

CHROM. 9494

GAS CHROMATOGRAPHIC-MASS SPECTROMETRIC EVALUATION OF EXHALED TOBACCO SMOKE

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SUMMARY

The impact of cigarette smoking on the distribution of organic substances in ambient air has been determined for the intermediate volatility range. A simple sampling procedure was employed, involving gas-solid adsorption onto an organic polymer followed by direct thermal elution onto a glass capillary column.

Aliphatic and substituted aromatic hydrocarbons are predominant in urban atmospheres. Depending on location and weather conditions the total concentration of such volatiles can differ by as much as a factor of 20. This high background variation makes it difficult to analyze for trace substances with low odor threshold values, such as encountered in cigarette smoke.

Standard cigarettes were smoked in a relatively small room, having no air filtration system. Air samples of approximately 3.5 l were taken. The amount of volatiles added to air by cigarette smoking is insignificant. Substances were analyzed and identified by gas chromatography and gas chromatography-mass spectrometry with glass capillary columns. Many compounds reported in cigarette smoke condensate have been confirmed.

INTRODUCTION

Cigarette smoking is clearly hazardous to health. Several states in the U.S.A. have recently enacted legislation which prohibits smoking in public buildings, and separate facilities for non-smokers are required in some parts of the country.

The composition of cigarette smoke is relatively well known, in spite of its tremendous complexity. A great deal of research has been devoted to the analysis of tobacco products, due to its general importance, but little is known about the substances non-smokers are exposed to in the presence of smokers. The analytical problems lie in both sampling and analysis. Significant advances have recently been made in sampling technology, and the analytical chemist now has several routes for the concentration of trace volatiles from air. Specialized analytical instrumentation

for such detailed analysis has been available for several years, but its use is still not widely accepted and generally restricted to laboratories which specialize in high-resolution separations.

The composition of volatile trace contaminants in air, especially urban air, has been investigated only within the last few years due to these experimental difficulties. Besides the permanent gases, water is the predominant substance in air. For obvious reasons, a preconcentration step is necessary prior to analysis. Its presence often causes problems for the analyst.

Surprisingly, the composition of organic volatiles in urban air closely resembles gasoline vapors^{1,2} in the intermediate volatility range to which this investigation has been directed. It is not clear to what extent loss of gasoline due to evaporation contributes or how much incomplete combustion in automobile engines is responsible. Alkanes and substituted aromatic hydrocarbons which make up the bulk of the organic material in urban air are relatively inert and only slowly undergo chemical change in the atmosphere. A higher reactivity, however, can be expected for unsaturates, oxygenated substances and similar labile compounds which take part in photochemical processes to various degrees. These substances are present only in relatively small concentrations, therefore, chromatographic profiles of urban air samples are relatively consistent.

Tobacco smoke can be expected to be much more reactive, and secondary reactions of sample components with each other, oxidation in air and photochemical reactions can produce many compounds which were not originally present in the smoke. On the other hand, other substances may be removed by absorption or may polymerize. The products obtained depend very much on the smoking conditions^{3,4}. Factors such as puff volume, puff rate, puff frequency, length of butt, the nature and type of the tobacco product, its history, and pretreatment as well as other extraneous variables such as moisture content, additives, texture and porosity of paper all influence the amount and distribution of components in tobacco smoke. Tobacco smoke analysts have agreed on standard smoking conditions, nevertheless, considerable variations can be expected from batch to batch even with the same tobaccos.

The standardized conditions used for the production of smoke condensate are not easily applicable for the analysis of tobacco smoke in air. The sampling conditions which were chosen in this investigation therefore represent a compromise between reproducibility and convenience. Since many of the substances generated by pyro-synthesis from plant material possess low odor and taste threshold values, as opposed to most contaminants in air, it is difficult to distinguish between compounds which are significant from the standpoint of biological activity or nuisance and substances which are relatively inert and do not represent a nuisance or health hazard.

SAMPLING CONSIDERATIONS

The preparation of air samples must be matched to the analytical technique to be used. Although the physical separation of sample components is not absolutely required even for a detailed analysis (high-resolution mass spectrometry (MS), especially with low-fragmentation ionization methods is another possibility), it is clearly desirable. Gas chromatography (GC) with high-resolution capillary columns is, at present, the most powerful approach for the type of analysis considered. The use of

such instruments requires relatively small samples, usually in the low μl range, with preferably low water content.

