The Direct Sampling Ion Trap Mass Spectrometer for the Rapid Analysis of Volatile Organic Contaminants in Groundwater Samples^(U)

Westinghouse Savannah River Company
Savannah River Site
Aiken, SC 29808

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C. A. Eddy-Dilek, J. Rossabi, and M. A. Keenan

Authentication: C. A. Eddy-Dilek

Approved by: D. B. Moore-Shedrow

D. B. Moore-Shedrow, Manager
Environmental Sciences Section
Savannah River Technology Center

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Abstract

Analytical results of volatile organic contaminant (VOC) concentrations in groundwater samples from A/M Area obtained using a direct sampling ion trap mass spectrometer (DSITMS) and a gas chromatograph (GC) with an electron capture detector (ECD) were comparable. Replicate water samples were collected at the Integrated Demonstration Site during four bi-weekly sampling periods and analyzed by both instruments. The calibration curves prepared for both the DSITMS and GC-ECD are essentially linear over the concentration range analyzed. The advantage of the DSITMS over the GC-ECD method is the rapid sample analysis time of the DSITMS. In order to validate the technology for use in the sample minimization efforts at SRS, duplicate groundwater samples from selected compliance wells were analyzed by DSITMS and GC-ECD. The DSITMS is appropriate to use for field screening water samples before offsite analysis. These analytical results will be compared with results from offsite labs contracted to perform contract lab program (CLP) analyses of regulatory samples when these analyses are available.

Background

An objective of the Savannah River Site (SRS) Integrated Demonstration (ID) Program is to demonstrate and evaluate new environmental characterization and monitoring technologies for environmental restoration of sites contaminated with volatile organic contaminants. Many developers of innovative technologies from industry, universities, and other government laboratories are interested in using the SRS ID site to test new technologies because the site is well characterized, well instrumented for baseline comparisons, and logistically friendly. As part of this effort, an ion trap mass spectrometer modified for realtime monitoring developed by Oak Ridge National Laboratory (ORNL) was transferred to SRS for use at the Integrated Demonstration Site and at Environmental Restoration (ER) waste sites. Recent efforts at SRS have focused on testing, procedure development, and operation of the instrument for analysis of field samples. The purpose of this report is to document the implementation of the modified DSITMS to use to analyze VOCs in groundwater and sediments.

The DSITMS uses a commercially available Finnegan-MAT Magnum ion trap mass spectrometer with three custom-designed modules for sample introduction. The three modules designed by Oak Ridge National Laboratory (ORNL) enable the analysis of water samples using a helium purge technique, gas samples using a valved gas mixing inlet, and sorbent traps using a thermal desorption unit. Mass spectrometry systems normally use a compound separation technique (e.g., gas chromatography column) to help to discriminate compounds with similar masses. These separation techniques slow the introduction of the sample to the mass spectrometer, adding up to 30

minutes to the time required for sample analysis of volatile compounds. The direct sample introduction modules on the DSITMS reduce time needed to analyze a sample consisting of a single or few chemical components. A typical groundwater sample from the A/M Area can be analyzed in less than three minutes with this system.

Experimental Protocols

Groundwater samples were collected from wells at the Integrated Demonstration Site and from M Area using dedicated submersible pumps in accordance with documented SRS well sampling protocols (3Q5). Bulk water parameters including temperature, pH, dissolved oxygen (DO), conductivity, and oxidation-reduction potential (ORP) were measured using a Hydrolab. Samples were collected for VOC analysis by GC-ECD in a headspace vial; and samples for analysis by DSITMS were collected in vials without a headspace. Samples from the Integrated Demonstration Site were collected by Savannah River Technology Center (SRTC) personnel. Quarterly compliance samples were collected by an independent contractor.

The VOC analyses by GC-ECD were performed on a Hewlett-Packard 5890 Gas Chromatograph, an HP 19395A Headspace Sampler, an HP 3392A Networking Integrator, and a 60 m $\times$ 0.75 mm i.d. Supelco VOCOL wide-bore capillary column coated with a 1.5 mm film. The instrument was calibrated using samples spiked with standard solution. The analytical techniques used are documented in WSRC procedure ESSOP-2-70, "Procedure for Analyzing Volatile Organic Contaminants in Sediment and Water Samples Using the Hewlett-Packard 5890 Gas Chromatograph", and are discussed in Eddy et al. 1991, and Looney, Eddy, and Sims in review.

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Compliance samples were analyzed according to EPA Standard Methods 8240 (GC-MS) and/or 8010 (GC).

Results

Water samples obtained from the Integrated Demonstration Site during bi-weekly samplings of water wells for the *in situ* bioremediation experiment were analyzed for four sampling periods using both the DSITMS and GC-MS (see Table 1). Four replicate samples were taken from each of the 16 wells. Two of the duplicates were run on the DSITMS and two were run on the GC. Figures 1 and 2 compare analytical results from the DSITMS using the helium purge unit for water samples with the GC-ECD using the headspace method. Figure 1 shows the results obtained for trichloroethylene (TCE) concentrations of the samples and Figure 2 shows the results obtained for (PCE) concentrations. Values for concentrations measured by both instruments are determined by comparing area counts of samples with calibration curves that consist of area counts plotted with respect to prepared standard concentrations. The calibration curves prepared for the DSITMS are essentially linear from 2 ug/l (Figures 3 and 4). The calibration curves prepared for the GC-ECD are linear in the lower concentration ranges (2-750 ug/l) where the ECD is used for quantitative analysis. Most of the water samples analyzed for this study are within this lower concentration range. In order to quantify samples with concentrations of greater than 750 ug/l TCE and 175 ug/l, a split of sample stream is measured with a flame ionization detector (FID). An FID detector was not used in this study.

