Results of the GCMS Effluent Gas Analysis for the Brine Processing Test

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The effluent gas for the Paragon Ionomer Water Processor (IWP), UMPQUA Ultrasonic Brine Dewatering System (UBDS), and the NASA Brine Evaporation Bag (BEB) were analyzed using Headspace GCMS Analysis in the recent AES FY14 Brine Processing Test. The results from the analysis describe the number and general chemical species of the chemicals produced. Comparisons were also made between the different chromatograms for each system, and an explanation of the differences in the results is reported.

Nomenclature

AES	=	Advanced Exploration Systems
BEB	=	Brine Evaporation Bag
GCMS	=	Gas Chromatography Mass Spectrometry
hrs	=	hours
ISS	=	International Space Station
IWP	=	Ionomer Water Processor
L	=	Liter
L/min	=	Liter per minute
mL	=	milliliter
MS	=	Mass Spectrum
NIST11	=	mass spectral identification program
UBDS	=	Ultrasonic Brine Dewatering System

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I. Introduction

THE Advanced Exploration Systems (AES) Program wanted to determine the performance characteristics of the brine dewatering technologies currently existing within NASA. Thus, the Brine Evaporation Bag (BEB) System,[1-4] the Ionomer Water Processor (IWP),[5] the Ultrasonic Brine Dewatering System (UBDS),[6] and the Forward Osmosis Brine Dryer (FOBD)[7] all participated in the AES Brine Processing Test in order to determine their performance characteristics.[8]

Part of the performance characterization includes the Gas Chromatograph Mass Spectrometry (GCMS) analysis of effluent gas being produced by each of the technologies. The motivation for the GCMS analysis of the effluent gas is because the working hypothesis is that the effluent gas from the system installed upon the ISS will be vented into the cabin. The ISS will then recycle the effluent gas as part of the normal cabin air recycling and any organics within the effluent gas will be handled by the ISS Trace Contaminate Control System. Thus, the system chosen will need to produce chemical concentration levels low enough that it would not cause the concentration of any of the chemicals produced to go above the Personal Exposure Limits (PELs) within the cabin.

GCMS analysis allows for the separation and identification of different chemical species within the sample mixture as well as the detection of very low levels of concentration. Thus, GCMS analysis is able to identify and quantitate the chemicals within the effluent gas. The analysis done here, however, is limited to the qualitative analysis between the different technologies.

II. GCMS Analysis

The premise of the GCMS analysis was that each of the processes will be releasing their effluent gas and water vapor into the ISS cabin. As such, the total quantity of hydrocarbons that would be discarded into the cabin is of interest. Due to the high flow volume of the IWP (several hundred liters per min), only 0.1% of the effluent gas was collected on Tenax AT for GCMS headspace analysis. The collected data would then be normalized for the volume of brine processed and the extent to which the brine was dewatered. For example, a 60% dewatered brine is processed for a shorter period of time than a 100% dewatered brine, and thus would need to be corrected for the shorter run time. Likewise, in comparing a 16 L batch to a 0.4 L batch, a correction must be applied for the amount of brine processed. Air backgrounds were also collected during the entire run so that intrinsic air contaminants could be corrected for in determining the contaminant load of the brine runs.

The data will be discussed in two parts. First, the GCMS chromatogram will be discussed, and then the GCMS mass spectral analysis will be discussed.

A. GCMS Chromatograms

The GCMS chromatograms were hand analyzed for identification and relative quantities. The identification was done by fingerprint matching of the mass spectrum (MS) to the NIST11 Mass Spectral Library. Relatively low matching factors were accepted for this identification. This is a tentative identification since only NIST11 MS fingerprinting was used. High accuracy identification would require the purchase and running of the tentatively identified compounds for cross verification of the retention times and the actual MS as produced by the reference compound.

The relative quantity of the components is hand calculated by the apparent peak area of each component; this is not quantitative. The same standards that could be used for identity verification above could also give quantitation of the identifiable peaks, but this was not done due to time and funding limitations. Peak identity verification and quantitation could be done provided funding and time.

1. UBDS

Figure 1 shows the GC Chromatogram for the only ISS Alternate Pretreatment Brine run of the UMPQUA UBDS. The red trace is the chromatogram collected from the effluent gas of the UBDS. The green trace is the chromatogram of an equivalent volume of lab air used as a background. The background was collected at the same time as the UBDS run.