The most important sampling requirements can be summarized as follows:

- (a) Concentration in the desired volatility range with minimal interference from moisture
- (b) Complete and nondiscriminatory collection
- (c) Quantitative and unaltered regeneration
- (d) Compatibility with the instrument used for analysis
- (e) Simplicity

Several different approaches have been offered in the past. Syringe injection, or sample loops⁵⁻¹⁰ are useful only for relatively concentrated samples, unless special selective and sensitive detection techniques are applied such as multiple ion detection by MS. Cryogenic condensation with containers or onto packed columns¹¹⁻²⁶ is limited by the presence of water which will condense. On the other hand, this approach is well suited for gases and reactive substances and application of a temperature gradient ensures excellent recovery²⁷. Drying agents have been used sometimes prior to condensation; their use, however, is questionable for less volatile substances, and labile or reactive compounds as found in tobacco smoke might be altered or absorbed.

Gas-solid adsorption onto carbonaceous adsorbents of high surface areas has been the most popular concentration method before synthetic polymers have become commercially available. Activated carbon²⁸⁻³⁵ has been frequently used, often in combination with solvent extraction^{1,36-41}. Carbon molecular sieve^{42,43} has also been applied, however, excessive temperatures are required for sample regeneration by thermal desorption. Adsorption onto surface-modified siliceous supports⁴⁴ has been described, but these materials are commercially not available.

Synthetic polymers of hydrophobic nature have been introduced within the last few years and are now becoming increasingly popular for the enrichment of organic substances from dilute media. Several types of commercially available polymers have been applied to the concentration of trace organics from air⁴⁵⁻⁵⁷. Thermal elution has considerable advantages over solvent extraction methods, if the adsorbent can meet certain requirements. Besides adequate capacity for the compounds to be analyzed, avoidance of artifacts due to outgassing products and inertness are of prime importance. Not all organic adsorbents fulfill these requirements. Specially treated graphitized carbon blacks have also been applied for air sampling⁵⁸.

There are advantages and disadvantages to each principle which is applicable for the concentration of trace organics from air. Unfortunately, there is no universal method which can be used for a very wide volatility range. Methods must be combined to achieve some overlap. Cigarette smoke unfortunately falls into this category, since it includes a large variety of substances of various polarity, ranging from permanent gases to virtually involatile polymers and other high-molecular-weight substances. In dilute cigarette smoke in room air, semivolatile substances seem to account for the bulk of the material nonsmokers are exposed to. Our investigation has been directed towards this volatility range. The restriction however is not by choice but is rather dictated by the analytical tools, including both sampling methods and analytical instrumentation, which are currently available.

EXPERIMENTAL

Sampling

Air samples were taken in a room having a total volume of 60 m³. The sampler consisted of a vacuum source, a flow meter and set of three parallel tubes containing the adsorbent. Pyrex glass tubes 115 × 7 mm O.D. × 5 mm I.D. were filled with Tenax GC 60-80 mesh (Applied Science, State College, Pa., U.S.A.) and Carbopack BHT (Supelco, Bellefonte, Pa., U.S.A.). Both adsorbents were also coated with 5% and 25% of OV-101 silicon fluid. The uncoated tubes were conditioned at 330° for 60 min with nitrogen as carrier gas, the coated tubes were conditioned overnight.

Cigarettes (standard reference cigarette, IRI, University of Kentucky, Lexington, Ky., U.S.A.) were smoked under standard conditions. Immediately after a cigarette had been smoked, an air sample of 3.5 l was taken in triplicate at a flow-rate of 220 ml/min per tube. Samples were usually analyzed immediately.

For comparison, cigarette smoke samples were taken with a simple sampler of our own design. The device (Fig. 1) consisted of three parallel adsorbent tubes connected to a vacuum source via a flow meter. A fine metering valve and a shut-off valve (Whitey, Oakland, Calif., U.S.A.) were located between vacuum source and flow meter. The conditions were adjusted to yield puffs of 35 ml volume and 2 sec duration. To obtain the desired amount of cigarette smoke from a 2-sec puff, one of the tubes, having a variable restriction, served as bypass. An aliquot of only 3 ml of the smoke was drawn through each of the two sampling tubes during a puff. The samples, as evidenced by their gas chromatograms were relatively reproducible, but no effort was made to study the variations. The air samples were taken in Houston, Texas, and Tuscaloosa, Ala., over a period of several weeks.