In Figure 1, the concentration data as determined by both the DSITMS and the GC for TCE are highly correlated for concentration values up to around 700 ug/l. Above this limit, the DSITMS values are consistently higher than those obtained from the GC. This can be explained by the loss of sensitivity of the ECD detector for concentrations above 700 ug/l TCE. This limited linear dynamic range is not experienced by the DSITMS for concentrations of TCE as high as 1500 ug/l. Figure 3 shows the linear response of the DSITMS for TCE standard measurements up to around 1500 ug/l. The linear pattern of the four highest concentration data points in Figure 1 give further evidence for the higher dynamic range of the DSITMS.

In Figure 2, PCE concentration values plotted for both instruments indicate a similar comparative response difference to the one described above. In this case, the linear response of the GC for PCE drops off at concentrations approaching 150 ug/l. The DSITMS linear response range extends to at least 1000 ug/l as shown in Figure 4. Again the lower concentrations (below 150 ug/l) compare advantageously.

Additional samples were collected during 4Q93 quarterly sampling of wells from M Area. The results from the DSITMS are tabulated in Table 2. A comparison of the results will be made when the results are obtained from contractor labs.

Summary

Analytical results of VOC concentrations in groundwater samples at A/M Area obtained using a direct sampling ion trap mass spectrometer and a gas chromatograph with an electron capture detector were comparable. Replicate water samples were collected at the Integrated Demonstration Site during four bi-weekly sampling periods and from M-Area wells during 4Q93 compliance monitoring sampling and analyzed by both instruments. The calibration curves prepared for both the DSITMS and GC-ECD are essentially linear over the concentration range of typical groundwater samples. The advantage of the DSITMS over the GC-ECD method is the rapid sample analysis time of the DSITMS. The DSITMS is appropriate for use in field screening of water samples prior to offsite analysis and will be included in the sample minimization efforts onsite.

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The Direct Sampling Ion Trap Mass Spectrometer for the Rapid
Analysis of Volatile Organic Contaminants in Groundwater Samples

Table 1. Bi-weekly Samplings for Four Periods (NA = Not Analyzed)

	TCE-ITMS	TCE-GC	PCE-ITMS	PCE-GC	VC-ITMS	VC-GC	DCE-ITMS	DCE-GC
<i>12/15/92</i>								
MHT 1C	226	207	98	82	17	NA	52	NA
MHT 2C	376	311	73	41	55	NA	58	NA
MHT 2D	87	ND	28	5	0	NA	0	NA
MHT 3C	479	517	83	69	83	NA	91	NA
MHT 4C	48	36	52	35	0	NA	0	NA
MHT 5C	181	193	157	140	10	NA	94	NA
MHT 5D	219	250	48	30	19	NA	13	NA
MHT 6C	150	179	331	193	11	NA	212	NA
MHT 7C	241	247	349	186	33	NA	241	NA
MHT 8C	1292	781	118	92	282	NA	238	NA
MHT 9B	326	378	364	179	70	NA	271	NA
MHT 9C	295	319	78	56	37	NA	49	NA
MHT 9D	124	116	33	8	0	NA	0	NA
MHT 10C	465	500	63	44	80	NA	76	NA
MHT 11C	48	42	33	12	0	NA	0	NA
MHT 12C	156	169	90	90	1.5	NA	47.5	NA
	TCE-ITMS	TCE-GC	PCE-ITMS	PCE-GC	VC-ITMS	VC-GC	DCE-ITMS	DCE-GC
<i>12/29/92</i>								
MHT 1C	238	255	104	86	0	NA	15	NA
MHT 2C	432	366	74	45	19	NA	16	NA
MHT 2D	96	75	27	5	0	NA	0	NA
MHT 3C	605	598	91	74	48	NA	44	NA
MHT 4C	47	42	56	42	0	NA	0	NA
MHT 5C	334	319	321	188	15	NA	123	NA
MHT 5D	263	248	56	30	0	NA	0	NA
MHT 6C	59	80	108	146	0	NA	0	NA
MHT 7C	291	280	412	202	8	NA	146	NA
MHT 8C	1841	914	144	108	226	NA	182	NA
MHT 9B	414	383	376	195	28	NA	148	NA
MHT 9C	365	344	91	62	12	NA	18	NA
MHT 9D	150	111	36	8	0	NA	0	NA
MHT 10C	516	533	88	68	35	NA	29	NA
MHT 11C	60	37	33	9	0	NA	0	NA
MHT 12C	194	121	106	58	0	NA	24	NA
	TCE-ITMS	TCE-GC	PCE-ITMS	PCE-GC	VC-ITMS	VC-GC	DCE-ITMS	DCE-GC
<i>1/11/93</i>								
MHT 1C	266	127	92	34	24	NA	17	NA
MHT 2C	304	267	57	32	27	NA	13	NA
MHT 2D	71	58	25	4	0	NA	0	NA
MHT 3C	582	568	86	65	62	NA	30	NA
MHT 4C	43	29	51	28	0	NA	1	NA
MHT 5C	212	213	198	161	22	NA	35	NA
MHT 5D	224	ND	47	ND	20	NA	9	NA
MHT 6C	153	109	320	168	15	NA	53	NA
MHT 7C	365	236	610	193	50	NA	104	NA
MHT 8C	2242	1013	148	132	250	NA	93	NA
MHT 9B	395	ND	306	ND	47	NA	60	NA