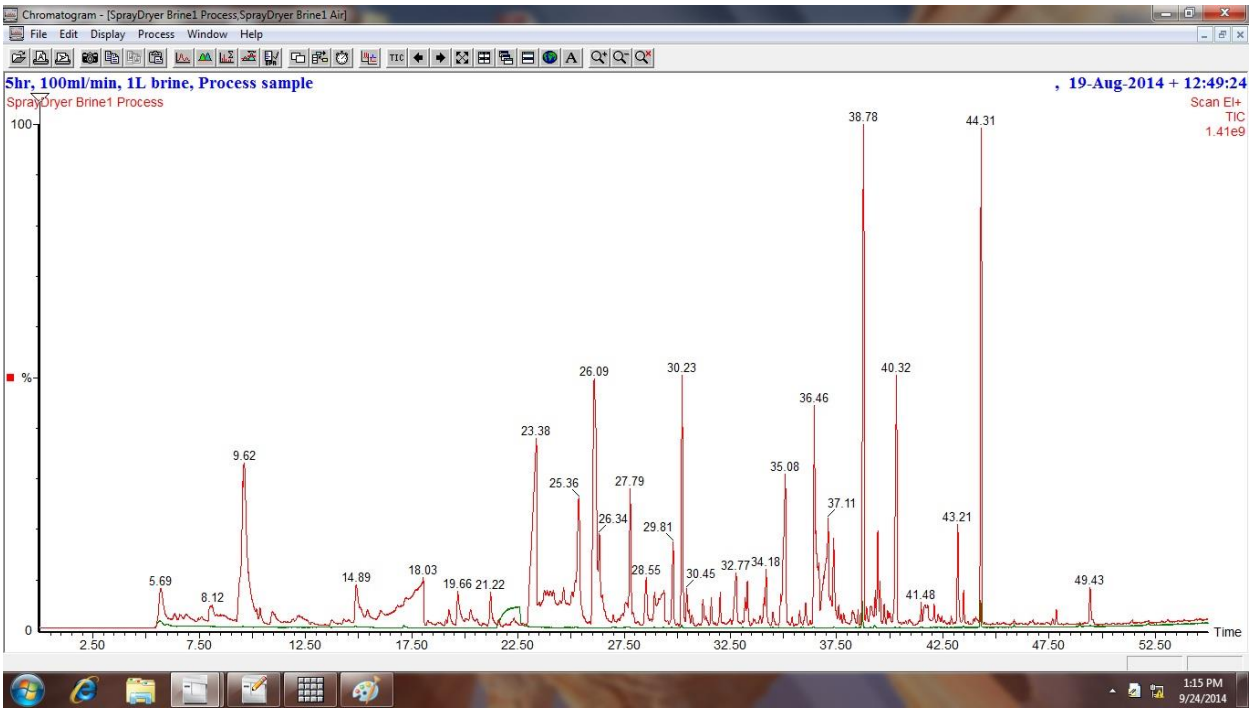

Figure 1. The red trace is the chromatogram for the effluent gas of the UBDS. The green trace is the chromatogram of an equivalent volume of lab air collected as a background.

Nearly 200 peaks were observed and are reported in Appendix B. They included alkanes, alkenes, alcohols, aldehydes, ketones, ethers, aliphatics, aromatics, disulfides, nitriles, and nitrogenous aromatic rings (pyrrole, pyridine, etc.).

Note: The UBDS completed only one ISS Alternate Pretreatment run and no Hygiene brine runs.

2. IWP

The IWP ran three ISS Alternate Pretreatment Brine at ARC. It also ran a Hygiene Brine run at ARC. The GC chromatograms for these runs are shown below (Figure 2, Figure 3, and Figure 4) with the process sample shown in red and the air background shown in green.

The first run (Figure 2) was run for a total of 20 days (run in several segments) and processed 16L of ISS Alternate Pretreatment brine to a nominal 84.5% water recovery. During part 2 of run 1, the WFRD and UBDS were also run and their effluent gases were released into the room with the IWP. This is most likely the source of the high air background in Figure 2.