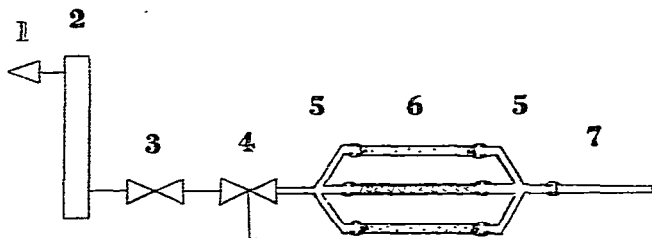


Fig. 1. Sampler for a small fraction of a standardized puff of fresh cigarette smoke. 1 = Vacuum source; 2 = flow meter; 3 = shutoff valve; 4 = fine metering valve; 5 = flow dividers and sample tube holders; 6 = adsorbent tubes and bypass tube; 7 = cigarette.

GC and GC-MS

A Hewlett-Packard GC 5830 with a flame ionization detector (FID), and a Hewlett-Packard GC 5720 with FID were used. Both instruments were modified to accept glass capillary columns. Additional injector ports were added to the instruments to accommodate the adsorbent tubes. Glass capillary columns of 0.35 mm I.D. and lengths between 25 and 55 m were drawn from soft glass, and either deactivated by Carbowax treatment according to Blomberg⁵⁹ or by standard silylation methods. OV-101 (Supelco, Bellefonte, Pa., U.S.A.) served as stationary phase. The columns were coated by either a modified plug method or the static procedure originally pro-

posed by Ilkova and Mistryukov⁶⁰. In the latter procedure in which the filled glass capillary is screwed into a hot oven, a heated mercury interface has been added. Columns were tested for efficiency and absorptive behavior. Average efficiencies, measured for *n*-decane at 100° were 2000–2600 effective plates per meter. Standards of phenolic compounds and aromatic amines were used to test the acid/base behavior of the column surfaces. Trapping periods of 30 min at 270° were allowed to compensate for the relatively large volume of the injector port. The purge gas passed through the entire column. No breakthrough was observed. Liquid nitrogen served as coolant.

Identifications were performed on a LKB 9000 gas chromatograph–mass spectrometer as described previously⁶¹. The column in the gas chromatograph–mass spectrometer was flow-controlled and rather reproducible over a period of several months. Mass spectra were deduced by comparison with reference spectra kept in our laboratory in files and with the use of standard tables⁶². In some cases where standards were available, small amounts of the references were added to the adsorbent tube by direct injection.

RESULTS AND DISCUSSION

Tobacco smoke analysis is one of the most challenging tasks for an analyst. Difficulties are encountered in both sampling procedures and the analysis itself. Nevertheless tobacco smoke condensate has been thoroughly investigated and its composition is now fairly well established. Grob applied capillary columns to cigarette smoke as early as 1962⁶³ and provided a comprehensive discussion on the analytical aspects with respect to sampling and especially column requirements^{64–66}. Others have also used capillary column GC-MS^{67–71} and further extended identifications.

Tobacco smoke analysts divide the total smoke into several overlapping fractions which have been well characterized. Little, however, is known about the fate of cigarette smoke condensate, as it ages and is exposed to air. It can be expected that variations in the smoke are reflected in the composition of volatiles found in air. Since a pyrolytic process is involved in the generation of the smoke, samples are often difficult to reproduce. For analysis, fresh cigarette smoke is desirable, but sample reproducibility may be low. Tobacco smoke condensate generated by smoking machines under standardized conditions is more reproducible, but changes inevitably occur during storage. The analyst is faced with the decision whether to apply a sampling technique which does deliver fresh tobacco smoke but which may not be easily reproducible from laboratory to laboratory or to use a more standardized technique which may generate additional artifacts.

It is common to distinguish between volatiles, semivolatiles and nonvolatiles. For the purpose of this investigation, the term "volatiles" refers to the material which can be collected and regenerated on an adsorbent, regardless if it is a true gaseous form or associated with particulate matter. As a basic rule, stable substances having boiling points between benzene and *n*-pentacosane fall into that category. To determine if significant differences could be determined between cigarette smoke in room air, filtered through a glass fiber filter and between unfiltered air, a short experiment was undertaken. Two tubes were connected in parallel and a glass fiber filter, as used for the collection of air particulate matter, was placed before the orifice of one tube. No significant differences were found.

