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GC Analysis of Human Breath with A Series-Coupled Column Ensemble and A Multibed Sorption Trap

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The combination of a tandem column ensemble and an on-line microsorption trap is used for the analysis of organic compounds in human breath samples. The four-bed sorption trap uses a series of discreet sorption beds containing three grades of graphitized carbon and a carbon molecular sieve to quantitatively remove most organic compounds from 0.8-L breath samples. The trap is then heated to 300 °C in ∼1.5 s and maintained at this temperature for 10 s. The resulting vapor plug width is in the range 0.7−1.3 s for the compounds found in the breath samples. The separation is performed with a 15-m-long, 0.25-mm-i.d. capillary using a 0.5-μm-thick film of nonpolar dimethyl polysiloxane coupled in series to a polar column, either trifluoropropylmethyl polysiloxane or poly(ethylene glycol). Both column combinations are successful in separating the early-eluting compounds acetone, isoprene, pentane, methyl alcohol, and ethyl alcohol, which are all common in breath samples. The poly(ethylene glycol) combination gave better separation but showed relatively fast deterioration for repeated analysis of wet samples. Breath samples were obtained under different conditions (smoker, nonsmoker, gum chewer), and 25 compounds were identified in the various samples. Many additional peaks are observed but not identified. Analytical curves (log−log) of peak area versus sample volume for test compounds are linear in the range 80−800 cm^3. Detection limits (3σ) for several volatile compounds in 800-cm^3 samples are in the 1−5 ppb range.

There is increasing interest in the determination of volatile organic compounds (VOCs) in human breath samples as a noninvasive method to replace or complement measurements from blood samples.[1−6] The organic constituents of exhaled breath are representative of their blood-borne concentrations through rapid gas exchange in the blood/gas interface in the lungs. The chemical composition of human exhaled breath can indicate a recent exposure to a drug or an environmental pollutant or a disease state of the individual. Moreover, the measurement of gas-phase analytes is much simpler than measurements in a complex biological sample such as blood,[7] and breath analysis will allow rapid on-site analysis when adequate portable devices become available.

Over 200 organic compounds have been detected in breath emissions from humans that include hydrocarbons, alcohols, ketones, and aldehydes at ppt to ppm levels.[2,5] The major VOCs in the breath of healthy individuals are isoprene, acetone, ethanol, methanol, and other alcohols.[5] The low concentrations of compounds in exhaled breath make necessary the use of a preconcentration technique prior to analysis. Preconcentration on solid sorbents followed by thermal desorption is the most frequent method for the analysis of breath samples,[8−15] including recommended EPA and ISO methods.[16,17] The wide range of VOCs present in breath results in no single sorbent being adequate to adsorb all the compounds, and a multicomponent sorbent is necessary.[10,18]

Two of the main problems associated with accurate measurements of breath samples are the short half-lives of some components in the collected samples and the high background concentrations of water vapor. Previous studies have demonstrated the possibility of using a sorbent trap coupled on-line with a separation GC column,[19−23] which eliminates the first problem as samples are measured immediately after collection in the trap.

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Different options have been evaluated to reduce the water vapor problem, such as the use of desiccants or water-sorbing polymers in front of the sampling tube, dry purge, or heating of the adsorbent during sampling[18,24,25]. However, there are limitations because of the possible loss of VOCs or introduction of contaminants. Another possibility is to avoid the use of carbon molecular sieves (CMSs) in the design of the trap, as these materials adsorb substantial amounts of water, corresponding to the volume of the micropores[24,26,27]. Unfortunately, sorbents as effectives as CMSs but resistant to water adsorption are currently unavailable,[28] and CMSs are needed to adsorb very volatile compounds. Carbotrap X, a graphitized carbon designed to adsorb very volatile compounds, fails to intercept quantitatively hydrocarbons more volatile than pentane, as well as low-molecular-weight compounds of high polarity.[29]

