INFICON

APPLICATION NOTE

Analysis of 58 Volatile Organic Compounds Using Two CMS5000 Monitoring Systems

OVERVIEW

This application note describes the benefits of using the fully automated on-site CMS5000 Monitoring System to identify and alert users to the presence of volatile organic compounds (VOCs) in water systems. Fifty-eight VOCs are analyzed using two CMS5000 systems in tandem.

INTRODUCTION

On-site monitoring of VOCs is essential for the timely evaluation of potential hazards throughout water system infrastructures. VOCs are often inadvertently introduced into drinking water as the result of spills, improper disposal or soil migration[1]. Many VOCs are known to cause severe health effects at low ppb concentrations[2].

CMS5000 employs SituProbe™ purge and trap sampling technology, gas chromatographic separation and Micro Argon Ionization Detection (MAID) to reliably monitor concentrations of multiple VOCs simultaneously in water, while in the presence of common interferences. The unit is designed to operate autonomously, analyzing numerous samples per day over several months without user supervision. The software generates an alarm if the concentrations exceed a user-defined threshold. Data collected from the calibrated CMS5000 allows users to make informed decisions based on their drinking water quality.

USEPA Methods 8260B and 5030 describe the analysis of approximately 90 VOCs in water by purge and trap. In order to analyze this number of compounds, the sample usually has to be analyzed using a mass spectrometer (MS). Most gas chromatography (GC) systems analyze 5-20 analytes. The separation of coeluting compounds when analyzing by GC is an analytical challenge.

In this application, 58 VOCs were analyzed on two separate CMS5000 systems with each employing complementary GC columns to improve separation of co-eluting compounds. The systems were nearly identical, except one system used a non-polar 100% polydimethylsiloxane (PDMS) column and the other used a slightly polar 4% cyanopropyl-penyl column.

EXPERIMENTAL

Calibration standards were prepared at 1, 3, 5 and 10 ppb by spiking 2 L of VOC-free water with the appropriate amount of a 200 µg/mL, 57 component VOC specialty mix in methanol and a 2000 µg/mL MTBE standard in methanol (SPEXCertiPrep). The standards were created by injecting 10.0 µL of the VOC specialty mix and 1.0 µL of the MTBE standard into 2 L of water and setting the concentrator fill time to 60, 180, 300 or 600 seconds.

Figure 1 and Figure 2 show chromatograms of the 1 ppb calibration standard. Using argon carrier gas, the analytes were purged from the calibration standard into the sampling tube headspace. The headspace sample was collected onto the Tri-Bed Concentrator. The analytes were thermally desorbed from the concentrator and then separated on a capillary column using a 51 minute temperature programmed method. A four point calibration curve with quadratic fit was generated from the data.

Calibration accuracy was measured by analyzing a 2 ppb calibration verification standard and calculating the percent recovery for each of the 58 compounds. See Table 1 for a list of compounds, the percent recovery, and the retention time of the compounds.

NOTE: MTBE, 2,2-dichloropropane, n-propylbenzene, 1,1,1,2-tetrachloroethane and 1,1,2,2-tetrachloroethane coeluted with a different compound on each column and could not be quantified by the software. The concentration of these compounds can be manually calculated by subtracting the concentration of the coeluting compound, determined on one column, from the concentration of the coeluting compounds on the other column. See Table 2.

CONCLUSION

The fully-automated CMS5000 Monitoring System is ideally suited to continually monitor VOCs in drinking water at low concentrations. The calibrated CMS5000 successfully separated, identified and quantified 58 VOCs at 1 to 10 ppb. Running an analysis with two complementary GC columns, with different stationary phases, reduced the number of coelutions and provided quantifiable data. These analyses demonstrate the utility of the CMS5000 for alerting users to unacceptable VOC concentrations in water, allowing water utilities to make fast, informed decisions to protect and ensure public health and well-being.