The purpose of this investigation was the determination of the nature and approximate quantity of volatiles non-smokers are exposed to in the presence of smokers. An investigation was therefore undertaken to determine the suitability of several adsorbents for the selective concentration of organics from air. Only adsorbents were considered which permit thermal elution of the substances of interest at a moderate temperature, without generation of artifacts or absorptive losses. These requirements eliminate most of the classical adsorbents, such as activated carbon or silica gel, because of high surface activity or high affinity for water. Our previous experiences with a number of different adsorbents also indicated that crosslinked DVB polymers would not be suitable for the purpose, due to their limited temperature stability and high background. Silica beads modified by surface esterification were excluded because of their small sample capacity and sensitivity towards hydrolysis.

Tenax GC and Carboxpack fulfill more requirements. Unfortunately, the capacities of these adsorbents are quite small and usually insufficient for substances being more volatile than benzene, unless a large quantity of adsorbent is used. In principle, the trapping efficiency can be improved by this method. In practice, the acceptable amount of adsorbent however is limited, primarily by an increase in background contamination from the adsorbent and by water which does accumulate on both sample tube and adsorbent. During desorption, small amounts of water can then cause a physical obstruction in a small-bore capillary column, disrupting the transfer process.

For quantitative analysis, it is important to ensure that the adsorbent has adequate capacity for the substances under investigation. Sample recovery at trace levels must also be confirmed, since irreversible losses can easily occur, especially for adsorbents which are not completely homogeneous.

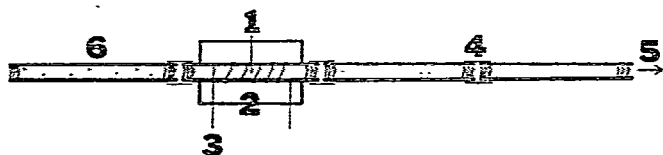


Fig. 2. Arrangement for the determination of breakthrough volumes and sample recoveries. 1 = Tube with small glass wool plug; 2 = thermal insulation; 3 = heating type; 4 = adsorbent tubes, in series; 5 = vacuum source; 6 = adsorbent tube for exclusion of air volatiles.

Fig. 2 shows the experimental arrangement which was used to evaluate breakthrough volumes and desorption efficiencies of some model compounds on Tenax GC. A standard was injected into a heated tube which preceded two sampling tubes in series, and a constant volume of air was drawn through the tubes. After injection, an additional tube was placed in front of the injection tube to exclude air volatiles. The adsorbent tubes were relatively small in size, 88×2.5 mm I.D., and contained approximately 70 mg of Tenax GC. Results are summarized in Table I. It should be noted that adsorption efficiencies depend on several parameters, such as sample size, amount of adsorbent, flow-rate, temperature, geometrical arrangement, etc. Fortunately, adsorbent capacity does not seem to be influenced to any extent by the moisture in the air⁷². Losses were estimated by difference with direct injections.

TABLE I

RECOVERY OF SELECTED COMPOUNDS ON TWO ADSORBENT TUBES CONNECTED IN SERIES

Conditions: tube, 88 × 2.2 mm I.D.; filled with Tenax GC, 60–80 mesh; flow-rate, 80 ml/min for 12 min; sampling temperature, 22–26°; desorption temperature, 320°; amount of single component, 30–100 ng.