Even when multibed sorbents are used, only the CMS bed determines water uptake in the system.[24,28] Helming and Vierling[24] suggested that procedures to reduce water uptake in multibed sorbents should be focused on reducing sample volume to the smallest possible value consistent with the required limits of detection. Gawrys et al.[28] found that at low relative humidity (RH), adsorption of water is slight and increases only slowly with increasing RH. Once a threshold value (RH_{th}) is surpassed, the increase becomes faster. They tested different CMSs and found that Carboxen 1000 has the highest RH_{th} value ($45 \pm 3\%$). Lu and Zellers[22] found that 1.8 mg of Carboxen 1000 in a multibed trap coupled on-line with a GC system is enough to have a 1-L breakthrough volume for acetone in 100% RH samples.

Recently, Pawliszyn et al.[30] used membrane extraction with sorption trap interface for the analysis of breath samples. The hydrophobic membrane blocks water vapor but passes volatile organic compounds, which are preconcentrated in a microsorption trap. The trap tube is resistively heated to inject a narrow vapor plug into the GC. Peak areas for acetone, benzene, and toluene show small increases with increasing RH in the range 10−90%. For ethyl alcohol, RH had no effect on peak area.

The work described here is part of a project devoted to the development of a portable GC device with an on-line preconcentration system for the near-real-time analysis of VOCs in breath samples. In this study, the behavior of a multibed trap connected on-line to a GC system using a series-coupled ensemble of two capillary columns with different stationary phases is explored. The effects of RH on peak areas and analytical-curve linearity are considered. The study also includes the evaluation of different chromatographic column combinations in order to obtain adequate separation of the less retained compounds and to obtain adequate robustness for the wet breath samples.

EXPERIMENTAL SECTION

Apparatus. The experimental system used for these studies is shown in Figure 1. Component separation is achieved by the use of a series-coupled (tandem) ensemble of two capillary columns, which is located in the oven of a Varian 3700 GC (Varian, Walnut Creek, CA). The Varian flame ionization detector (FID) is used for all experiments. Several column combinations were evaluated in order to obtain adequate separation of the early-eluting compounds as well as adequate robustness for extended operation with wet samples. In all cases, 0.25-mm-i.d. wall-coated open-tubular (capillary) columns were used. For one set of studies, C_2 was a 15-m length of nonpolar 5% phenyl dimethyl polysiloxane column with a 0.5-μm film (Rtx-5, Restek Corp., Bellefonte, PA), and C_1 was a polar poly(ethylene glycol) column with a 0.25-μm film and length ranging from 0 to 11 m (Rtx-Wax, Restek). For another set of studies, C_1 was a 15-m length of nonpolar 5% phenyl dimethyl polysiloxane column with a 0.5-μm film (Rtx-5, Restek), and C_2 was a moderately polar trifluoropropylmethyl polysiloxane column with a 0.25-μm film and length ranging from 0 to 15 m (Rtx-200, Restek).

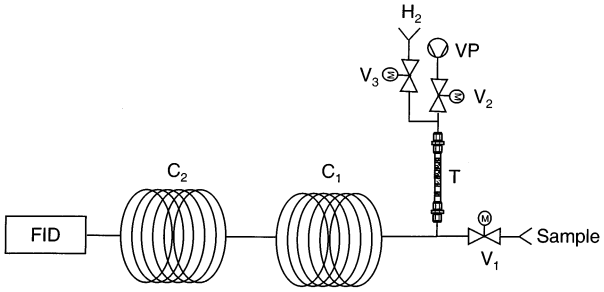

Figure 1. Multibed sorption trap and series-coupled dual-column ensemble used for human breath analysis: T, trap; C_1 and C_2, capillary columns; FID, flame ionization detector; V_1 and V_2, low-dead volume valves; VP, vacuum pump; H_2, carrier gas. See text for details.

