Oral Diseases (2005) 11 (Suppl. 1), 48–50
 1601-5665/05
http://www.blackwellmunksgaard.com

ORIGINAL ARTICLE

Breath odor evaluation by detection of volatile sulfur compounds – correlation with organoleptic odor ratings

CM Hunter[1], HP Niles[1], J Vazquez[1], C Kloos[1], R Subramanyam[1], MI Williams[1], D Cummins[1], PA Lenton[2], GJ Majerus[2]

[1]*Oral Care Advanced Technology, Colgate-Palmolive Company Technology Center, Piscataway, NJ;* [2]*Department of Preventive Sciences, University of Minnesota, School of Dentistry, Minneapolis, MN, USA*

BACKGROUND: Detection of oral volatile sulfur compounds (VSC) by gas chromatography (GC) is a widely used method for evaluating breath odor. Air aspirated from the mouth is injected into the GC column for analysis. To eliminate discrepancies caused by variations in operator sampling or injection techniques, a new GC system designed to aspirate breath samples directly into the GC was developed.
OBJECTIVE: A clinical study was performed to compare this new automated breath-sampling GC system to organoleptic evaluation by two trained odor judges.
METHODS: A randomized, two-cell, double-blind, parallel design was used in which subjects were tested before and 3 h after using either a mouthrinse containing zinc or a matching placebo rinse. Thirteen subjects used the zinc mouthrinse, and 12 used the placebo. Subjects with a wide range of VSC levels were studied. The average organoleptic ratings for each subject at each time-point were compared with the average VSC measurements made with the GC, and Pearson product–moment correlation coefficients between the corresponding GC and organoleptic measurements were determined.
RESULTS: The correlation between the GC and organoleptic assessment methods were highly significant ($P \leq 0.001$) for: total VSC, 0.65; H_2S, 0.63; CH_3SH, 0.61; and $(CH_3)_2S$, 0.46. The correlation between the two judges was also highly significant (0.823, $P < 0.001$).
CONCLUSION: These results demonstrate the utility of the automated GC method for evaluating breath odor.
Oral Diseases (2005) **11** (Suppl. 1), 48–50

Keywords: volatile sulfur compounds; gas chromatography; halitosis; oral malodor; breath

Correspondence: Dr Catherine M. Hunter, Colgate-Palmolive Technology Center, 909 River Road, Piscataway, NJ 08855-1343, USA. Tel: 732 878 7162, Fax: 732 878 7880,
E-mail: cathy_hunter@colpal.com

Introduction

Detection of volatile sulfur compounds (VSC) by gas chromatography (GC) is a widely used method for evaluating breath odor (Tonzetich, 1971; Solis-Gaffar *et al*, 1975). Air aspirated from the mouth is directly injected into the GC column for analysis. To eliminate discrepancies caused by variations in operator sampling or injection techniques, a new GC system designed to aspirate breath samples directly into the GC was developed. This method allows individual quantification of the three main VSC's in mouth air, hydrogen sulfide, methyl mercaptan, and dimethyl sulfide. A clinical study was performed to compare this new automated breath-sampling GC system to organoleptic evaluation by two trained odor judges.

Methods

A randomized, two-cell, double-blind, parallel design was used in which subjects were tested before and 3 h after using either a prototype mouthrinse containing 0.4% zinc acetate or a matching placebo rinse without zinc. During the 7-day period prior to the study, all subjects used a regular fluoride dentifrice (Colgate-Palmolive Company, New York, NY, USA). Thirteen subjects rinsed with 15 ml of the zinc mouthrinse, and 12 with 15 ml of the placebo for 60 s. Subjects with a wide range of VSC levels were studied. On the morning of the study, subjects arrived at the clinical facility, without eating, drinking, or performing oral hygiene, for baseline evaluations. After a limited breakfast, subjects rinsed with their assigned product for 1 min and returned 3 h later for post-treatment evaluations.

Instrumental analysis of breath air was performed using a GC system consisting of an Agilent 6890 gas chromatograph (Wasson-ECE Instrumentation, Ft Collins, CO, USA) with a flame photometric detector and an automated system that aspirates gaseous samples from the mouth and injects them onto the column. The chromatography method used was able to quantify the three individual volatile sulfur species hydrogen sulfide, methyl mercaptan, and dimethyl sulfide, at levels

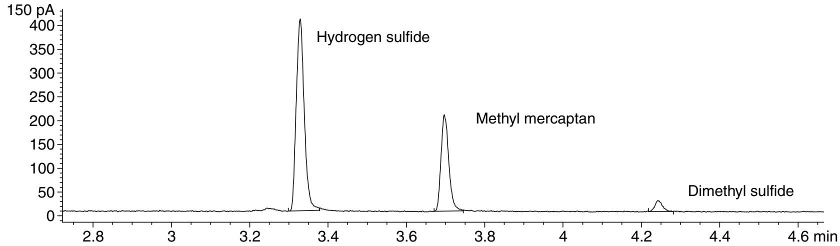

Figure 1 Sample chromatogram of mouth air

Table 1 Organoleptic rating scale

Mouth odor rating	*Malodor*
0	None
1	Barely
2	Slight
3	Moderate
4	Strong
5	Very strong

commonly found in the mouth (Tonzetich, 1971, 1977). For each sample, concentrations of these three species were calculated and added to determine the total VSC concentration. A sample chromatogram is shown in Figure 1.