Compound	MW	B.p. (°C)	Recovery (%) [*]		Lost ^{**}
			Tube 1	Tube 2	
<i>Alcohols</i>					
Methanol	32	65	< 2	< 4	>90
Ethanol	46	79	< 3	< 5	>90
Isopropanol	60	82	55	20	25
1-Hexanol	103	158	>90	< 5	< 5
1-Octanol			>95	< 5	< 3
<i>Ketones</i>					
Acetone	58	56	35	25	40
Methyl isobutyl ketone	100	117	95	< 5	< 3
2-Octanone	128	173	95	< 5	< 3
<i>Alkanes</i>					
<i>n</i> -Pentane	72	36	35	30	35
<i>n</i> -Hexane	86	69	65	20	15
<i>n</i> -Octane	114	126	>95	< 5	< 3
<i>n</i> -Decane	143	174	>95	< 5	< 3
<i>n</i> -Tetradecane	198	254	>95	< 5	< 3
<i>n</i> -Octadecane	255	316	>95	< 5	< 3
Cyclohexane	84	81	75	15	10
<i>Alkenes</i>					
1-Octene	112	121	>95	< 5	< 3
<i>Esters</i>					
Ethyl acetate	88	77	65	25	10
Butyl acetate	116	126	>95	< 5	< 3
<i>Halogenated hydrocarbons</i>					
Dichloromethane	85	40	15	20	65
Chloroform	119	62	85	10	5
Bromoform	253	150	>95	< 5	< 3
Trichlorotrifluoroethane	187	478	15	15	20
<i>Aromatic hydrocarbons</i>					
Benzene	78	80	65	30	5
Toluene	92	111	>95	< 5	< 3
Ethylbenzene	106	136	>95	< 5	< 3
Cumene	120	152	>95	< 5	< 3
Mesitylene	120	165	>95	< 5	< 3

^{*} Average results from 3 runs.

^{**} Calculated by difference.

In another series of experiments, Tenax GC and Carbo-pack BHT, having surface areas of approximately 20 m²/g and 90 m²/g (ref. 73) were compared to each other. Data are summarized in Table II. It can be seen that Carbo-pack BHT retains low-molecular-weight compounds slightly better than Tenax GC. Additional coating of these adsorbents with a high-temperature liquid phase of low viscosity should extend

TABLE II
RELATIVE TRAPPING EFFICIENCIES FOR COATED VERSUS NONCOATED TENAX GC AND CARBOPACK BHT

	Tenax 60-80		Tenax 5% OV-101		Tenax 25% OV-101		Carbopack BHT		Carbopack 5% OV-101		Carbopack 25% OV-101	
	Outer	Inner	Outer	Inner	Outer	Inner	Outer	Inner	Outer	Inner	Outer	Inner
C_6H_6	100	100	100	45	100	80	100	100	100	100	170	≈ 100
$C_6H_5-CH_3$	100	<2	100	4	100	7	100	<5	100	100	<5	0
$C_6H_5-C_2H_5$	100	0	100	0	100	<3	100	≈ 0	100	100	30	≈ 0

the usefulness of either adsorbent towards more volatile compounds. The data obtained support this prediction, the improvement, however, is smaller than expected. In general, Carbo-pack BHT and Tenax GC are comparable in performance.

Selective concentration of trace organics from air at ambient temperature followed by direct desorption is an attractive sampling approach, but the method has some inherent contradictions which limit its usefulness. The adsorbent, on one hand, should provide adequate and nonspecific retentions for substances of a wide boiling point range. This requirement can be met by choosing an adsorbent with a larger surface area. On the other hand, desorption temperatures, necessary for complete sample regeneration, especially of less volatile compounds also increases with increasing adsorbent activity. Obviously, a compromise must be found.

It is conceivable that the overall usable range of such gas-solid adsorption-thermal elution processes could be extended by the use of several adsorbents having different surface areas or by multilayer traps. In the latter, high-molecular-weight substances would be adsorbed on a less active adsorbent in the front section of the sample tube and only the more volatile compounds would move to the more active adsorbent layers. Sample regeneration could be done under relatively mild conditions. Preliminary experiments are still unsatisfactory and more work is needed to establish this procedure for practical use.

Most volatiles in urban air are clearly associated with gasoline. The absolute levels vary considerably depending primarily on sample location and weather conditions. Samples were taken within a short time interval to avoid drastic changes of the background. The contribution of cigarette smoke to the volatiles already present in an urban atmosphere is smaller than may be expected from its general appearance and odor perception. It is difficult to distinguish between the relatively small additions of volatiles coming from tobacco smoke under such background variations, but no effort was made to suppress the hydrocarbon background or to enhance the concentration of the cigarette smoke beyond a level which would not relate to conditions usually encountered in practice. Cigarettes were smoked in relatively large rooms and the cigarette smoke was strongly diluted under these circumstances. No attempt was made to analyze tobacco smoke itself. Cigarette smoke samples were only taken for purposes of comparison.

Fig. 3 shows the total ion current monitor profiles obtained from a 3.5-l sample of urban air, from a sample of the same volume, after a cigarette had been smoked, and from a 3-ml puff of the cigarette used for the experiment. Differences between the air samples are primarily in the higher molecular weight range.