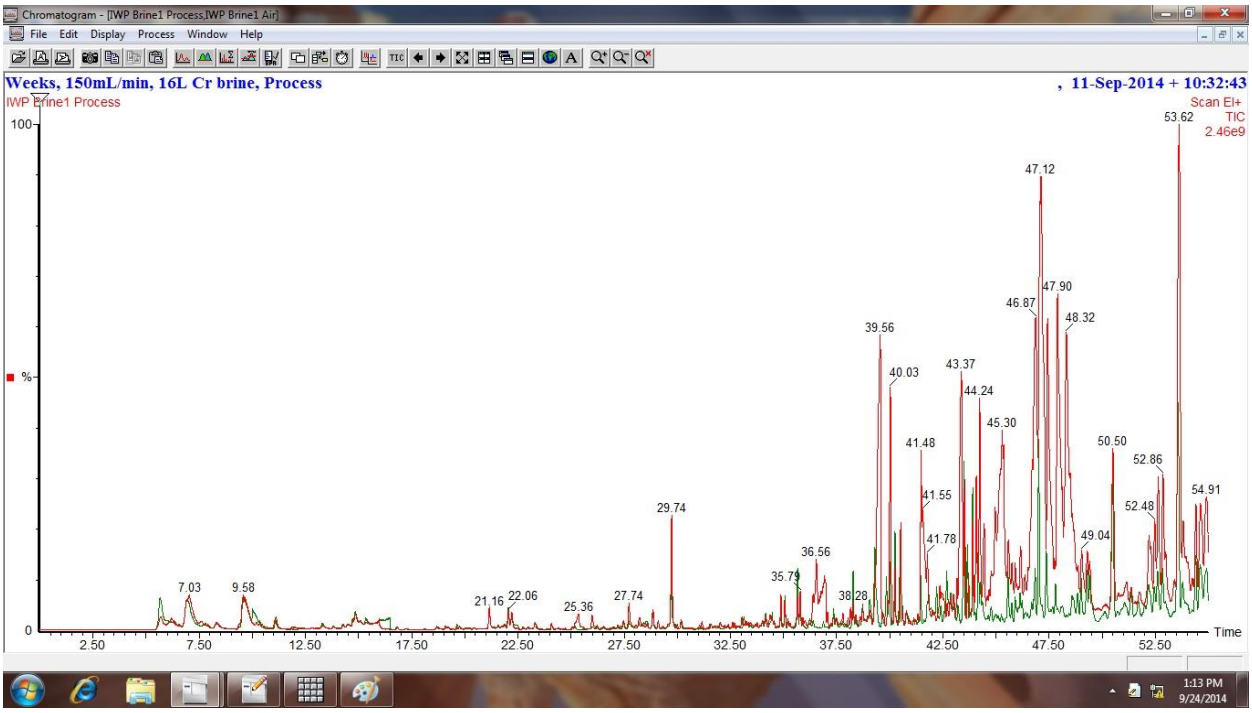

Figure 2. The red trace is the chromatogram collected from the effluent gas of the first ISS Alternate Pretreatment brine run of the IWP. The green trace is the chromatogram of an equivalent volume of lab air collected as a background. The high background is due to other processors running within the lab during part 2 of the first run.

The second IWP ISS Alternate Pretreatment run was reconfigured to recycle its air flow. Thus, the background for Figure 3 is that of a cleaned adsorbent tube with no air collection. The second run lasted for 1.7 days and processed 16 L of brine to 38.7% water recovery.

The third IWP ISS Alternate Pretreatment run also recycled its air. Its chromatogram is shown in Figure 4. The system processed 16L of brine over 6.1 days to 71.3% water recovery.

Figure 5 compares the three ISS Alternate Pretreatment brine runs. The first run is in red, the second run is in green, and the third run is in purple.

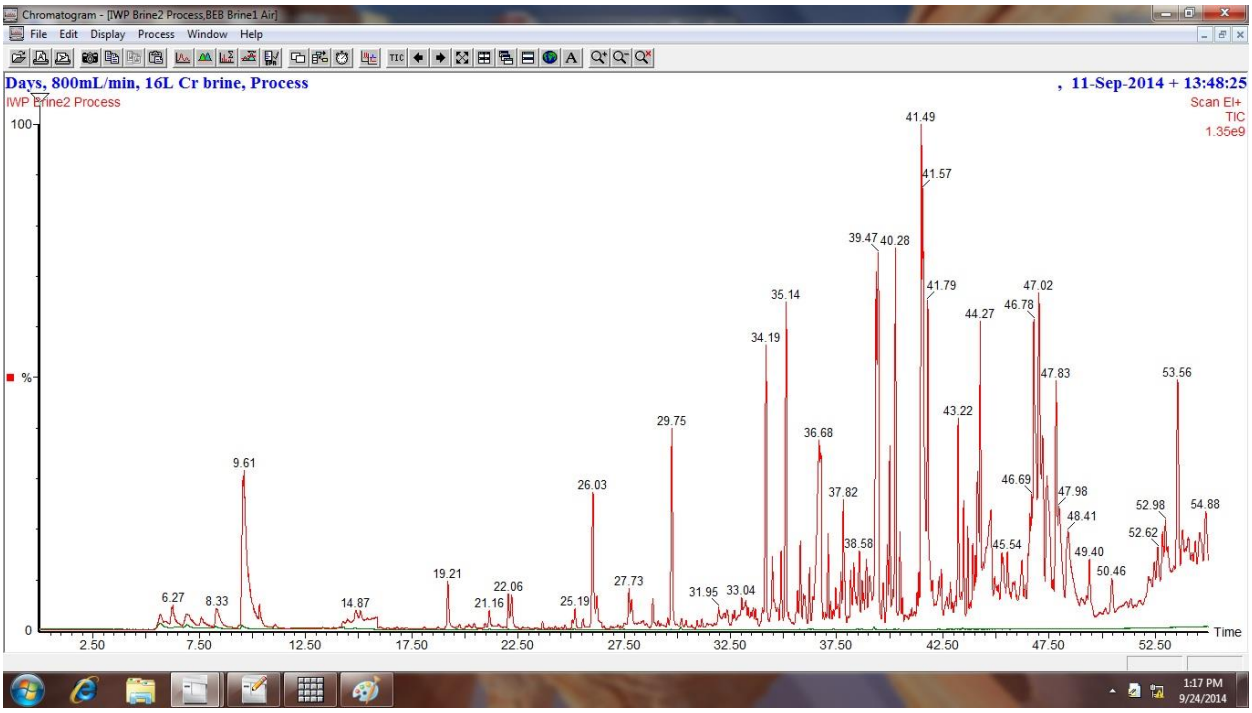

Figure 3. The red trace is the chromatogram collected from the effluent gas of the second ISS Alternate Pretreatment brine run of the IWP. The green trace is the chromatogram of the adsorbent used. No air background is presented since the IWP was converted to recycle its airflow.