Table 1. Bi-weekly Samplings for Four Periods (NA = Not Analyzed) (contd)

	TCE-ITMS	TCE-GC	PCE-ITMS	PCE-GC	VC-ITMS	VC-GC	DCE-ITMS	DCE-GC
<i>1/11/93</i>								
MHT 9C	338	254	79	42	36	NA	20	NA
MHT 9D	147	ND	36	ND	11	NA	4	NA
MHT 10C	581	595	82	66	66	NA	30	NA
MHT 11C	56	41	30	9	0	NA	0	NA
MHT 12C	173	184	87	88	16	NA	19	NA
	TCE-ITMS	TCE-GC	PCE-ITMS	PCE-GC	VC-ITMS	VC-GC	DCE-ITMS	DCE-GC
<i>1/26/93</i>								
MHT 1C	246	244	88	80	30	NA	31	NA
MHT 2C	318	344	54	43	42	NA	26	NA
MHT 2D	115	101	23	8	5	NA	7	NA
MHT 3C	644	605	90	74	98	NA	63	NA
MHT 4C	37	32	41	32	0	NA	5	NA
MHT 5C	223	196	260	173	34	NA	83	NA
MHT 5D	243	244	46	32	35	NA	24	NA
MHT 6C	438	448	1094	249	98	NA	289	NA
MHT 7C	363	378	528	220	67	NA	153	NA
MHT 8C	1629	881	119	97	250	NA	120	NA
MHT 9B	374	297	350	182	64	NA	108	NA
MHT 9C	291	257	72	53	42	NA	29	NA
MHT 9D	106	97	22	7	8	NA	5	NA
MHT 10C	457	427	71	59	72	NA	44	NA
MHT 11C	53	48	21	11	0	NA	0	NA
MHT 12C	236	195	185	143	33	NA	63	NA

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Table 2. Quarterly Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = Trichloroethylene, TCLEE = tetrachloroethylene).

Bold ug/l numbers are low range calibration. All others are full range calibration. Full range calibration only goes as high as 3650 ug/l TCE, and 2500 ug/l PCE. Keep this in mind when looking at results, unless a dilution was made that was within the range of the calibration curve results above curve. Results above curve were not accurate. (Italicized numbers)

Well ID	TCE ug/l	PCE ug/l
MSB-1B	408	5
MSB-1C	65	263
MSB-1CC	46	33
MSB-1D	8	7
MSB-2B	<i>12308</i>	<i>5356</i>
MSB-2C	<i>5261</i>	<i>8253</i>
MSB-2D	602	768
MSB-3B	820	92
MSB-3C	<i>10212</i>	<i>22888</i>
MSB-3D	31380	<i>1234640</i>
MSB-4B	1086	32
MSB-4C	<i>8906</i>	<i>7296</i>
MSB-4D	105	42
MSB-5A	2	5
MSB-5B	35	4
MAB-5C	11	193
MSB-6A	2	4
MSB-6B	1155	36
MSB-6C	6	21
MSB-7A	1	3
MSB-7B	24	11
MSB-7C	20	36
MSB-8A	17	74
MSB-8B	19	9
MSB-8C	78	103
MSB13A	189	1
MSB-13B	5	51
MSB-13CC	10	15
MSB-13D	33	54
MSB-75D	27	47
MSB-58D	705	1173
MSB-59D	<i>4352</i>	<i>116765</i>
MSB-60D	52	90
MSB-62B	32	35
MSB-62C	73	223
MSB-62D	177	624
MSB-63B	316	26
MSB-63C	12	32
MSB-63D	58	315
MSB-64B	1815	113
MSB 64C	94	390
MSB-64D	9	23
<i>F-Area Rubble Pit (100069)</i>		
10001115	9	24
10001116	10	23

Dilution Made; TCE within CAL Range, PCE above

Table 1 Quarterly Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene). (contd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Batch	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB1B	716C	071493	071993	0803931140	ITS1	FC	403	TRCLE	ITMS PURGE	2	415	UGL	0	1	MS	MK	0
MSB1B	716C	071493	071993	0803931140	ITS1	FC	403	TCLEE	ITMS PURGE	2	5	UGL	0	1	MS	MK	0
MSB1B	716C	071493	071993	0803931145	ITS1	FC	404	1TRCLE	ITMS PURGE	2	401	UGL	0	1	MS	MK	0
MSB1B	716C	071493	071993	0803931145	ITS1	FC	404	1TCLEE	ITMS PURGE	2	4	UGL	0	1	MS	MK	0
MSB1C	716D	071893	071993	0803931152	ITS1	FC	405	TRCLE	ITMS PURGE	2	67	UGL	0	1	MS	MK	0
MSB1C	716D	071893	071993	0803931152	ITS1	FC	405	TCLEE	ITMS PURGE	2	266	UGL	0	1	MS	MK	0
MSB1C	716D	071893	071993	0803931156	ITS1	FC	406	1TRCLE	ITMS PURGE	2	63	UGL	0	1	MS	MK	0
MSB1C	716D	071893	071993	0803931156	ITS1	FC	406	1TCLEE	ITMS PURGE	2	260	UGL	0	1	MS	MK	0
MSB1CC	716E	071893	071993	0803931202	ITS1	FC	407	TRCLE	ITMS PURGE	2	47	UGL	0	1	MS	MK	0
MSB1CC	716E	071893	071993	0803931202	ITS1	FC	407	TCLEE	ITMS PURGE	2	34	UGL	0	1	MS	MK	0
MSB1CC	716E	071893	071993	0803931206	ITS1	FC	408	1TRCLE	ITMS PURGE	2	45	UGL	0	1	MS	MK	0
MSB1CC	716E	071893	071993	0803931206	ITS1	FC	408	1TCLEE	ITMS PURGE	2	32	UGL	0	1	MS	MK	0
MSB1D	716F	071893	071993	0804930900	ITS2	FC	409	TRCLE	ITMS PURGE	2	9	UGL	0	1	MS	MK	0
MSB1D	716F	071893	071993	0804930900	ITS2	FC	409	TCLEE	ITMS PURGE	2	7	UGL	0	1	MS	MK	0
MSB1D	716F	071893	071993	0804930905	ITS2	FC	410	1TRCLE	ITMS PURGE	2	7	UGL	0	1	MS	MK	0
MSB1D	716F	071893	071993	0804930905	ITS2	FC	410	1TCLEE	ITMS PURGE	2	6	UGL	0	1	MS	MK	0
MSB2B	7170	071593	071993	0804930908	ITS2	FC	411	TRCLE	ITMS PURGE	2L	12376	UGL	0	1	MS	MK	0
MSB2B	7170	071593	071993	0804930908	ITS2	FC	411	TCLEE	ITMS PURGE	2L	5396	UGL	0	1	MS	MK	0
MSB2B	7170	071593	071993	0804930912	ITS2	FC	412	1TRCLE	ITMS PURGE	2L	12239	UGL	0	1	MS	MK	0
MSB2B	7170	071593	071993	0804930912	ITS2	FC	412	1TCLEE	ITMS PURGE	2L	5316	UGL	0	1	MS	MK	0