Table III lists the identifications of both volatiles in urban air and the additions which result from the action of cigarette smoking. The quantitations are only semi-quantitative, since many of the peaks are composed of several unresolved substances. Some breakthrough of components has been observed over the entire range of the chromatogram, regardless of boiling point or substance type. This phenomenon still needs to be explained. Sample loss due to insufficient retention, however, is minor for the substances eluting after toluene (peak 42). For compounds eluting between benzene and toluene, adsorbent capacity might have been exceeded by a factor of 2 or 3. The picture gets progressively worse for the compounds eluting before benzene. These regions have therefore been omitted from quantitation.

It would be interesting to investigate the retention of tobacco smoke compo-

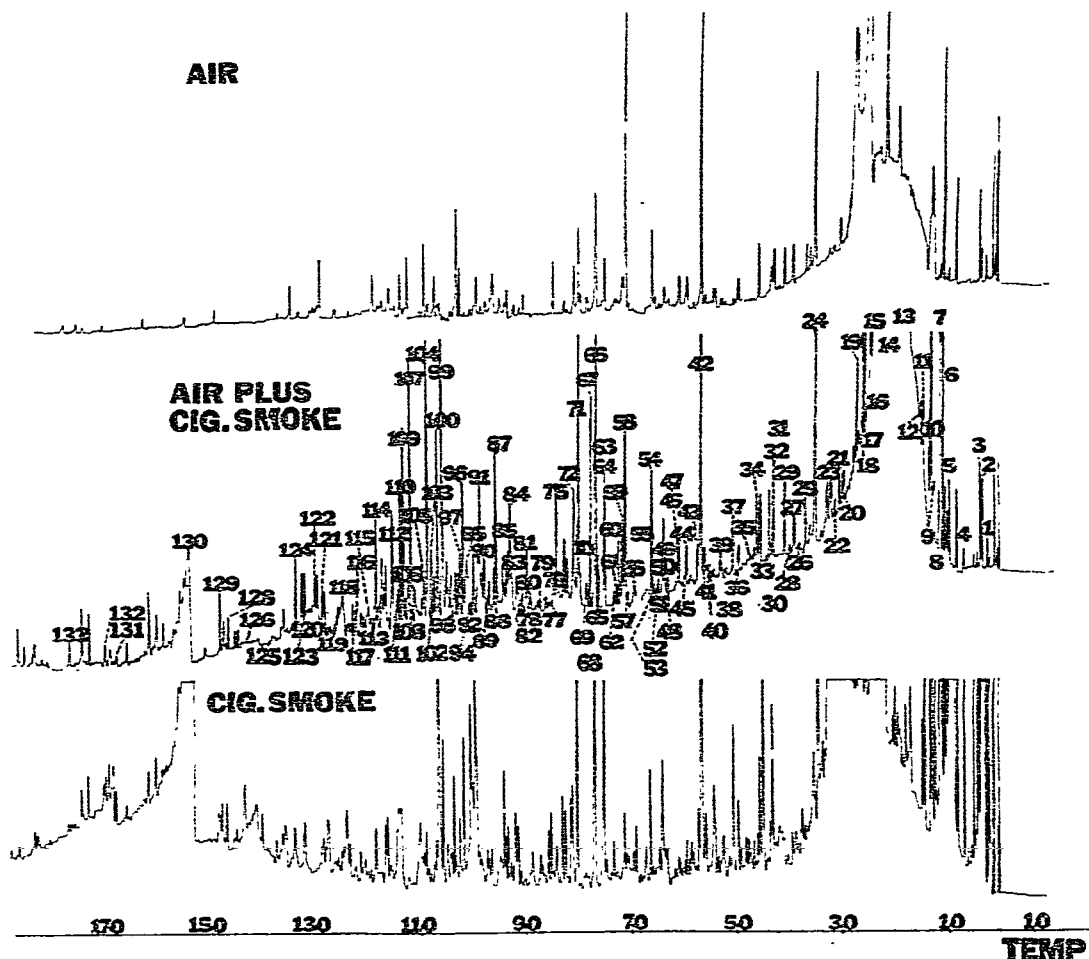


Fig. 3*. Total ion current chromatograms of urban air, air contaminated by cigarette smoke and cigarette smoke. Sample size of air samples, 3.5 l; sample size of cigarette puff, 3 ml; glass capillary column: 38 m \times 0.35 mm I.D., coated with OV-101; carrier gas (helium) flow-rate, 3 ml/min; temperature program: 20° for 8 min, 20–200° at 2°/min. For identification of peaks, see Table III.

nents in lung tissue. Preliminary investigations indicate that compounds found in tobacco smoke are still exhaled for a considerable time after the smoking process. An investigation into aspects of selective retention of some smoke constituents is presently underway.