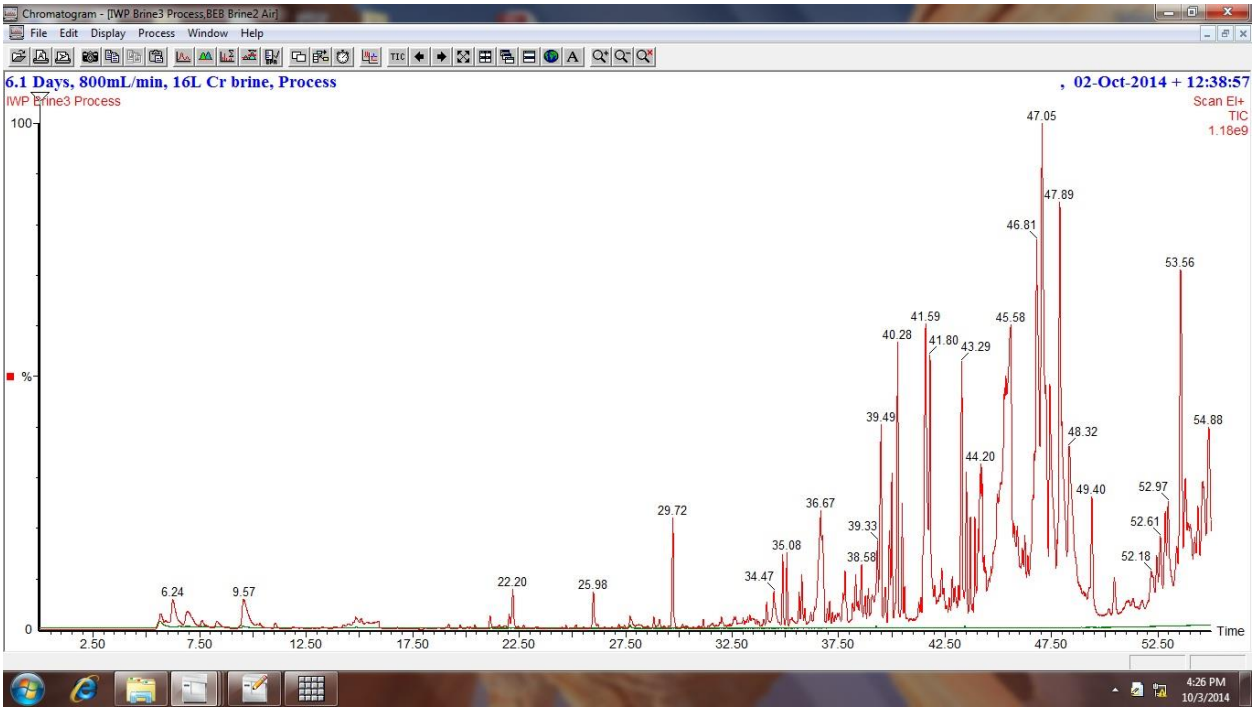

Figure 4. The red trace is the chromatogram collected from the effluent gas of the third ISS Alternate Pretreatment brine run of the IWP. The green trace is the chromatogram of an adsorbent background. No air background is presented since the IWP was converted to recycle its airflow.