The on-line multibed sorption trap T has been discussed in detail.[23] The device uses an 80-mm-long, 1.35-mm-i.d. tube made of a Ni−Co alloy (Inconel 600, Accu-Tube Corp., Englewood, CO). The tube contains a graded ensemble of four adsorbent materials separated by glass-wool plugs. Each bed contains between 2.2 and 2.5 mg of adsorbent. The adsorbents from top to bottom in Figure 1 are Carboxen 1000, Carbopack X, Carbopack B, and Carbopack Y. These materials were obtained from Supelco Corp. (Bellefonte, PA). Carboxen 1000 is a carbon molecular sieve, and the three Carbopack materials are graphitized carbon. The adsorbent strengths for organic compounds are graded with Carboxen 1000 the strongest and Carbopack Y the weakest.

To collect a breath sample from a gas-sampling bag, valves V_1 and V_2 (model LFVA1230113H, The Lee Co., Westbrook, CT) are opened, and the sample is pulled through the trap by vacuum pump VP (model UN86KNI, KNF Newberger, Inc., Trenton, NJ). During sample collection, valve V_3 is closed to isolate the carrier gas supply, and the column ensemble is back-flushed with gases from the FID. This back-flush flow passes through the trap, but its flow is much smaller than the sample gas flow, and chromatograms from samples of purified air show no evidence of contamination or degradation of trap performance.

The highest molecular weight components in the sample are captured by the first (weakest) bed encountered (Carbopack Y) and thus never reach the last (strongest) bed (Carboxen 1000) from which they would be very difficult to desorb at temperatures that would not destroy the adsorbent materials or result in thermal

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Table 1. Volatile and Semivolatile Compounds Detected in Breath Samples

peak no.	compound name	boiling point (°C)
1	methanol*	64.7
2	*n*-pentane*	35−36
3	isoprene	34
4	acetone*	56.2
5	ethanol*	78
6	2-propanol*	82.4
7	*n*-hexane*	69
8	butanone	80
9	1-propanol	97
10	2-butanol	98
11	benzene*	80.1
12	2-pentanone	100−101
13	toluene	110.6
14	octane	125−127
15	hexanal	131
16	ethylbenzene	136.2
17	*m*-xylene	139.1
17	*p*-xylene	138.3
18	*o*-xylene	143−145
19	nonane	150.8
20	α-pinene	155
21	*β*-pinene	167
22	decane	174
23	limonene	175.5
24	1,2-dichlorobenzene	180
25	undecane	196

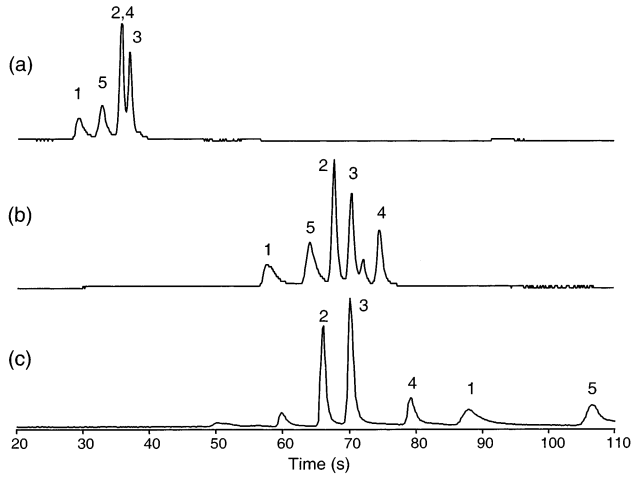

Figure 2. Separation of volatile compounds with a 15-m-long, 0.25-mm-i.d., 0.50-μm-thick film nonpolar 5% phenyl dimethyl polysiloxane column (a) and with the addition of 9 m of 0.25-mm-i.d., 0.25-μm-thick film trifluoropropylmethyl polysiloxane column (b) and the addition of 9 m of 0.25-mm-i.d., 0.25-μm-thick film poly(ethylene glycol) column (c). Peak numbers correspond to compound numbers in Table 1. A sample collection time of 10 s at a flow rate of 1.33 cm^3/s was used for all chromatograms.