REFERENCES

1 http://www.health.state.mn.us/divs/eh/hazardous/topics/vocs.html

2 Zogorski, J. S. (2006). Volatile Organic Compounds in the Nation's Ground Water and Drinking-Water Supply Wells. Reston, VA: U.S. Department of the Interior U.S. Geological Survey.

Figure 1 Chromatogram of 58 compounds at 1.0 ppb run on a DB-1 column

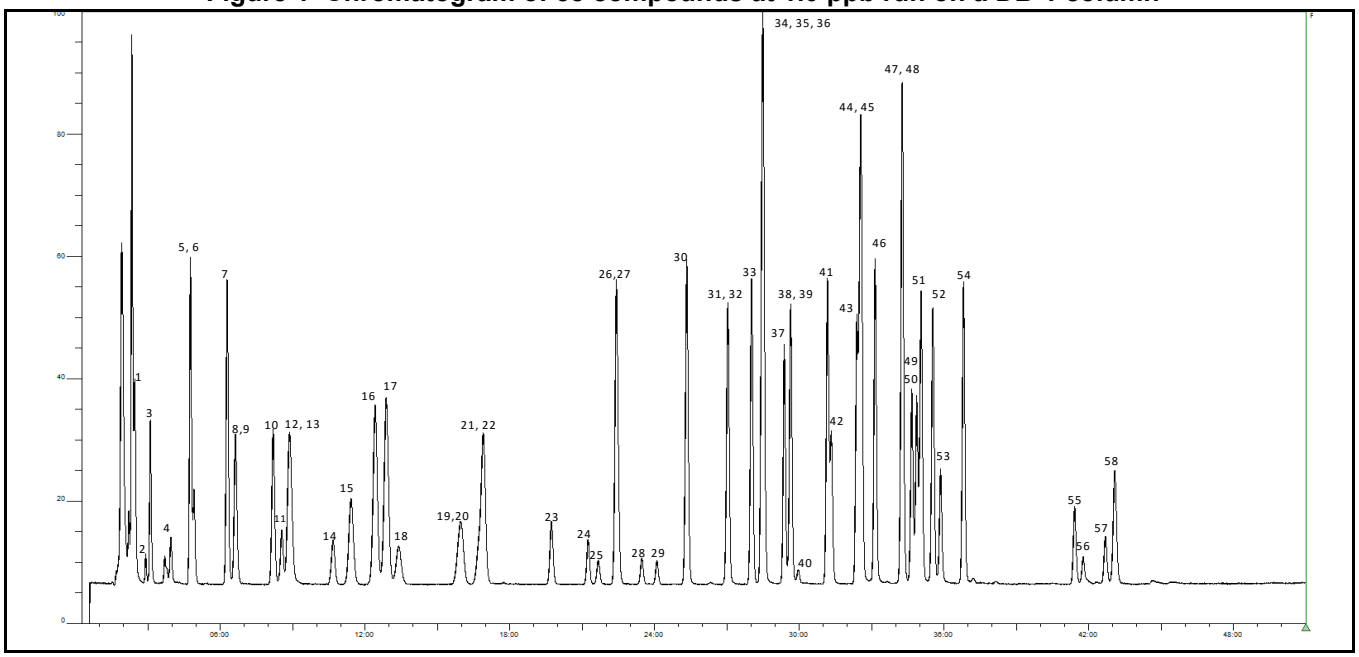

Figure 2 Chromatogram of 58 compounds at 1.0 ppb run on a DB-624 column

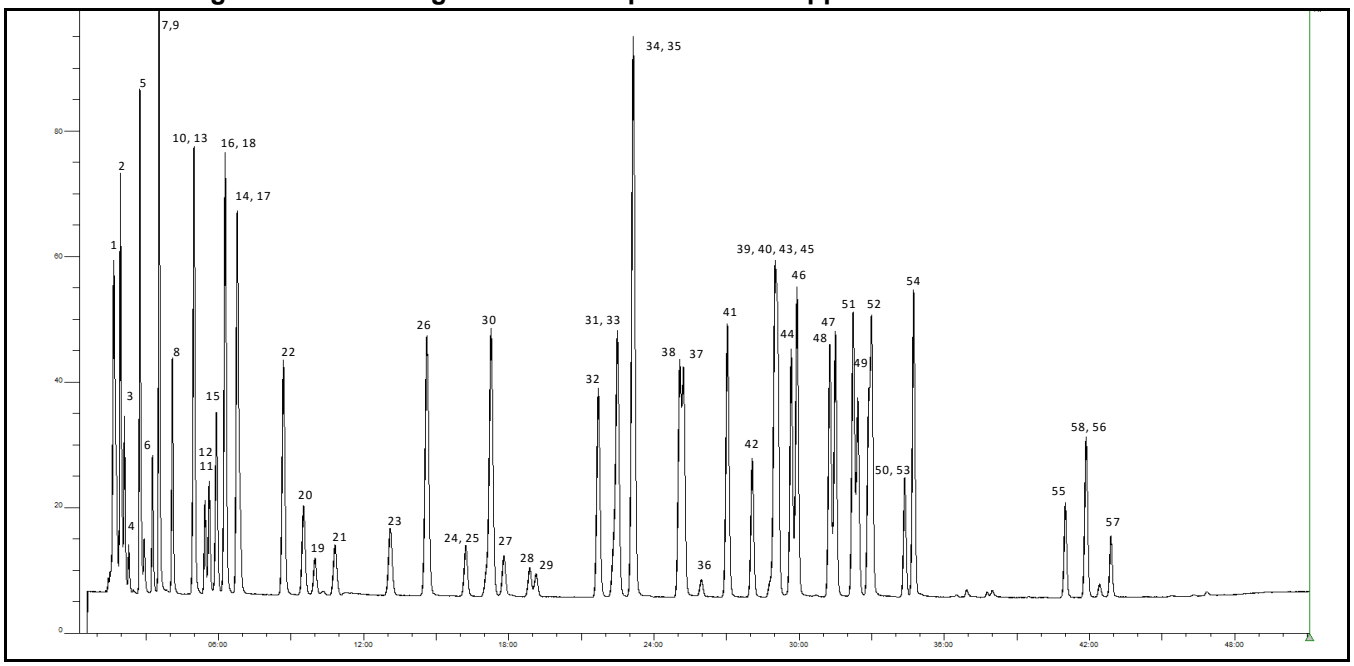

Table 1 Recovery and retention times of 58 compound standard

No.	Compound	RT DB-1	% Rec DB-1	RT DB-624	% Rec DB-624
1	vinyl chloride	2:27	93	1:48	NA
2	bromomethane	2:55	168	1:55	NA
3	chloroethane	3:07	96	2:08	99
4	trichlorofluoromethane	3:58	125	2:20	97
5	1,1-dichloroethene	4:46	92	2:47	91
6	methylene chloride	4:46	92	3:17	97
7	trans-1,2-dichloroethene	6:17	99	3:34	93
8	1,1-dichloroethane	6:38	97	4:07	94
9	MTBE	6:38	97	3:34	93
10	cis-1,2-dichloroethene	8:12	100	5:01	82
11	bromochloromethane	8:33	103	5:29	115
12	chloroform	8:52	93	5:39	104
13	2,2-dichloropropane	8:52	93	5:01	82