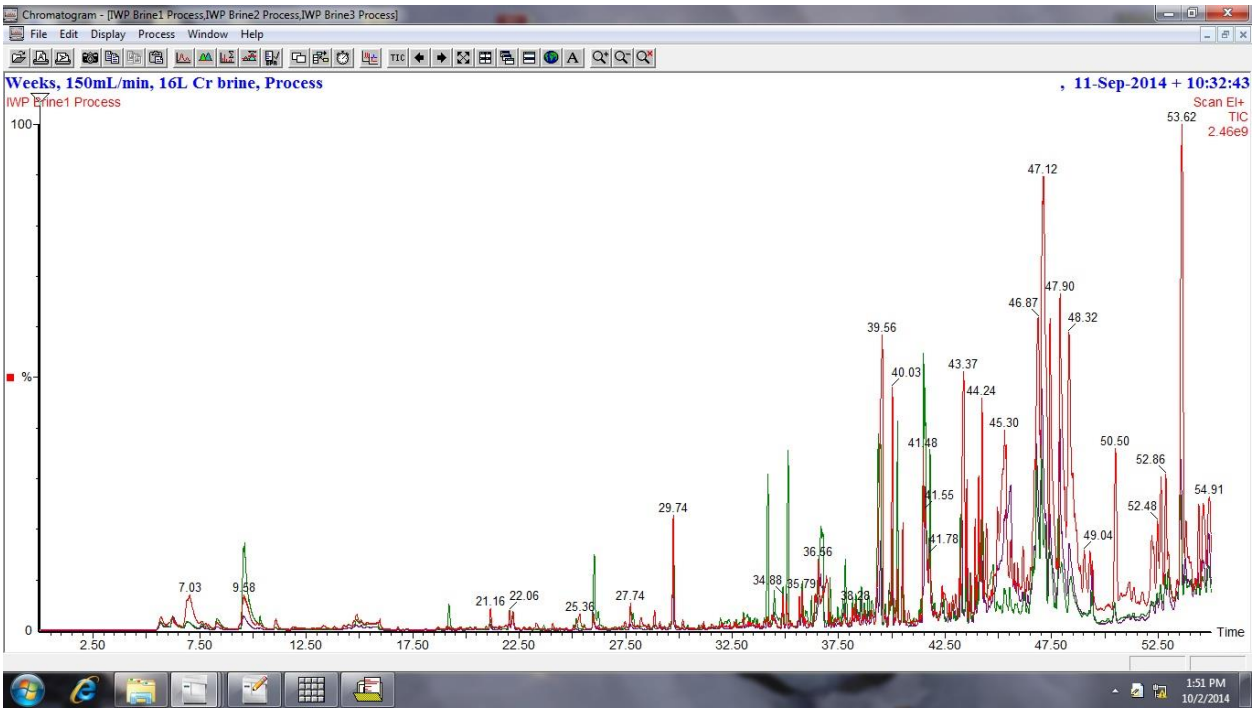

Figure 5. Comparison of the three ISS Alternate Pretreatment brine runs. The first run is in red, the second run is in green, and the third run is in purple. The three runs lasted for 20, 1.7, and 6.1 day, respectively.

The IWP produced similar chemicals to the UBDS with the exception that it did not produce any nitriles or nitrogenous compounds. The chemicals are listed in Appendix A.

3. BEB

The BEB processed approximately 400 mL of brine per batch. The BEB system ran three ISS Alternate Pretreatment brine batches and three Hygiene Brine batches. An air sample and a process sample were collected for each of the runs. The samples were collected for the entire duration of the run. The ISS Alternate Pretreatment brine runs took nominally 4 hrs (nominally 100% water recovery). The ISS Alternate Pretreatment runs took 2.75 hrs to reach 85% water recovery. Figure 6, Figure 7, and Figure 8 show the process and air samples for each of the first, second, and third ISS Alternate Pretreatment brine runs, respectively.

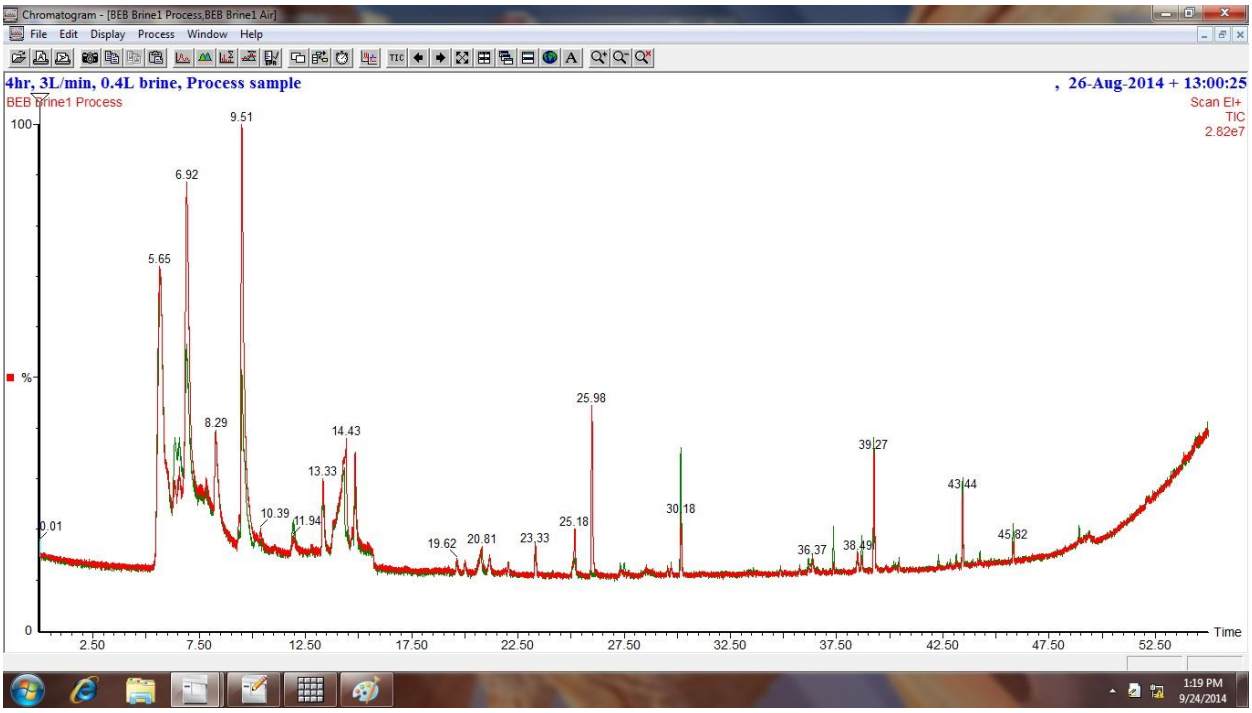

Figure 6. Chromatograms for effluent gas samples collected from the process (red) and air (green) for the first ISS Alternate Pretreatment brine run.