WSRC-TR-93-563

Table 2. Quality Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene). (contd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Date	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB2C	7171	071593	071993	0804930922	ITS2	FC	413	TRCLE	ITMS PURGE	2L	5296	UGL	0	1	MS	MK	0
MSB2C	7171	071593	071993	0804930922	ITS2	FC	413	TCLEE	ITMS PURGE	2L	8310	UGL	0	1	MS	MK	0
MSB2C	7171	071593	071993	0804930926	ITS2	FC	414	ITRCLE	ITMS PURGE	2L	5226	UGL	0	1	MS	MK	0
MSB2C	7171	071593	071993	0804930926	ITS2	FC	414	ITCLEE	ITMS PURGE	2L	8196	UGL	0	1	MS	MK	0
MSB2D	7172	071593	071993	0804930930	ITS2	FC	415	TRCLE	ITMS PURGE	2	605	UGL	0	1	MS	MK	0
MSB2D	7172	071593	071993	0804930930	ITS2	FC	415	TCLEE	ITMS PURGE	2	775	UGL	0	1	MS	MK	0
MSB2D	7172	071593	071993	0804930933	ITS2	FC	416	ITRCLE	ITMS PURGE	2	599	UGL	0	1	MS	MK	0
MSB2D	7172	071593	071993	0804930933	ITS2	FC	416	ITCLEE	ITMS PURGE	2	760	UGL	0	1	MS	MK	0
MSB3B	7173	071993	072093	0804931346	ITS2	FC	451	TRCLE	ITMS PURGE	2	856	UGL	0	1	MS	MK	0
MSB3B	7173	071993	072093	0804931346	ITS2	FC	451	TCLEE	ITMS PURGE	2	100	UGL	0	1	MS	MK	0
MSB3B	7173	071993	072093	0804931349	ITS2	FC	452	ITRCLE	ITMS PURGE	2	784	UGL	0	1	MS	MK	0
MSB3B	7173	071993	072093	0804931349	ITS2	FC	452	ITCLEE	ITMS PURGE	2	83	UGL	0	1	MS	MK	0
MSB3C	7174	072093	072093	0804931406	ITS2	FC	453	TRCLE	ITMS PURGE	2L	1320	UGL	1	8	MS	MK	0
MSB3C	7174	072093	072093	0804931406	ITS2	FC	453	TCLEE	ITMS PURGE	2L	2950	UGL	1	8	MS	MK	0
MSB3C	7174	072093	072093	0804931412	ITS2	FC	454	ITRCLE	ITMS PURGE	2L	1233	UGL	1	8	MS	MK	0
MSB3C	7174	072093	072093	0804931412	ITS2	FC	454	ITCLEE	ITMS PURGE	2L	2772	UGL	1	8	MS	MK	0
MSB3D	7175	072293	072293	0805931653	ITS3	FC	465	TRCLE	ITMS PURGE	2	932	UGL	1	40	MS	MK	0
MSB3D	7175	072293	072293	0805931653	ITS3	FC	465	TCLEE	ITMS PURGE	2L	12817	UGL	1	40	MS	MK	0
MSB3D	7175	072293	072293	0805931656	ITS3	FC	466	ITRCLE	ITMS PURGE	2	637	UGL	1	40	MS	MK	0
MSB3D	7175	072293	072293	0805931656	ITS3	FC	466	ITCLEE	ITMS PURGE	2L	48915	UGL	1	40	MS	MK	0

The Direct Sampling Ion Trap Mass Spectrometer for the Rapid Analysis of Volatile Organic Contaminants in Groundwater Samples