degradation of sample components. For sample injection, valves V_1 and V_2 are closed and V_3 is opened. Carrier gas (H_2) reverses the gas flow direction in the trap. The trap is then resistively heated by a power supply to a temperature of 300 °C. Peak temperature is reached in ∼1.5 s and maintained for 10 s. The heating source and control circuitry have been described.[23]

The ordering of the four sorbent beds and the gas flow direction reversal in the trap tube after sample collection greatly facilitate thermal desorption. Previous studies have shown that desorption is complete for a 300 °C, 10-s-long heating pulse, and no memory effects are observed for a subsequent heating cycle.[23] In addition, the combination of on-line operation, which results in rapid removal of desorbed sample components from the hot environment of the trap tube, and the design of the trap with graded bed strength and flow reversal after sample collection reduces the risk of sample decomposition during sample injection. Previous studies have shown that no significant changes in peak areas occur for desorption temperatures in the range 200−300 °C suggesting minimal decomposition. At a desorption temperature of 350 °C, extensive decomposition of terpines, including α-pinene, *β*-pinene, and limonene, was observed. Injection plug widths are in the range from ∼0.7 s for the most volatile compounds to ∼1.5 s for the least volatile compounds.

Materials and Procedures. In a previous study,[23] 46 volatile compounds were used to challenge a sorption trap similar in design to the one used here. Of these compounds, 25 were found in the breath samples described in this report. These compounds are listed in Table 1. All of these compounds have previously been detected in human breath samples.[2,5,14] Peak identification was accomplished by spiking with the pure compounds. The compounds marked with asterisks were used to construct calibration plots for quantitative analysis. All materials used as calibration standards are reagent grade or better. Standards were prepared by injecting microliter quantities of mixtures into 12-L Tedlar gas sampling bags (SKC Inc., Eighty Four, PA) and diluting with dry, pruified air. Vapor concentrations were in the range 8−46 ppm (v/v). Ten-fold dilutions were made by drawing aliquots of the vapor samples, injecting them into clean gas-sampling bags, and further diluting with dry, purified air. However, uncertainties in the mixing volumes obtained with available equipment render the concentrations in these dilute samples less reliable. Humidified standards were prepared by using water-saturated air obtained by bubbling purified air through water. Breath samples were collected in 1-L Tedlar bags from University of Michigan Chemistry Department employees. For each sample, ∼800 cm^3 was pulled through the sorption trap at a rate of 80 cm^3/min.

Hydrogen carrier gas was used after purification by traps for water vapor, hydrocarbons, and oxygen. Chromatograms were obtained with an initial 2.0-min. isothermal interval at 30 °C followed by a 15 °C/min temperature program to 150 °C. Instrument control and data acquisition were provided by a 16-bit A/D board (CIO-DAS16/F, Measurement Computing Corp., Middleboro, MA). A sampling rate of 10 Hz was used.

RESULTS AND DISCUSSION

Column Selectivity. Several major constituents in human breath are very volatile, and their separation is difficult. These components include isoprene, acetone, methyl alcohol, and ethyl alcohol. Preliminary studies with a 5% phenyl dimethylpolysiloxane (Rtx-5) column indicated that adequate retention could not be achieved at 30 °C with a 0.25-μm-thick film, and all further studies used a 15-m-long column with a 0.5-μm-thick film.