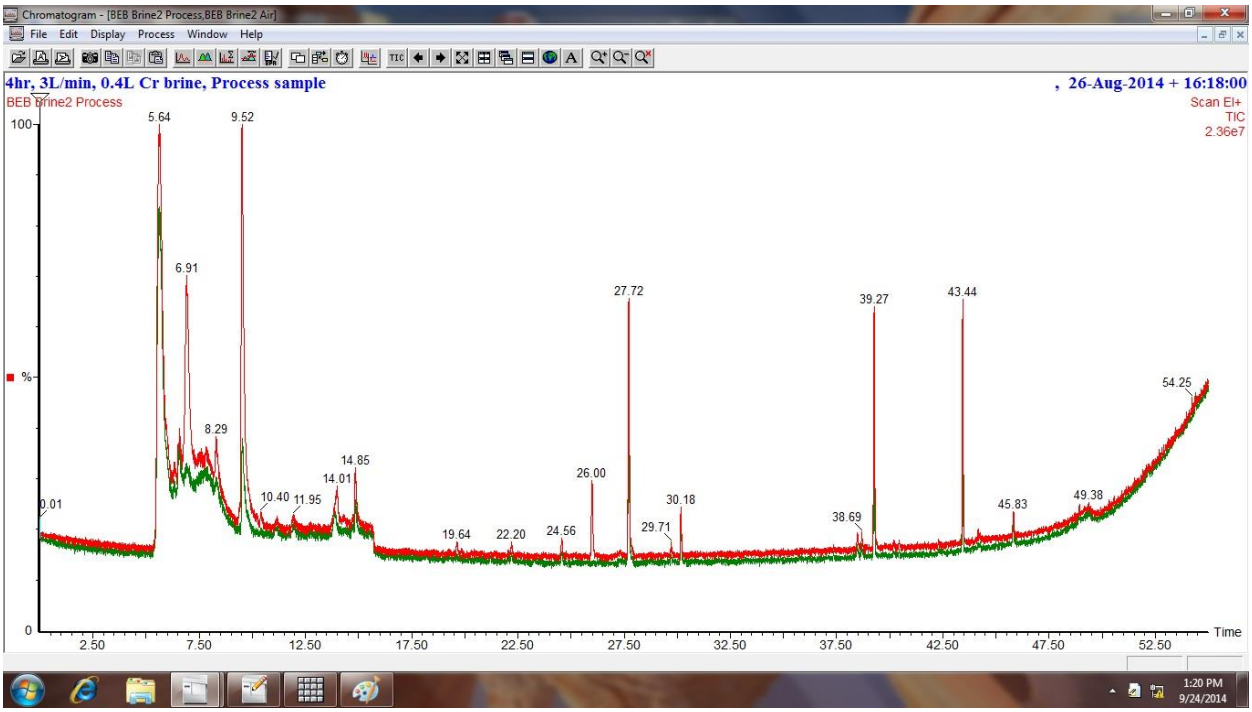

Figure 7. Chromatograms for effluent gas samples collected from the process (red) and air (green) for the second ISS Alternate Pretreatment brine run.

