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A critical review on the diverse preconcentration procedures on bag samples in the quantitation of volatile organic compounds from cigarette smoke and other combustion samples

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ABSTRACT

It is challenging to analyze environmental tobacco smoking (ETS) samples given the diversity of hazardous toxic components and the difficulty of collecting/treating the samples. As one of the simple means to quantify volatile organic compounds (VOCs) in ETS samples, researchers have used such combinations as the bag sampling method and in-bag solid-phase microextraction for GC-MS analysis. In this review, we describe various factors involved in the application of paired sampling/preconcentration procedures for the analysis of VOCs, especially in ETS samples (and other combustion sources). The reliability of such paired procedures is also evaluated by considering several components, e.g., as the factors controlling QA/QC, the associated sources of bias, and the effect of temporal stability (on bag sampling). Accordingly, it is recommended that several QA-related terms involved in such application (e.g., accuracy, robustness, high throughput, and quantitativeness) ought to be assessed properly and reported in a more objective manner.

Contents

1. Introduction

In order to evaluate smoking-related health issues, numerous experimental protocols have been proposed to accurately quantify the chemicals in tobacco smoke. In both its vapor and particulate phases, cigarette smoke contains a variety of pollutants. These chemicals result from the intrinsic incomplete combustion (pyrolysis) of biomass macromolecules in a smoldering flame. For example, Table 1

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Table 1
Delivery of aromatic volatile organic compounds in the mainstream cigarette smoke of 41 U.S. brands[a]