Figure 2a shows the chromatogram of these four components plus *n*-pentane using the 15-m Rtx-5 column with the 0.5-μm film. Peak numbers correspond to the compound numbers in Table 1. The sample collection time was 10 s at a flow rate of 1.33 cm^3/s (80 cm^3/min). The chromatogram was obtained at 30 °C during the 2-min isothermal interval prior to the start of the temperature

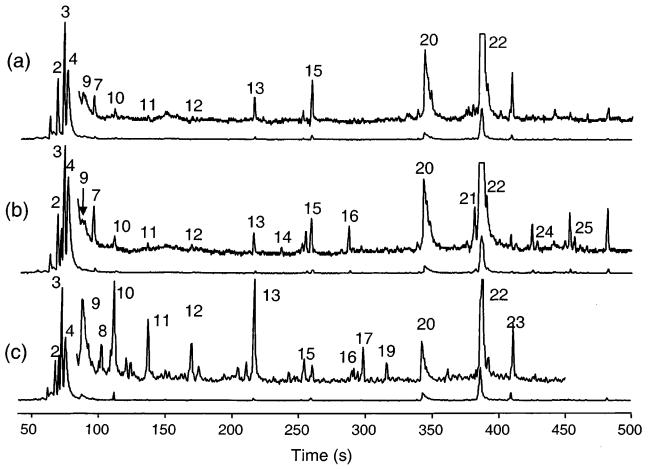

Figure 3. Chromatograms of breath samples from two nonsmoking (a, b) and one smoking (c) individual. The sample size was 0.8 L. Peak numbers correspond to compound numbers in Table 1. Chromatograms are presented on two different vertical scales so that the large range of peak heights can be displayed. The 15-m 5% phenyl dimethylpolysiloxane column with the 9-m trifluoropropylmethyl polysiloxane column was used.

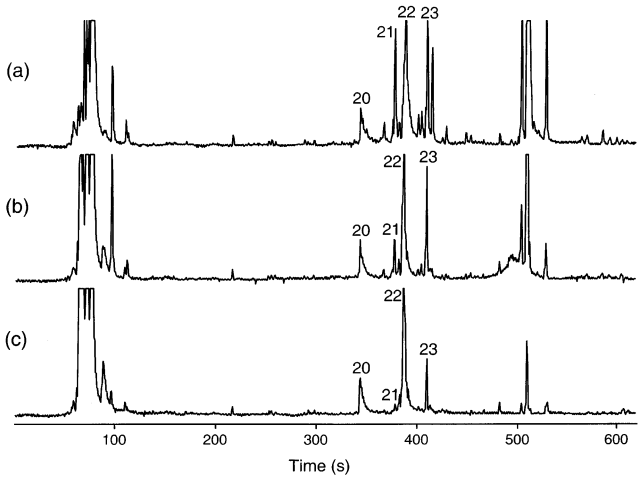

Figure 4. Breath samples from a nonsmoker immediately after chewing mint-flavored gum (a), 1 h later (b), and 4 h later (c). The sample size was 0.8 L. Peak numbers correspond to compound numbers in Table 1. Columns were the same as for Figure 3.

program. The two alcohols (peaks 1 and 5) are completely separated, but *n*-pentane and acetone completely coelute, and isoprene (peak 3) is not adequately separated. To enhance the separation of these early-eluting compounds, various lengths of trifluoropropylmethyl polysiloxane (Rtx-200) and poly(ethylene glycol) (Rtx-Wax) were coupled to the Rtx-5 column. Both polar columns used 0.25-μm-thick films.

Figure 2b shows the chromatogram using the 15-m Rtx-5 column coupled to a 9-m-long Rtx-200 column. The pattern of peaks is quite different from for chromatogram 2a with an elution order change for peaks 3 and 4. All of the target compounds are completely separated with the added Rtx-200 column. Figure 2c shows the chromatogram using the 15-m Rtx-5 column coupled to a 9-m-long Rtx-Wax column. The pattern of peaks is again very different with peaks 2, 3, and 4 showing greater separation relative to chromatogram b and peaks 1 and 5 for the alcohols shifted from the first two peaks to elute from the Rtx-5/Rtx-200 ensemble to the last two peaks to elute from the Rtx-5/Rtx-Wax ensemble.