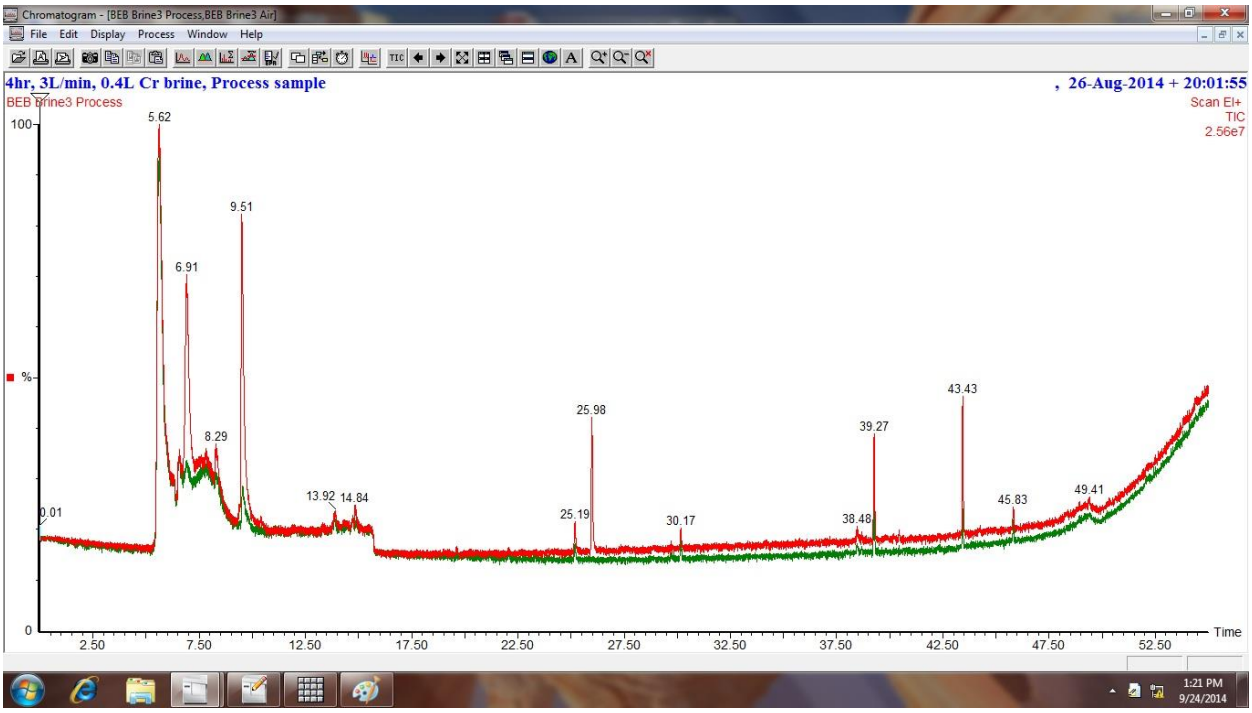

Figure 8. Chromatograms for effluent gas samples collected from the process (red) and air (green) for the third ISS Alternate Pretreatment brine run.

The BEB had very few bands present in the chromatograms as compared to the IWP and UBDS. The observed peaks are reported in Appendix C.

The limited number of chemicals is presumably due to the short period of time required for the BEB run (<4hrs compared to the several days of the IWP run). Additionally, if the amount of organics released were based upon Henry's Law and the flow of air through the reactor, then the BEB would have substantially less organics since its gas flow rate is only 0.1 L/min compared to the 100L/min for the UBDS or the 800 L/min for the IWP.
Finally, the condensation of the water vapor could also be stripping the organics from the effluent gas since there is very little air compared to the volume of steam.

4. Comparison of the BEB, IWP, and UBDS

The first observation is that the BEB's process chromatogram shows fewer organics than the IWP and UBDS. Figure 9 shows a comparison of the BEB, IWP, and UBDS chromatograms; all on the same scale. The intensity of the BEB's chromatogram is much weaker than that of the IWP and UBDS, and is just barely above the x-axis. The UBDS, which ran for approximately the same duration and processed a similar quantity of brine as the BEB, shows many more peaks with greatly larger intensity. This is likely due to the UBDS using an electrostatic precipitator which ran at 200 °C. This high temperature causes charring and burning of the organics producing the bands observed. The IWP, which runs at a low temperature similar to the BEB, also shows many peaks that are much more intense than those produced by the BEB. This is assumed to be due to the length of time required for the IWP process to operate and the volume of air that the IWP requires.