Table 2. Quality Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene). (contd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Date	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB4B	7176	071593	071993	0804930951	ITS2	FC	417	TRCLE	ITMS PURGE	2	1058	UGL	0	1	MS	MK	0
MSB4B	7176	071593	071993	0804930951	ITS2	FC	417	TCLEE	ITMS PURGE	2	33	UGL	0	1	MS	MK	0
MSB4B	7176	071593	071993	0804930954	ITS2	FC	418	1TRCLE	ITMS PURGE	2	1114	UGL	0	1	MS	MK	0
MSB4B	7176	071593	071993	0804930954	ITS2	FC	418	1TCLEE	ITMS PURGE	2	31	UGL	0	1	MS	MK	0
MSB4C	7177	071693	071993	0804930958	ITS2	FC	419	TRCLE	ITMS PURGE	2L	8703	UGL	0	1	MS	MK	0
MSB4C	7177	071693	071993	0804930958	ITS2	FC	419	TCLEE	ITMS PURGE	2L	6969	UGL	0	1	MS	MK	0
MSB4C	7177	071693	071993	0804931001	ITS2	FC	420	1TRCLE	ITMS PURGE	2L	9109	UGL	0	1	MS	MK	0
MSB4C	7177	071693	071993	0804931001	ITS2	FC	420	1TCLEE	ITMS PURGE	2L	7623	UGL	0	1	MS	MK	0
MSB4D	7178	071793	071993	0804931011	ITS2	FC	421	TRCLE	ITMS PURGE	2	104	UGL	0	1	MS	MK	0
MSB4D	7178	071793	071993	0804931011	ITS2	FC	421	TCLEE	ITMS PURGE	2	40	UGL	0	1	MS	MK	0
MSB4D	7178	071793	071993	0804931016	ITS2	FC	422	1TRCLE	ITMS PURGE	2	106	UGL	0	1	MS	MK	0
MSB4D	7178	071793	071993	0804931016	ITS2	FC	422	1TCLEE	ITMS PURGE	2	43	UGL	0	1	MS	MK	0
MSB5A	7179	071893	071993	0804931019	ITS2	FC	423	TRCLE	ITMS PURGE	2	3	UGL	0	1	MS	MK	0
MSB5A	7179	071893	071993	0804931019	ITS2	FC	423	TCLEE	ITMS PURGE	2	6	UGL	0	1	MS	MK	0
MSB5A	7179	071893	071993	0804931026	ITS2	FC	424	1TRCLE	ITMS PURGE	2	0	UGL	0	1	MS	MK	0
MSB5A	7179	071893	071993	0804931026	ITS2	FC	424	1TCLEE	ITMS PURGE	2	3	UGL	0	1	MS	MK	0
MSB5B	717A	070693	070693	0804931040	ITS2	FC	425	TRCLE	ITMS PURGE	2	33	UGL	0	1	MS	MK	0
MSB5B	717A	070693	070693	0804931040	ITS2	FC	425	TCLEE	ITMS PURGE	2	5	UGL	0	1	MS	MK	0
MSB5B	717A	070693	070693	0804931045	ITS2	FC	426	1TRCLE	ITMS PURGE	2	3	UGL	0	1	MS	MK	0
MSB5B	717A	070693	070693	0804931045	ITS2	FC	426	1TCLEE	ITMS PURGE	2	3	UGL	0	1	MS	MK	0

WSRC-TR-93-563

Table 2. Quality Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene). (contd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Date	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB5C	717B	071093	071093	0803931133	ITS1	FC	401	TRCLE	ITMS PURGE	2	12	UGL	0	1	MS	MK	0
MSB5C	717B	071093	071093	0803931133	ITS1	FC	401	TCLEE	ITMS PURGE	2	195	UGL	0	1	MS	MK	0
MSB5C	717B	071093	071093	0803931137	ITS1	FC	402	TRCLE	ITMS PURGE	2	10	UGL	0	1	MS	MK	0
MSB5C	717B	071093	071093	0803931137	ITS1	FC	402	TCLEE	ITMS PURGE	2	191	UGL	0	1	MS	MK	0
MSB6A	717C	071893	071993	0804931048	ITS2	FC	427	TRCLE	ITMS PURGE	2	3	UGL	0	1	MS	MK	0
MSB6A	717C	071893	071993	0804931048	ITS2	FC	427	TCLEE	ITMS PURGE	2	4	UGL	0	1	MS	MK	0
MSB6A	717C	071893	071993	0804931053	ITS2	FC	428	TRCLE	ITMS PURGE	2	1	UGL	0	1	MS	MK	0
MSB6A	717C	071893	071993	0804931053	ITS2	FC	428	TCLEE	ITMS PURGE	2	4	UGL	0	1	MS	MK	0
MSB6B	717D	071993	072093	0805931353	ITS3	FC	455	TRCLE	ITMS PURGE	2	1181	UGL	0	1	MS	MK	0
MSB6B	717D	071993	072093	0805931353	ITS3	FC	455	TCLEE	ITMS PURGE	2	40	UGL	0	1	MS	MK	0
MSB6B	717D	071993	072093	0805931357	ITS3	FC	456	TRCLE	ITMS PURGE	2	1129	UGL	0	1	MS	MK	0
MSB6B	717D	071993	072093	0805931357	ITS3	FC	456	TCLEE	ITMS PURGE	2	32	UGL	0	1	MS	MK	0
MSB6C	717E	071893	071993	0804931109	ITS2	FC	429	TRCLE	ITMS PURGE	2	6	UGL	0	1	MS	MK	0
MSB6C	717E	071893	071993	0804931109	ITS2	FC	429	TCLEE	ITMS PURGE	2	21	UGL	0	1	MS	MK	0
MSB6C	717E	071893	071993	0804931112	ITS2	FC	430	TRCLE	ITMS PURGE	2	6	UGL	0	1	MS	MK	0
MSB6C	717E	071893	071993	0804931112	ITS2	FC	430	TCLEE	ITMS PURGE	2	21	UGL	0	1	MS	MK	0
MSB7A	717F	071893	071993	0804931116	ITS2	FC	431	TRCLE	ITMS PURGE	2	1	UGL	0	1	MS	MK	0
MSB7A	717F	071893	071993	0804931116	ITS2	FC	431	TCLEE	ITMS PURGE	2	5	UGL	0	1	MS	MK	0
MSB7A	717F	071893	071993	0804931120	ITS2	FC	432	TRCLE	ITMS PURGE	2	0	UGL	0	1	MS	MK	0
MSB7A	717F	071893	071993	0804931120	ITS2	FC	432	TCLEE	ITMS PURGE	2	1	UGL	0	1	MS	MK	0