Order	Classification	% vent	benzene	toluene	styrene	o-xylene	m/p-xylene	Et-benzene	3-Et-toluene
A. Full flavored brands									
1	Basic	0	49.8 ± 5.9	69.0 ± 9.6	4.3 ± 0.4	2.4 ± 0.1	13.1 ± 1.2	6.1 ± 0.7	2.3 ± 0.3
2	Camel (M)	0	52.9 ± 3.6	74.6 ± 5.8	5.0 ± 0.6	2.7 ± 0.3	15.0 ± 1.3	6.9 ± 0.6	2.8 ± 0.7
3	Newport (M)	0	50.7 ± 2.5	72.3 ± 3.7	4.3 ± 0.0	2.4 ± 0.0	13.2 ± 0.4	6.3 ± 0.3	2.2 ± 0.6
4	Salem (M)	0	56.8 ± 6.9	81.2 ± 12.7	5.3 ± 1.1	2.9 ± 0.5	16.0 ± 2.8	7.5 ± 1.2	2.9 ± 0.9
5	Camel Jade (M)	1	57.1 ± 3.5	82.4 ± 3.7	5.4 ± 0.4	3.0 ± 0.3	16.4 ± 1.4	7.8 ± 0.7	2.7 ± 1.1
6	Kool (M)	1	50.5 ± 4.5	73.1 ± 3.1	4.2 ± 0.2	2.3 ± 0.2	13.4 ± 0.9	6.2 ± 0.3	1.8 ± 0.4
7	GPC	5	56.4 ± 0.7	75.0 ± 2.8	4.7 ± 0.2	2.6 ± 0.1	14.4 ± 0.8	6.9 ± 0.3	2.4 ± 0.0
8	Marlboro	12	46.8 ± 0.5	67.0 ± 3.6	3.9 ± 0.3	2.2 ± 0.1	12.8 ± 0.4	5.6 ± 0.2	2.3 ± 0.3
9	Benson & Hedges	13	50.7 ± 2.4	73.8 ± 6.4	3.8 ± 0.9	2.4 ± 0.4	14.1 ± 2.2	6.1 ± 0.9	2.4 ± 0.8
10	Camel	15	56.6 ± 0.9	76.1 ± 2.0	4.8 ± 0.1	2.7 ± 0.1	14.7 ± 0.6	6.7 ± 0.2	2.6 ± 0.2
11	Marlboro (M)	16	42.8 ± 3.3	62.4 ± 6.2	3.2 ± 0.2	1.9 ± 0.2	11.1 ± 1.0	5.1 ± 0.4	1.6 ± 0.3
12	Kent	20	38.3 ± 2.1	57.2 ± 5.8	3.0 ± 0.4	1.7 ± 0.1	9.8 ± 0.3	4.6 ± 0.7	1.3 ± 0.9
13	Doral	22	50.0 ± 7.4	66.0 ± 12.0	4.6 ± 0.7	2.7 ± 0.4	14.6 ± 1.5	6.3 ± 0.6	2.9 ± 0.7
14	Winston	23	51.5 ± 1.5	68.9 ± 1.7	4.1 ± 0.3	2.4 ± 0.1	13.7 ± 0.1	6.1 ± 0.2	2.2 ± 0.1
B. Medium or mild brands									
15	GPC	12	43.8 ± 3.6	57.9 ± 8.5	3.1 ± 0.2	1.7 ± 0.1	9.7 ± 0.9	4.8 ± 0.3	1.3 ± 0.2
16	Marlboro (M)	13	43.9 ± 3.1	62.0 ± 5.2	3.0 ± 0.4	1.9 ± 0.2	10.8 ± 0.9	5.2 ± 0.5	1.5 ± 0.2
17	Newport (M)	20	42.2 ± 4.2	58.5 ± 6.1	3.2 ± 0.5	1.8 ± 0.2	10.0 ± 1.3	4.7 ± 0.6	1.7 ± 0.3
18	Marlboro	22	41.9 ± 4.3	57.6 ± 7.5	3.0 ± 0.3	1.9 ± 0.1	11.0 ± 0.9	4.9 ± 0.5	1.6 ± 0.2
C. Light brands									
19	Basic	15	42.0 ± 0.7	55.1 ± 1.4	2.9 ± 0.2	1.8 ± 0.1	10.1 ± 0.3	4.7 ± 0.1	1.6 ± 0.4
20	GPC	21	38.2 ± 3.5	50.3 ± 4.3	2.5 ± 0.4	1.5 ± 0.2	8.5 ± 1.0	4.1 ± 0.5	1.4 ± 0.3
21	Marlboro	22	40.4 ± 3.0	55.4 ± 6.5	2.7 ± 0.1	1.8 ± 0.2	10.4 ± 1.2	4.6 ± 0.5	1.8 ± 0.3
22	Newport (M)	23	31.6 ± 3.1	43.2 ± 5.4	1.8 ± 0.4	1.2 ± 0.1	6.8 ± 0.9	3.3 ± 0.5	0.9 ± 0.2
23	Camel Jade (M)	24	42.8 ± 3.8	60.3 ± 4.7	3.4 ± 0.3	1.9 ± 0.2	10.9 ± 1.1	5.3 ± 0.5	1.6 ± 0.4
24	Camel (M)	25	39.6 ± 3.9	57.1 ± 9.3	2.8 ± 0.6	1.6 ± 0.3	9.7 ± 1.8	4.8 ± 1.0	1.1 ± 0.6
25	Marlboro (M)	25	37.0 ± 5.9	51.3 ± 9.4	2.3 ± 0.3	1.4 ± 0.3	8.6 ± 1.7	4.1 ± 0.6	0.9 ± 0.5
26	Doral	26	38.2 ± 5.8	53.4 ± 6.9	2.9 ± 0.6	1.8 ± 0.3	10.0 ± 1.4	4.4 ± 0.7	1.8 ± 0.2
27	Camel	30	39.4 ± 3.5	52.6 ± 6.6	2.6 ± 0.3	1.6 ± 0.2	9.0 ± 1.1	4.2 ± 0.5	1.4 ± 0.3
28	Winston	30	44.5 ± 3.4	57.2 ± 5.7	2.9 ± 0.4	1.9 ± 0.2	10.4 ± 1.4	4.8 ± 0.5	1.5 ± 0.2
29	Misty	49	30.7 ± 2.6	39.9 ± 3.3	1.8 ± 0.3	1.2 ± 0.1	6.9 ± 0.8	3.2 ± 0.3	0.9 ± 0.1
30	Misty (M)	50	25.4 ± 1.5	32.3 ± 1.9	1.2 ± 0.3	0.8 ± 0.1	4.8 ± 0.5	2.2 ± 0.2	0.5 ± 0.0
D. Ultralight brands									
31	Basic	32	25.6 ± 5.0	32.0 ± 6.7	1.4 ± 0.5	1.0 ± 0.3	5.6 ± 1.7	2.7 ± 0.7	0.7 ± 0.4
32	Marlboro	47	25.5 ± 2.8	33.6 ± 4.8	1.4 ± 0.3	1.0 ± 0.2	5.9 ± 1.1	2.7 ± 0.3	0.8 ± 0.4
33	GPC	49	26.7 ± 3.5	34.5 ± 4.0	1.9 ± 0.3	1.2 ± 0.2	6.5 ± 1.0	3.0 ± 0.4	1.1 ± 0.4
34	Camel	52	29.3 ± 1.1	39.7 ± 2.5	2.1 ± 0.3	1.4 ± 0.1	7.6 ± 0.6	3.4 ± 0.3	1.3 ± 0.4
35	Marlboro (M)	53	27.3 ± 2.6	33.3 ± 3.3	1.2 ± 0.3	1.0 ± 0.1	5.8 ± 0.5	2.7 ± 0.3	0.7 ± 0.1
36	Winston	55	26.6 ± 0.2	31.7 ± 1.8	1.5 ± 0.3	1.1 ± 0.1	6.2 ± 0.4	2.8 ± 0.3	0.9 ± 0.1
37	Doral	61	19.7 ± 1.9	27.7 ± 2.9	1.2 ± 0.2	1.0 ± 0.0	5.7 ± 0.3	2.5 ± 0.2	0.8 ± 0.2
38	Misty (M)	67	15.7 ± 1.3	21.0 ± 3.1	0.7 ± 0.2	0.7 ± 0.1	4.0 ± 0.8	1.7 ± 0.2	0.4 ± 0.3
39	TRUE	68	15.0 ± 1.1	18.8 ± 2.1	0.9 ± 0.3	0.6 ± 0.1	3.7 ± 0.3	1.7 ± 0.2	0.5 ± 0.0
40	Carlton	77	6.3 ± 0.6	7.3 ± 0.7	0.3 ± 0.1	0.3 ± 0.1	1.9 ± 0.3	1.0 ± 0.1	0.2 ± 0.1
41	Carlton (M)	78	3.7 ± 0.9	4.5 ± 1.3	0.3 ± 0.3	0.2 ± 0.1	1.5 ± 0.4	0.8 ± 0.2	0.0 ± 0.0