* *Editor's note:* Fig. 3 contains very valuable information. It compares 3.5 l of air from a room in which a cigarette was smoked to a 3.5-ml puff of cigarette smoke. The 3.5-l volume is approximately the vital capacity (*i.e.*, the average volume which a person inspires and expires during normal respiration). From comparing the two chromatograms, it is evident that a person breathing in a room where one cigarette was smoked inspires the equivalent of a 3.5-ml puff of cigarette smoke (with 10 to 12 respirations per minute). Thus, I cannot agree to the authors' statement that "the amount of volatiles added to air by cigarette smoking is insignificant". *Editor of J. Chromatogr.*

TABLE III

IDENTIFICATION OF VOLATILES IN AIR AND AIR CONTAMINATED BY TOBACCO SMOKE

Peak No.	Compound	MW	Approximate concentration (ppb)		Method
			In air without cigarette smoke	In air with cigarette smoke	
1	1-Pentene	70			MS
2	C ₅ H ₁₂	72			MS
3	Acetaldehyde	44			MS
4	C ₅ H ₁₂	72			MS
5	<i>n</i> -Pentane	72			GC-MS
6	Acrolein	46			MS
7	Isoprene	68			MS
8	C ₆ H ₁₂	84			MS
9	2-Methylbutane	70			MS
10	Furan	68			GC-MS
11	Diethylether	74			MS
12	Dichloromethane	84			GC-MS
13	2-Methylpentane	86			MS
14	3-Methylpentane	86			MS
15	C ₆ H ₁₂	84			GC-MS
16	<i>n</i> -Hexane	86			GC-MS
17	Dimethylbutene	84			MS
18	Chloroform	118			GC-MS
19	Ethylacetate	88			MS
20	4-Methyl-2-pentene	84			MS
21	2-Methylcyclopentane	84			MS
22	C ₆ H ₁₂	84			MS
23	Dichloroethylene	96			MS
24	Benzene	78			GC-MS
25	C ₈ H ₁₂	108			MS
26	C ₆ H ₁₀	82			MS
27	Methylhexane	100			MS
28	1,5-Hexadiene	82			MS
29	C ₇ H ₁₆	100			MS
30	Cyclohexene	82			MS
31	1,2-Dimethylcyclopentane	98			MS
32	C ₇ H ₁₄	98			MS
33	Trichloroethylene	130			MS
34	<i>n</i> -Heptane	100			MS
35	<i>n</i> -C ₇ H ₁₄	98			GC-MS
36	C ₂ -Alkylcyclopentane	98			MS
37	2-Methyl-2-hexene	98			MS
38	2,4-Dimethylhexane	114			MS
39	C ₈ H ₁₆	112			
40	C ₈ H ₁₈	114			MS
41	2-Methylheptane	114			MS
42	Toluene	92	40	45	GC-MS
43	C ₈ H ₁₈	114		2	
44	2,5-Dimethylhexane	114	2	2	MS
45	3-Methylheptane	114		1	MS
46	1,1-Dimethylcyclohexane	112	2	4	MS

(Continued on p. 782)

TABLE III (continued)