The Direct Sampling Ion Trap Mass Spectrometer for the Rapid Analysis of Volatile Organic Contaminants in Groundwater Samples

Table 2. Quality Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene). (contd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Date	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB7B	7180	071893	071993	0804931130	ITS2	FC	433	TRCLE	ITMS PURGE	2	24	UGL	0	1	MS	MK	0
MSB7B	7180	071893	071993	0804931130	ITS2	FC	433	TCLEE	ITMS PURGE	2	11	UGL	0	1	MS	MK	0
MSB7B	7180	071893	071993	0804931136	ITS2	FC	434	ITRCLE	ITMS PURGE	2	23	UGL	0	1	MS	MK	0
MSB7B	7180	071893	071993	0804931136	ITS2	FC	434	ITCLEE	ITMS PURGE	2	11	UGL	0	1	MS	MK	0
MSB7C	7181	071893	071993	0804931141	ITS2	FC	435	TRCLE	ITMS PURGE	2	3	UGL	1	8	MS	MK	0
MSB7C	7181	071893	071993	0804931141	ITS2	FC	435	TCLEE	ITMS PURGE	2	5	UGL	1	8	MS	MK	0
MSB7C	7181	071893	071993	0804931144	ITS2	FC	436	ITRCLE	ITMS PURGE	2	2	UGL	1	8	MS	MK	0
MSB7C	7181	071893	071993	0804931144	ITS2	FC	436	ITCLEE	ITMS PURGE	2	4	UGL	1	8	MS	MK	0
MSB8A	7182	071793	071993	0804931231	ITS	FC	437	TRCLE	ITMS PURGE	2	17	UGL	0	1	MS	MK	0
MSB8A	7182	071793	071993	0804931231	ITS2	FC	437	TCLEE	ITMS PURGE	2	74	UGL	0	1	MS	MK	0
MSB8A	7182	071793	071993	0804931236	ITS2	FC	438	ITRCLE	ITMS PURGE	2	17	UGL	0	1	MS	MK	0
MSB8A	7182	071793	071993	0804931236	ITS2	FC	438	ITCLEE	ITMS PURGE	2	74	UGL	0	1	MS	MK	0
MSB8B	7183	071793	071993	0804931240	ITS2	FC	439	TRCLE	ITMS PURGE	2	19	UGL	0	1	MS	MK	0
MSB8B	7183	071793	071993	0804931240	ITS2	FC	439	TCLEE	ITMS PURGE	2	9	UGL	0	1	MS	MK	0
MSB8B	7183	071793	071993	0804931245	ITS2	FC	440	ITRCLE	ITMS PURGE	2	19	UGL	0	1	MS	MK	0
MSB8B	7183	071793	071993	0804931245	ITS2	FC	440	ITCLEE	ITMS PURGE	2	8	UGL	0	1	MS	MK	0
MSB8C	7184	071793	071993	0804931255	ITS2	FC	441	TRCLE	ITMS PURGE	2	103	UGL	0	1	MS	MK	0
MSB8C	7184	071793	071993	0804931255	ITS2	FC	441	TCLEE	ITMS PURGE	2	93	UGL	0	1	MS	MK	0
MSB8C	7184	071793	071993	0804931259	ITS2	FC	442	ITRCLE	ITMS PURGE	2	52	UGL	0	1	MS	MK	0
MSB8C	7184	071793	071993	0804931259	ITS2	FC	442	ITCLEE	ITMS PURGE	2	113	UGL	0	1	MS	MK	0