Adequate separation of the early-eluting components was achieved for both column combinations, but substantially greater separation is obtained when the poly(ethylene glycol) column is used in the ensemble. In general, fewer coeluting pairs were observed for the Rtx-5/Rtx-Wax combination. However, it should be noted that the wet samples encountered in breath analysis caused gradual deterioration of the poly(ethylene glycol) column, and after about a month of daily operation, the separation between components 2 and 3 significantly deteriorated. Relatively frequent column replacement thus is required. The trifluoropropylmethyl polysiloxane column appears to tolerate water vapor for at least several months of daily operation, and this column ensemble was used for further work.

Qualitative Analysis. For these studies, 800-cm^3 samples were collected at a flow rate of 80 cm^3/min. Figure 3 shows a comparison of breath sample chromatograms for two nonsmoking employees at the University of Michigan (a, b) and a smoking employee (c). The early-eluting peaks are much larger than the other peaks in the chromatograms, and each of the chromatograms is shown on two different vertical scales to accommodate the large range of peak heights. Vertical scales are the same for all three samples. Numerous peaks are observed in all of the chromatograms. Peak numbers correspond to the compound numbers in Table 1. Substantial differences are observed in the two chromatograms for the two nonsmokers. In particular, components 16 (ethylbenzene), 21 (β-pinene), and 25 (*n*-undecane) are detected only in chromatogram b.

The breath sample from the smoker was obtained ~15 min after smoking a cigarette. Many peaks are observed in chromatogram c for the smoker that are either absent or present at substantially lower concentrations for the two nonsmokers. Peaks 11 and 17 are for benzene and *m*/*p*-xylene, respectively. These aromatic compounds are observed only in the breath sample from the smoker. Peak 13 for toluene and peak 10 for 2-butanol also are much larger for the smoker. Peak 23, limonene, is a common terpene that may be a combustion product or a flavor/fragrance additive. Note that limonene is also present at significant concentration in chromatogram a for a nonsmoker.

Figure 4 shows chromatograms for a nonsmoker immediately after chewing mint-flavored gum (a), 1 h later (b), and 4 h later (c). Peaks 21 (β-pinene) and 23 (limonene), which are common flavor and fragrance components, are much larger in the chromatogram in Figure 4a than in the chromatograms in Figure 3. Note that α-pinene (peak 20), which is a normal constituent of breath samples (see Figure 3), shows little change for the three chromatograms in Figure 4. A number of smaller peaks are also observed in Figure 4a for the time window from 400 to 600 s, which are not observed in Figure 3. These peaks appear in the retention range associated with monoterpenes and oxygen-containing terpene structures commonly used in the flavor and fragrance industries. Chromatograms b and c in Figure 4 show a gradual decrease in peak heights for these compounds as they are eliminated from the lungs.

It is clear from Figures 3 and 4 that breath samples contain a great deal of chemical information that should be useful in assessing chemical exposure. A principal limitation for the more widespread use of this type of information is the lack of low-cost,

portable, and reliable instrumentation, which allows for on-line sample collection and analysis.

Water Vapor and Analyte Recovery. Breath samples are saturated with water vapor, and this has been shown to degrade the performance of sorption traps using carbon molecular sieves.[24,28] Several methods have been used to reduce the water vapor problem including the use of a water barrier such as a hydrophobic membrane,[18,30] the use of desiccants,[18] and gentle heating of the sorption trap during sample collection.[14,24,28] All of these methods risk the partial loss of some components in the sample. Other sample losses, particularly for more polar compounds, can occur if condensed water forms in the gas-sampling bag as the breath samples cool from body temperature to ambient temperature.[31] This problem can be reduced by dilution of the sample with dry air or by the use of more specialized breath-sampling devices.[30]

To evaluate the effects of trap heating during sample collection, two chromatograms from the same breath sample where obtained in rapid succession. For the first sample, the multibed sorption trap was maintained at room temperature during sample collection, and for the second sample, the trap was heated to 40 °C during sample collection in order to reduce the amount of water vapor collected in the trap. A large decrease in peak amplitude was observed for the more volatile compounds, which elute in less than ~200 s, when the trap is heated during sample collection relative to when the trap is at room temperature during sample collection. No significant change is observed for the less volatile compounds, which elute later in the chromatogram.