[a] All analytes are expressed as micrograms per cigarette along with the corresponding standard deviation, (M) denotes a mentholated brand.

lists the delivery of aromatic volatile organic compounds (e.g., benzene) in the mainstream cigarette smoke of 41 U.S. brands. Therefore, in order to accurately assess the health impacts, it is crucial to understand the chemical composition of environmental tobacco smoke (ETS) based on proper quantification approaches.

The analysis of key ETS components (and more recently, e-cigarette emissions) has been conducted most commonly and reliably with chromatographic methods, including either high-performance liquid chromatography (HPLC) or gas chromatography (GC) [1, 2]. HPLC is preferable to GC for the determination of carbonyls, and related compounds. For nicotine analysis, the industry standard is by GC while LCMS is mainly employed for the analysis of trace-level nicotine [3]. In contrast, GC, including flame ionization detection (FID) or mass spectrometric (MS) detection, is commonly chosen for the determination of volatile organic compounds (VOCs). However, the quantitation of most trace-level VOCs is not possible by means of direct sample injection into the GC system. Therefore, it is imperative to combine GC with diverse sampling/pretreatment methods. Accordingly, various paired options have been proposed regarding sampling (bag, canister, and sorbent tube) and pretreatment stages (solvent extraction, solid-phase microextraction, and thermal desorption).

Among all of the possible options, the combination of bag sampling and SPME has been suggested as one of the most feasible choices to allow high throughput in ETS analysis. For instance, Sampson et al. [4] reported an improved methodology for the analysis of 22 structurally diverse VOCs (e.g., benzene and substituted benzenes, aldehydes and ketones, furans, acrylonitrile, 1,3-butadiene, vinyl chloride, and nitromethane) in cigarette smoke. Similar approaches have been reported in which samples of tobacco cigarette and/or e-cigarette smoke were collected into bags [4–13] or environmental chambers [13–16]. There have also been many advances with regard to sample collection approaches. However, it appears that considerable analytic discrepancies remain when the bag sampling method is paired with SPME analysis, making these options less desirable [4, 9, 12]. Therefore, we provide detailed descriptions of the sampling methods available for ETS samples. The limitations of bag sampling/SPME are discussed with respect to precautions and considerations for the proper quantitation of ETS. Our review further assesses the reliability of these applications in