Table 2. Quality Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene). (contd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Date	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB13A	7185	071893	071993	0804931303	ITS2	FC	443	TRCLE	ITMS PURGE	2	194	UGL	0	1	MS	MK	0
MSB13A	7185	071893	071993	0804931303	ITS2	FC	443	TCLEE	ITMS PURGE	2	1	UGL	0	1	MS	MK	0
MSB13A	7185	071893	071993	0804931306	ITS2	FC	444	1TRCLE	ITMS PURGE	2	184	UGL	0	1	MS	MK	0
MSB13A	7185	071893	071993	0804931306	ITS2	FC	444	1TCLEE	ITMS PURGE	2	0	UGL	0	1	MS	MK	0
MSB13B	7186	071493	071993	0804931317	ITS2	FC	445	TRCLE	ITMS PURGE	2	5	UGL	0	1	MS	MK	0
MSB13B	7186	071493	071993	0804931317	ITS2	FC	445	TCLEE	ITMS PURGE	2	52	UGL	0	1	MS	MK	0
MSB13B	7186	071493	071993	0804931321	ITS2	FC	446	1TRCLE	ITMS PURGE	2	4	UGL	0	1	MS	MK	0
MSB13B	7186	071493	071993	0804931321	ITS2	FC	446	1TCLEE	ITMS PURGE	2	50	UGL	0	1	MS	MK	0
MSB13CC	7187	071893	071993	0804931324	ITS2	FC	447	TRCLE	ITMS PURGE	2	10	UGL	0	1	MS	MK	0
MSB13CC	7187	071893	071993	0804931324	ITS2	FC	447	TCLEE	ITMS PURGE	2	15	UGL	0	1	MS	MK	0
MSB13CC	7187	071893	071993	0804931328	ITS2	FC	448	1TRCLE	ITMS PURGE	2	10	UGL	0	1	MS	MK	0
MSB13CC	7187	071893	071993	0804931328	ITS2	FC	448	1TCLEE	ITMS PURGE	2	15	UGL	0	1	MS	MK	0
MSB13D	7188	071893	071993	0804931337	ITS2	FC	449	TRCLE	ITMS PURGE	2	33	UGL	0	1	MS	MK	0
MSB13D	7188	071893	071993	0804931337	ITS2	FC	449	TCLEE	ITMS PURGE	2	54	UGL	0	1	MS	MK	0
MSB13D	7188	071893	071993	0804931342	ITS2	FC	450	1TRCLE	ITMS PURGE	2	33	UGL	0	1	MS	MK	0
MSB13D	7188	071893	071993	0804931342	ITS2	FC	450	1TCLEE	ITMS PURGE	2	54	UGL	0	1	MS	MK	0
MSB57D	7189	072993	072993	0805931454	ITS3	FC	467	TRCLE	ITMS PURGE	2	29	UGL	0	1	MS	MK	0
MSB57D	7189	072993	072993	0805931454	ITS3	FC	467	TCLEE	ITMS PURGE	2	50	UGL	0	1	MS	MK	0
MSB57D	7189	072993	072993	0805931459	ITS3	FC	468	1TRCLE	ITMS PURGE	2	24	UGL	0	1	MS	MK	0
MSB57D	7189	072993	072993	0805931459	ITS3	FC	468	1TCLEE	ITMS PURGE	2	44	UGL	0	1	MS	MK	0

The Direct Sampling Ion Trap Mass Spectrometer for the Rapid Analysis of Volatile Organic Contaminants in Groundwater Samples

Table 2. Quality Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene. (contd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Date	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB58D	718A	072093	072093	0805931400	ITS3	FC	457	TRCLE	ITMS PURGE	2	722	UGL	0	1	MS	MK	0
MSB58D	718A	072093	072093	0805931400	ITS3	FC	457	TCLEE	ITMS PURGE	2	1223	UGL	0	1	MS	MK	0
MSB58D	718A	072093	072093	0805931403	ITS3	FC	458	1TRCLE	ITMS PURGE	2	687	UGL	0	1	MS	MK	0
MSB58D	718A	072093	072093	0805931403	ITS3	FC	458	1TCLEE	ITMS PURGE	2	1123	UGL	0	1	MS	MK	0
MSB59D	718B	072093	072093	0805931421	ITS3	FC	459	TRCLE	ITMS PURGE	2L	4508	UGL	0	1	MS	MK	0
MSB59D	718B	072093	072093	0805931421	ITS3	FC	459	TCLEE	ITMS PURGE	2L	114134	UGL	0	1	MS	MK	0
MSB59D	718B	072093	072093	0805931427	ITS3	FC	460	1TRCLE	ITMS PURGE	2L	4196	UGL	0	1	MS	MK	0
MSB59D	718B	072093	072093	0805931427	ITS3	FC	460	1TCLEE	ITMS PURGE	2L	119395	UGL	0	1	MS	MK	0
MSB60D	718C	072993	072993	0805931512	ITS3	FC	469	TRCLE	ITMS PURGE	2	53	UGL	0	1	MS	MK	0
MSB60D	718C	072993	072993	0805931512	ITS3	FC	469	TCLEE	ITMS PURGE	2	92	UGL	0	1	MS	MK	0
MSB60D	718C	072993	072993	0805931515	ITS3	FC	470	1TRCLE	ITMS PURGE	2	51	UGL	0	1	MS	MK	0
MSB60D	718C	072993	072993	0805931515	ITS3	FC	470	1TCLEE	ITMS PURGE	2	88	UGL	0	1	MS	MK	0
MSB62B	718D	080293	080293	0805931518	ITS3	FC	471	TRCLE	ITMS PURGE	2	32	UGL	0	1	MS	MK	0
MSB62B	718D	080293	080293	0805931518	ITS3	FC	471	TCLEE	ITMS PURGE	2	35	UGL	0	1	MS	MK	0
MSB62B	718D	080293	080293	0805931522	ITS3	FC	472	1TRCLE	ITMS PURGE	2	32	UGL	0	1	MS	MK	0
MSB62B	718D	080293	080293	0805931522	ITS3	FC	472	1TCLEE	ITMS PURGE	2	34	UGL	0	1	MS	MK	0
MSB62C	718E	080293	080293	0805931533	ITS3	FC	473	TRCLE	ITMS PURGE	2	77	UGL	0	1	MS	MK	0
MSB62C	718E	080293	080293	0805931533	ITS3	FC	473	TCLEE	ITMS PURGE	2	235	UGL	0	1	MS	MK	0
MSB62C	718E	080293	080293	0805931538	ITS3	FC	474	1TRCLE	ITMS PURGE	2	69	UGL	0	1	MS	MK	0
MSB62C	718E	080293	080293	0805931538	ITS3	FC	474	1TCLEE	ITMS PURGE	2	211	UGL	0	1	MS	MK	0