Peak No.	Compound	MW	Approximate concentration (ppb)		Method
			In air without cigarette smoke	In air with cigarette smoke	
47	C ₈ H ₁₆	112		4	MS
48	C ₈ H ₁₆	112		1	MS
49	C ₈ H ₁₆	112		8	MS
50	2,5-Dimethy-1,2-hexene	112	1	8	MS
51	1,3-Dimethylcyclohexane	112		1	MS
52	Tetrachloroethylene	164		1	GC-MS
53	C ₈ H ₁₈	114		1	MS
54	C ₈ H ₁₆	112	6	6	MS
55	C ₈ H ₁₈	114		10	MS
56	C ₇ -Cyclohexane	106		1	
57	Trimethylcyclopentane	110		2	
58	C ₈ H ₁₆	112	50	45	MS
59	C ₃ -Cyclopentane	112		7	MS
60	1,1,3-Trimethylcyclohexane	128		6	MS
61	C ₉ H ₁₈	126		1	MS
62	C ₃ -Cyclohexane	126		3	MS
63	Ethylbenzene	106	5	12	GC-MS
64	C ₃ -Cyclohexane	126		12	MS
65	C ₉ H ₁₆	124		5	MS
66	<i>m</i> -Xylene + <i>p</i> -xylene	106	18	50	GC-MS
67	Methyloctane	128		25	MS
68	C ₉ H ₁₈	126	1	2	
69	3-Ethylheptane	128		4	MS
70	Diethylpentane	128	1		MS
71	Styrene	104	5	35	MS
72	<i>o</i> -Xylene	106	3	7	GC-MS
73	C ₉ H ₁₆	124		3	GC-MS
74	C ₉ H ₁₈	126		5	MS
75	<i>n</i> -Nonane	128		8	GC-MS
76	C ₉ H ₁₈	126		1	MS
77	C ₁₀ H ₂₀	140		1	
78	Cumene	120		2	GC-MS
79	<i>n</i> -Nonyne	124		2	MS
80	C ₃ -Benzene	120		2	MS
81	α -Pinene	136	2	7	GC-MS
82	C ₁₀ H ₂₀	140		3	MS
83	C ₃ -Benzene	120	1	5	MS
84	C ₃ -Benzene	120	2	15	MS
85	C ₃ -Benzene	120		4	MS
86	C ₁₀ H ₂₀	140	2	2	MS
87	C ₁₀ H ₂₂	142	3	20	MS
88	β -Pinene	36	1	4	MS
89	5-Methyldecane	156	1	3	MS
90	Methylstyrene	118		6	MS
91	C ₃ -Benzene	156	3	12	MS
92	C ₁₀ H ₂₀	190		7	MS
93	C ₁₁ H ₂₄	156	1		MS
94	1,3-Dichlorobenzene	146		3	GC-MS
95	C ₁₁ H ₂₄	156		7	MS
96	<i>n</i> -Decane	142	10	13	GC-MS
97	C ₃ -Benzene	120		6	MS

TABLE III (continued)

Peak No.	Compound	MW	Approximate concentration (ppb)		Method
			In air without cigarette smoke	In air with cigarette smoke	
98	C ₆ -Benzene	134		5	MS
99	Limonene	178		40	GC-MS
100	C ₁₀ H ₂₆	170	5	18	MS
101	C ₁₁ H ₂₂	154	2	1	MS
102	C ₆ -Benzene	134		5	MS
103	C ₁₁ H ₂₂	154	6	2	MS
104	C ₁₁ H ₂₄	156		25	MS
105	C ₆ -Benzene	134	1	6	MS
106	C ₆ -Benzene	134		4	MS
107	Undecane	156	6	23	GC-MS
108	C ₆ -Benzene	134		6	MS
109	C ₁₂ H ₂₆	170	4	15	MS
110	Methyldecane	156		13	MS
111	C ₆ -Benzene	134		3	MS
112	C ₁₂ H ₂₆	170	4	9	MS
113	C ₆ -Benzene	134		7	MS
114	2-Methyldecane	156		10	MS
115	C ₆ -Benzene	134		1	MS
116	C ₁₂ H ₂₆	170		2	MS
117	1-Methylindane	132		3	MS
118	C ₅ -Benzene	148		5	MS
119	C ₅ -Benzene	148		4	MS
120	C ₅ -Benzene	148		1	MS
121	Naphthalene	128		3	MS
122	1-Methyl-(1,2,3,4-tetrahydronaphthalene)	156		3	MS
123	C ₅ -Benzene	148		3	MS
124	n-Dodecane	170		7	GC-MS
125	Phenylhexane	162		2	MS
126	2-Methylnaphthalene	142		1	MS
127	C ₁₂ H ₂₄	168		2	MS
128	1-Methylnaphthalene	142		3	MS
129	Tridecane	184		7	GC-MS
130	Nicotine			40	MS
131	Phenyloctane	190		2	MS
132	Dimethylphthalate	194		2	MS
133	Diethylphthalate	222		3	MS

ACKNOWLEDGEMENT

We would like to thank E. Anderson and H. Mayfield for experimental assistance.

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