14	1,2-dichloroethane	10:42	99	6:48	100
15	1,1,1-trichloroethane	11:26	100	5:56	103
16	1,1-dichloropropene	12:26	101	6:18	93
17	benzene	12:54	101	6:48	100
18	carbon tetrachloride	13:25	96	6:18	93
19	dibromomethane	15:59	99	10:00	99
20	1,2-dichloropropane	15:59	99	9:32	103
21	bromodichloromethane	16:55	103	10:50	100
22	trichloroethene	16:55	103	8:42	104
23	cis-1,3-dichloropropene	19:44	103	13:07	103
24	trans-1,3-dichloropropene	21:15	98	16:14	102
25	1,1,2-trichloroethane	21:40	102	16:14	102
26	toluene	22:26	101	14:38	101
27	1,3-dichloropropane	22:26	101	17:49	103
28	dibromochloromethane	23:29	91	18:52	103
29	1,2-dibromoethane	24:06	102	19:08	103
30	tetrachloroethene	25:21	100	17:17	98
31	1,1,1,2-tetrachloroethane	27:02	103	22:30	101
32	chlorobenzene	27:02	103	21:43	103
33	ethylbenzene	28:02	100	22:30	101
34	m-xylene	28:30	95	23:09	101
35	p-xylene	28:30	95	23:09	101
36	bromoform	28:30	95	25:58	99
37	styrene	29:23	92	25:09	109
38	o-xylene	29:39	92	24:57	105
39	1,1,2,2-tetrachloroethane	29:39	92	29:01	87
40	1,2,3-trichloropropane	29:58	100	29:01	87