WSRC-TR-93-563

Table 2. Quality Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene). (cont'd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Date	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB62D	718F	072093	072093	0805931430	ITS3	FC	461	TRCLE	ITMS PURGE	2	243	UGL	0	1	MS	MK	0
MSB62D	718F	072093	072093	0805931430	ITS3	FC	461	TCLEE	ITMS PURGE	2	904	UGL	0	1	MS	MK	0
MSB62D	718F	072093	072093	0805931434	ITS3	FC	462	ITRCLE	ITMS PURGE	2	110	UGL	0	1	MS	MK	0
MSB62D	718F	072093	072093	0805931434	ITS3	FC	462	ITCLEE	ITMS PURGE	2	343	UGL	0	1	MS	MK	0
MSB63B	7190	080193	080293	0805931542	ITS3	FC	475	TRCLE	ITMS PURGE	2	326	UGL	0	1	MS	MK	0
MSB63B	7190	080193	080293	0805931542	ITS3	FC	475	TCLEE	ITMS PURGE	2	27	UGL	0	1	MS	MK	0
MSB63B	7190	080193	080293	0805931545	ITS3	FC	476	ITRCLE	ITMS PURGE	2	306	UGL	0	1	MS	MK	0
MSB63B	719	080293	080293	0805931545	ITS3	FC	476	ITCLEE	ITMS PURGE	2	25	UGL	0	1	MS	MK	0
MSB63C	7191	080293	080293	0805931556	ITS3	FC	477	TRCLE	ITMS PURGE	2	12	UGL	0	1	MS	MK	0
MSB63C	7191	080293	080293	0805931556	ITS3	FC	477	TCLEE	ITMS PURGE	2	33	UGL	0	1	MS	MK	0
MSB63C	7191	080293	080293	0805931559	ITS3	FC	478	ITRCLE	ITMS PURGE	2	11	UGL	0	1	MS	MK	0
MSB63C	7191	080293	080293	0805931559	ITS3	FC	478	ITCLEE	ITMS PURGE	2	31	UGL	0	1	MS	MK	0
MSB63D	7192	080293	080293	0805931603	ITS3	FC	479	TRCLE	ITMS PURGE	2	60	UGL	0	1	MS	MK	0
MSB63D	7192	080293	080293	0805931603	ITS3	FC	479	TCLEE	ITMS PURGE	2	321	UGL	0	1	MS	MK	0
MSB63D	7192	080293	080293	0805931606	ITS3	FC	480	ITRCLE	ITMS PURGE	2	56	UGL	0	1	MS	MK	0
MSB63D	7192	080293	080293	0805931606	ITS3	FC	480	ITCLEE	ITMS PURGE	2	308	UGL	0	1	MS	MK	0
MSB64B	7193	071993	072093	0805931446	ITS3	FC	463	TRCLE	ITMS PURGE	2	1875	UGL	0	1	MS	MK	0
MSB64B	7193	071993	072093	0805931446	ITS3	FC	463	TCLEE	ITMS PURGE	2	117	UGL	0	1	MS	MK	0
MSB64B	7193	071993	072093	0805931449	ITS3	FC	464	ITRCLE	ITMS PURGE	2	1755	UGL	0	1	MS	MK	0
MSB64B	7193	071993	072093	0805931449	ITS3	FC	464	ITCLEE	ITMS PURGE	2	109	UGL	0	1	MS	MK	0

The Direct Sampling Ion Trap Mass Spectrometer for the Rapid Analysis of Volatile Organic Contaminants in Groundwater Samples

Table 2. Quality Compliance Monitoring Sample Analysis: Results are listed in format required for input into the SRS analytical database (TRCLE = trichloroethylene, TCLEE = tetrachloroethylene). (contd)

Well Name	CoC No.	Sample Date	Date Rec'd	Analysis Date and Time	Analysis Date	Lab Code	Lab Sample ID	Test Name	Analysis Method	Detection Limit	Results	Results Unit	No. of Dilutions	Dilution Factor	Inst.	Analyst	Nominal Conc.
MSB64C	7194	080293	080293	0805931622	ITS3	FC	481	TRCLE	ITMS PURGE	2	95	UGL	0	1	MS	MK	0
MSB64C	7194	080293	080293	0805931622	ITS3	FC	481	TCLEE	ITMS PURGE	2	393	UGL	0	1	MS	MK	0
MSB64C	7194	080293	080293	0805931627	ITS3	FC	482	1TRCLE	ITMS PURGE	2	92	UGL	0	1	MS	MK	0
MSB64C	7194	080293	080293	0805931627	ITS3	FC	482	1TCLEE	ITMS PURGE	2	386	UGL	0	1	MS	MK	0
MSB64D	7195	080293	080293	0805931636	ITS3	FC	483	TRCLE	ITMS PURGE	2	8	UGL	0	1	MS	MK	0
MSB64D	7195	080293	080293	0805931636	ITS3	FC	483	TCLEE	ITMS PURGE	2	23	UGL	0	1	MS	MK	0
MSB64D	7195	080293	080293	0805931639	ITS3	FC	484	1TRCLE	ITMS PURGE	2	9	UGL	0	1	MS	MK	0
MSB64D	7195	080293	080293	0805931639	ITS3	FC	484	1TCLEE	ITMS PURGE	2	23	UGL	0	1	MS	MK	0

Figure 1. GC vs. DSITMS TCE Comparison

Figure 2. GC vs. DSITMS PCE Comparison

Figure 3. DSITMS Standard Curve for TCE

Figure 4. DSITMS Standard Curve for PCE

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