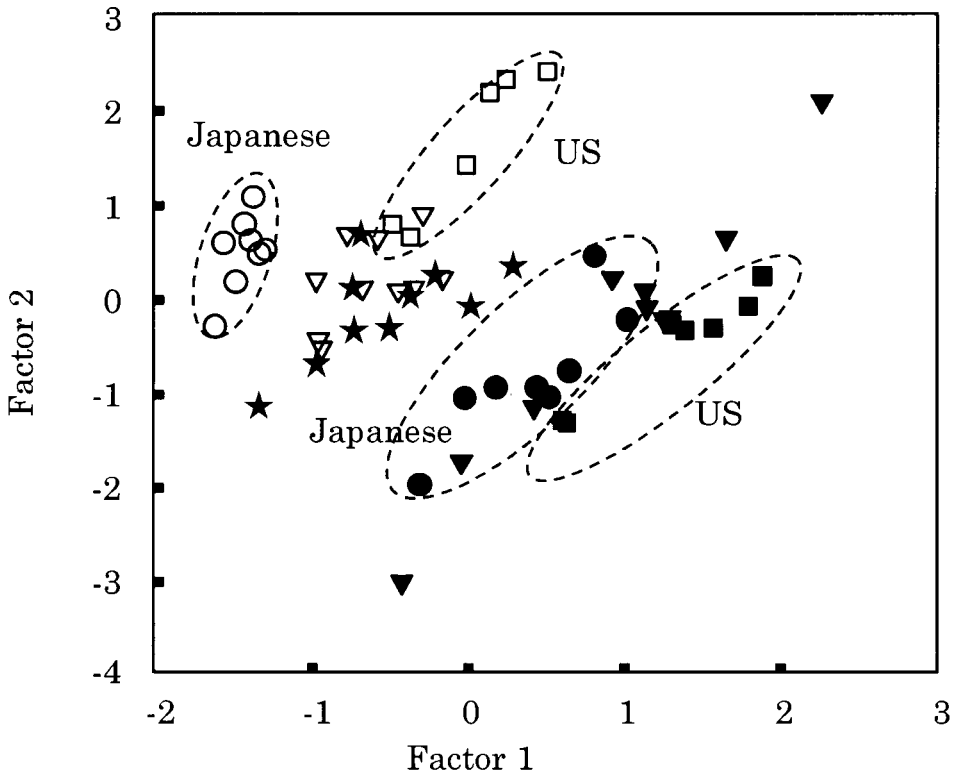

Figure 16.
Principal component scores (vapor phase and semivolatile components).
(★: Oriental; □ : flue-cured USA; ○ : flue-cured Japan; ▽ : flue-cured other countries; ■ : Burley USA; ● : Burley Japan; ▼ : Burley other countries)

identified the varieties and counties of origin of total tobacco leaves most clearly of all three PCA approaches. On the chart of factor loadings, scatter plots are also divided into three groups of oxygen-containing components, hydrocarbons and nitrogen-containing components. In the chart of principal component scores, the distribution of plots for each group such as Japanese flue-cured was elliptic. The expanded distribution of plots for each group may be attributable to the presence of vapor phase components such as hydrocarbons.

DISCUSSION

Usefulness of vapor phase component analysis

The analytical method discussed here enables simple and precise determination of vapor phase components. The data from this analysis may be used to classify tobacco leaves. Although the vapor phase component data alone fail to provide sufficient information to clearly classify tobacco leaves by variety and by country of origin, when they are combined with semivolatile component data, more clear-cut classification is possible. The combined data also provide other useful information such as stalk positions. Furthermore, the data may be used to determine how irritable a particular tobacco leaf or cigarette is because some of vapor phase components are irritants. The multivariate analysis used in this study will also help to trace the precursors of vapor phase components the procedure for which has been highly complex.

Qualitative differences between vapor phase and semivolatile component data

While the vapor phase component data successfully identified the variety of total tobacco leaves, as far as countries of origin are concerned, the distribution of the plots did not separate into distinctive groups and even partially overlapped for both flue-cured and Burley tobacco. On the other hand, semivolatile component data successfully identified the variety of total tobacco leaves more clearly. Although semivolatile component data provide more information about flue-cured tobacco leaves than those on vapor phase do, the plots for US Burley tobacco were completely contained in the plot area for Japanese Burley. From the fact that the combined data clearly characterized Burley tobacco, vapor phase components seem to have useful information about Burley tobacco.

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