Table 1 Recovery and retention times of 58 compound standard (continued)

No.	Compound	RT DB-1	% Rec DB-1	RT DB-624	% Rec DB-624
41	isopropylbenzene	31:10	100	27:02	98
42	bromobenzene	31:20	103	28:04	105
43	2-chlorotoluene	32:23	100	29:01	87
44	4-chlorotoluene	32:33	98	29:41	103
45	n-propylbenzene	32:33	98	29:01	87
46	1,3,5-trimethylbenzene	33:09	102	32:45	98
47	1,2,4-trimethylbenzene	34:17	98	31:29	101
48	tert-butylbenzene	34:17	98	31:17	98
49	1,3-dichlorobenzene	34:41	103	32:26	103
50	1,4-dichlorobenzene	34:52	103	34:21	103
51	sec-butylbenzene	35:03	102	32:15	95
52	4-isopropyltoluene	35:32	99	33:51	90
53	1,2-dichlorobenzene	35:51	96	34:21	103
54	n-butylbenzene	36:49	102	34:44	96
55	1,2,4-trichlorobenzene	41:23	103	41:00	102
56	naphthalene	41:44	102	41:50	97
57	1,2,3-trichlorobenzene	42:42	105	42:51	100
58	hexachlorobutadiene	43:05	102	41:50	97

Table 2 Determination of the concentration of compounds which coelute on both columns

Conc. of Cmpd. (ppb)	Equation
MTBE (1)	(Conc. of MTBE + 1,1-dichloroethane) DB-1 - (Conc. of 1,1-dichloroethane) DB-624 = Conc of MTBE
MTBE (2)	(Conc. of MTBE + trans-1,2-dichloroethene) DB-624 - (Conc. of trans-1,2-dichloroethane) DB-1 = Conc. of MTBE
2,2-dichloropropane (1)	(Conc. of 2,2-dichloropropane + chloroform) DB-1 - (Conc. chloroform) DB-624 = Conc of 2,2-dichloropropane
2,2-dichloropropane (2)	(Conc. of 2,2-dichloropropane + cis-1,2-dichloroethene) DB-624 = Conc. of 2,2-dichloropropane
1,1,1,2-tetrachloroethane (1)	(Conc. of 1,1,1,2-tetrachloroethane + chlorobenzene) DB-1 - (Conc. of chlorobenzene) DB-624 = Conc. of 1,1,1,2-tetrachloroethane
1,1,1,2-tetrachloroethane (2)	(Conc. of 1,1,1,2-tetrachloroethane + ethylbenzene) DB-624 - (Conc. of ethylbenzene) DB-1 = Conc. of 1,1,1,2-tetrachloroethane
1,1,2,2-tetrachloroethane	(Conc. of 1,1,2,2-tetrachloroethane + o-xylene) DB-1 - (Conc. of o-xylene) DB-624 = Conc. of 1,1,2,2-tetrachloroethane
n-propylbenzene	(Conc. of n-propylbenzene + 4-chlorotoluene) DB-1 - (Conc. of 4-chlorotoluene) DB-624 = Conc. of n-propylbenzene