The later-eluting compounds should be completely adsorbed by the graphitized carbon beds, which do not retain water. It is likely that only compounds trapped in the carbon molecular sieve bed (Carboxen 1000) will be at all influenced by the water vapor in the sample. Based on these results, no further studies were made using trap heating during sample collection.

To evaluate sample recovery by the multibed trap as a function of the mass of analyte challenging the trap, plots of log peak area versus log sample collection time were prepared for both wet and dry samples. Figure 5 shows plots for test mixtures containing acetone (a), methyl alcohol (b), and ethyl alcohol (c). For the solid-line plots, the samples were diluted with dry air, and for the broken-line plots, the samples were diluted with air that was saturated with water vapor by bubbling purified air through water. Analytes were present at concentrations of 25, 46, and 32 ppm (v/v), respectively. These concentrations are larger than typically found in breath samples, and this limited sample collection times to less than 60 s in order to prevent overloading both the trap and the column with the target analytes. Reliable standards could not be made for realistic concentrations found in breath samples (ppb and ppt levels) with available equipment. Since the dry and wet samples for each of the three compounds were prepared with the same concentrations, direct comparison can be made.

For acetone (a), there is no significant difference for the dry and wet samples. Similar results were obtained for *n*-pentane and *n*-hexane. Methyl alcohol (b) shows nonlinear plots for both the wet and the dry samples, indicating extensive sample loss. The plots for ethyl alcohol are linear with peak areas for the wet sample lower than for the dry sample by 9.5% for the shortest sampling

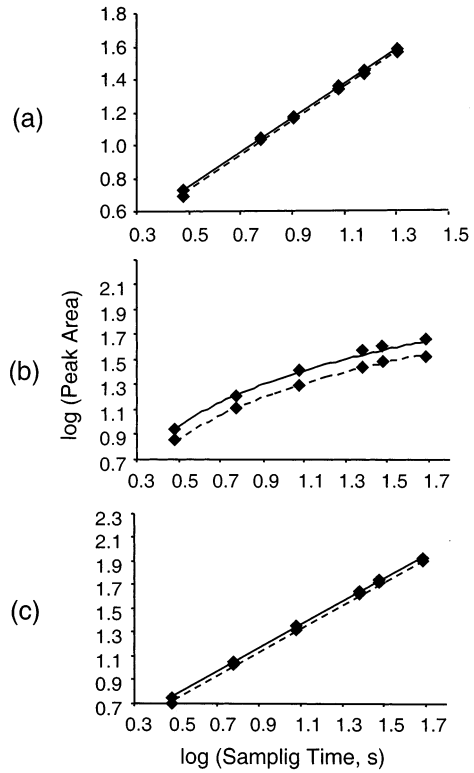

Figure 5. Log−log plots of peak area versus sampling time for acetone (a), methyl alcohol (b), and ethyl alcohol (c). Solid-line plots are for dry samples, and broken-line plots are for wet samples (100% RH). Sample collection times ranged from 5 to 60 s. Columns were the same as for Figure 3.

time (5 s) and by 4.0% for the longest sampling time (60 s). From Figure 5, it appears that only the most volatile and polar of the compounds found in human breath break through the three graphitized carbon beds and are trapped (partially) in the Carboxen 1000 bed. Peak areas from other compounds, which are quantitatively trapped in the graphitized carbon beds, should not be influenced by the presence of water vapor in the breath samples.