Sensory breath evaluation was performed by two trained, calibrated breath examiners. Mouth air samples were collected from each subject in triplicate using a specially designed mouthpiece and 20-ml polypropylene syringes. Following mouth air sampling, the syringes were blindly and randomly presented to each odor judge for assessment using a scale of 0–5 (Table 1). The scores given each sample by the two judges were averaged to determine an overall organoleptic rating for that sample. The average organoleptic ratings for each subject at each time-point were compared with the average VSC measurements made with the GC, and Pearson product–moment correlation coefficients between the corresponding GC and organoleptic measurements were determined.

Individual product effects were determined by comparing the initial pretreatment ratings to the 3-h ratings for each product tested using a paired *t*-test. The effects of the two products were compared using an ANCOVA performed on the 3-h measurements with the products and the baseline measurements as covariants.

Results

Table 2 lists the correlation coefficients between the individual and total VSC measurements and the organoleptic ratings. The significance level (*P*-value) of each correlation is also listed. The correlations between the organoleptic ratings and both total VSC and the individual sulfur species were all statistically significant ($P < 0.001$), with the total VSC having the highest correlation to the mouth odor ratings. The correlation between the two judges was also highly significant ($P < 0.001$) with a correlation coefficient of 0.823, indicating a strong degree of agreement between the perceptions of mouth odor by the two judges.

Table 2 Correlation coefficients between GC measurements and organoleptic ratings

GC measurement	R^a	*Statistical significance*
Total VSC	0.6481	<0.001
H_2S	0.6336	<0.001
CH_3SH	0.6120	<0.001
$(CH_3)_2S$	0.4642	<0.001

[a]Pearson product–moment correlation coefficients (*R*) and significance levels for comparisons between specific GC measurements and organoleptic ratings.
GC, gas chromatography; VSC, volatile sulfur compounds.

Table 3 Baseline and 3-h levels for each treatment group (mean ± s.d.)

	0.4% zinc acetate rinse		*Placebo rinse*	
	Baseline	*3-h*	*Baseline*	*3-h*
Total VSC (p.p.b.)	532 ± 346	35 ± 68	574 ± 468	397 ± 378
Organoleptic ratings	3.6 ± 1.0	1.2 ± 0.8	3.1 ± 1.0	2.3 ± 1.1

Mean organoleptic ratings and mean total VSC at each time-point are shown with standard deviations in Table 3. Compared with baseline, both the GC method and the organoleptic method demonstrated a statistically significant 3-h effect for the zinc-containing mouth rinse ($P < 0.05$) and no significant effect for the placebo ($P > 0.05$). Both methods also demonstrated a statistically significantly greater effect for the active rinse compared with the placebo ($P < 0.05$).

Discussion and conclusion

The results of this study, demonstrate that there is a statistically significant correlation between VSC in mouth air as measured by the breath-sampling GC system and organoleptic evaluations of mouth odor. Compared with the results presented by Schmidt *et al* (1978), the VSC measurements observed here indicate comparable or stronger correlations with the organoleptic ratings. The two methods also performed similarly in evaluating the effects of the two mouthrinses tested. Features of the current system that contribute to this performance include the automated breath-sampling assembly, a chromatographic method specially designed to separate and detect VSCs found in the oral cavity, and computerized data acquisition and analysis methods. These results demonstrate the utility of the automated GC method for evaluating breath odor.

Acknowledgment

Data reprinted with permission from Dental Learning Systems.

Hunter CM, Niles HP, Lenton PA *et al* (2003). Breath odor evaluation by detection of volatile sulfur compounds – correlation with organoleptic odor ratings. *Compend Contin Educ Dent* **24** (Suppl. 9): 25–28.

References

Schmidt N, Missan S, Tarbet WJ (1978). The correlation between organoleptic mouth-odor ratings and levels of volatile sulfur compounds. *Oral Surg* **45:** 560–567.

Solis-Gaffar M, Niles H, Rainieri WC, Kestenbaum RC (1975). Instrumental evaluation of mouth odor in a human clinical study. *J Dent Res* **54:** 351–357.

Tonzetich J (1971). Direct gas chromatographic analysis of sulfur compounds in mouth air in man. *Arch Oral Biol* **16:** 587–597.

Tonzetich J (1977). Production and origin of oral malodor: a review of mechanisms and methods of analysis. *Periodontology* **48:** 13–20.