Additional test were made for more dilute (~10-fold) samples where longer sample collection times could be used thus increasing the amount of water vapor passing through the sorption trap. However, these lower concentrations could not be accurately reproduced with available equipment, and thus, a direct comparison of peak areas for wet and dry samples could not be made. For these very dilute samples, sample collection times were in the 120−600-s range. Statistical data for plots of log peak area versus log sampling time for these samples as well as for the higher concentration samples described in Figure 5 are presented in Table 2.

For the shorter sampling time data from the wet samples, ~1.5 mg of water vapor passes through the trap for the 60-s sampling time. For the longer sampling times, ~15 mg of water vapor passes through the trap for the 10-min sampling time. This is nearly twice the total mass of the sorption bed. Despite this relatively large amount of water vapor, all of the log−log slopes except for ethyl alcohol with the longer sampling times are near the 1.0 value expected for peak area linearity with sample mass. Correlation coefficients for the shorter sampling times are all greater than 0.999 except for acetone in wet air, which has a value of 0.9988.

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Table 2. Slopes and Correlations Coefficients for Short and Long Sampling Times in Dry and Humid Conditions

	dry samples		humid samples	
compound	slope	R^2	slope	R^2
	Short Sampling Time (5−60 s)			
pentane	1.05 ± 0.01	0.9992	1.12 ± 0.01	0.9990
acetone	1.02 ± 0.01	0.9999	1.07 ± 0.01	0.9988
ethanol	0.99 ± 0.02	0.9995	1.00 ± 0.02	0.9994
2-propanol	1.00 ± 0.02	0.9993	1.01 ± 0.02	0.9994
hexane	1.02 ± 0.01	0.9999	1.06 ± 0.01	0.9995
	Long Sampling Time (120−600 s)			
pentane	1.17 ± 0.03	0.9926	1.05 ± 0.03	0.9981
acetone	1.00 ± 0.02	0.9999		
ethanol	0.81 ± 0.05	0.9808	0.80 ± 0.05	0.9994
2-propanol			1.08 ± 0.04	0.9894
hexane			1.17 ± 0.02	0.9950
benzene	1.17 ± 0.02	0.9992		

Correlation coefficients for the longer sampling times are somewhat poorer with two of the values less than 0.99. Extrapolations of the plots in Figures 5 to a signal-to-noise ratio of 3.0 give detection limits (v/v) in the 10−50 ppb range for 60-s sampling time. This would give detection limits of 1−5 ppb for 600-s sampling time (800-mL samples).

CONCLUSIONS

Human breath analysis has great potential as a noninvasive diagnostic tool for monitoring human exposure to a variety of substances. The use of breath analysis for medical diagnostic purposes also has potential, but the lack of reliable, portable instruments is presently a barrier to its development. The work described here shows that a simple, on-line adsorption trap coupled to a GC using a column ensemble designed to enhance the separation of the volatile components in human breath, including acetone, *n*-pentane, and isoprene, has adequate selectivity and sensitivity for this application. The combination of a nonpolar dimethyl polysiloxane column and a trifluoropropylmethyl polysiloxane column has adequate selectivity for the volatile compounds and is sufficiently robust for water-containing samples.

Quantitative recovery for wet or dry samples can be achieved for most organic compounds with the exception of the lower-molecular-weight alcohols. However, even ethyl alcohol shows peak area linearity with sample collection time for times less than 1 min. The breath analysis system described here is simple and straightforward to operate. The relatively high sampling flow rate allows for 800-mL samples to be collected in 10 min. Resulting detection limits using FID detection are in the low-ppb range.

The human breath chromatograms shown in this report have numerous unidentified peaks. Mass spectrometric detection will be used to more fully characterize human breath samples. Future work will also involve the reduction of instrument size and weight. Air as a carrier gas will also be investigated since this has proven useful for other applications and would obviate the need for cylinders of carrier gas. Other detection methods that require no compressed gases including photoionization also will be investigated so that a portable instrument can be developed requiring only electrical power. In addition, an alternative sample collection device to replace gas-sampling bags is under investigation.

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