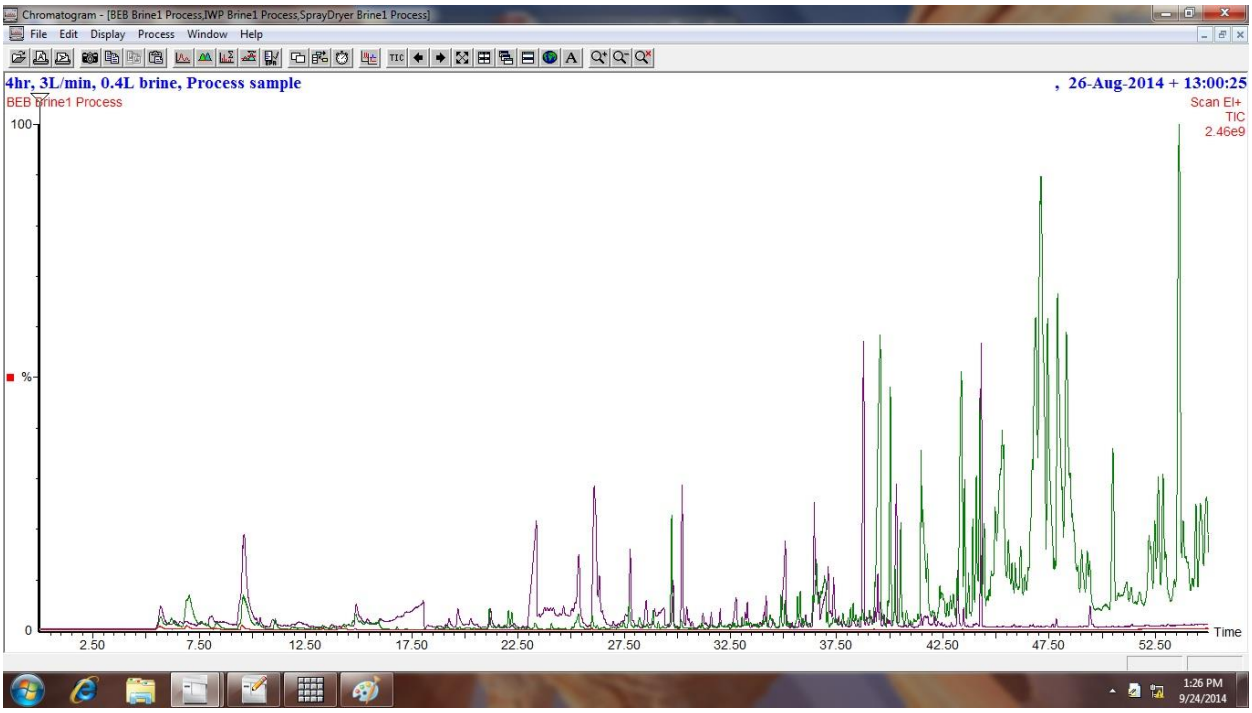

Figure 9. The chromatograms of the BEB (red), IWP (green), and UBDS (purple) are shown, all on the same scale. The chromatogram for the BEB (red), on this scale, is at the baseline.

A qualitative comparison of the organics produced by the three processes will be presented within the next section.

B. GCMS Mass Spectrum

The chromatograms of the ISS Alternate Pretreatment brine runs were band fit for the peak area of the observed peaks. The air chromatogram for the run was used as the base line, and to identify which chemicals were present in the air and not due to the process. For bands that were present in both the air and process chromatograms, the area of the air peak was subtracted out from the area of the process peak to determine the peak area.

This analysis is peak area only, and is not a determination of concentration or quantity since no calibration curve was used. A direct comparison between peak areas of the same chemical can be made with the ratio of the peak areas equaling the ratio of the quantities collected (the comparison is between peaks of the same chemical, and does not apply to comparisons of different chemicals). It should also be pointed out that correction for the volume of brine processed and the extent of brine dewatering must be taken into consideration when comparing the raw data. The raw data is presented in Appendices A, B, and C.

Table 1 shows the Total Area, the Area/L of brine processed, the Area/Day, and the Area/Liter of air for the BEB, IWP, and UBDS. The scaling for percent dewatering is done linearly, even though, each additional percent of dewatering takes increasingly longer. The BEB produces only about 0.1% of the total organics produced by the IWP and UBDS. Additionally, the BEB produces a greater concentration of organics within the effluent gas (Area/Vol air) indicating that the effluent gas of the BEB may be saturated. Thus, the total organics that are being evolved from the BEB is limited because of the limited volume of purge gas; a consequence of Henry's Law.

Table 1. Comparison of organics produced by the BEB, IWP and UBDS.

	BEB			IWP		UBDS
	Run 1	Run 2	Run 3	Run 1	Run 2	Run 1
Total area	5	5	5	5969	8437	2239
Area / L	12	12	14	441	1363	2239
Area / day	29	28	33	352	12458	9772
Area / Vol. air	200	192	227	0.3	11	68

5. IWP

The IWP produced an effluent gas that contained a wide variety of chemicals that included alkanes, alkenes, cyclic, and aromatic carbon bonds, as well as alcohols, aldehydes, ketones, ether, and carboxylic acid oxygen species. In addition, a number of cyclic compounds were seen where one or more of the atoms within the ring were an oxygen or sulfur. Finally, a number of thiol and disulfide compounds were also observed.

6. UBDS

The UBDS also produced a broad spectrum of chemicals similar to the IWP with the addition that the UBDS also produced a number of nitrogen containing ring compounds, amines, and nitriles. The nitrogenous compounds are most likely the result of the high temperatures and the electric field of the electrostatic precipitator within the UBDS. Many nitrogenous aromatics and nitrile compounds are produced by the chemical reaction of their aromatic and oxygenous counter parts reacting with ammonia, i.e., furan reacts with ammonia to become pyrrole, and benzene becomes benzonitrile.

7. BEB

The BEB chromatogram for the ISS Alternate Pretreatment brine produced less than a dozen peaks compared to the nearly 200 peaks produced by the IWP and UBDS. However, the difference in number and area of peaks could have been a result of the low air flow and short collection time. Additionally, the peaks that are present may be so weak in intensity that they cannot be resolved from the baseline by visual inspection of the chromatogram.

In order to increase the intensity of any weak peaks that are being lost within the baseline of the chromatogram, the volume of effluent gas collected for the third hygiene run was increased by a factor of 40. The factor of 40 is based on the ratio of the 16 L ran by the IWP to the 0.4 L ran by the BEB, so that a direct comparison of the chromatograms between the BEB and the IWP could be made. This direct comparison would show if there is an actual difference in the quantity of organics produced by the two systems on a per Liter of brine basis. The process effluent gas for the third hygiene brine run was collected at a flow rate of 100 ml/min with the identical setup as was used for the IWP and UBDS. This comparison is shown in Figure 10.

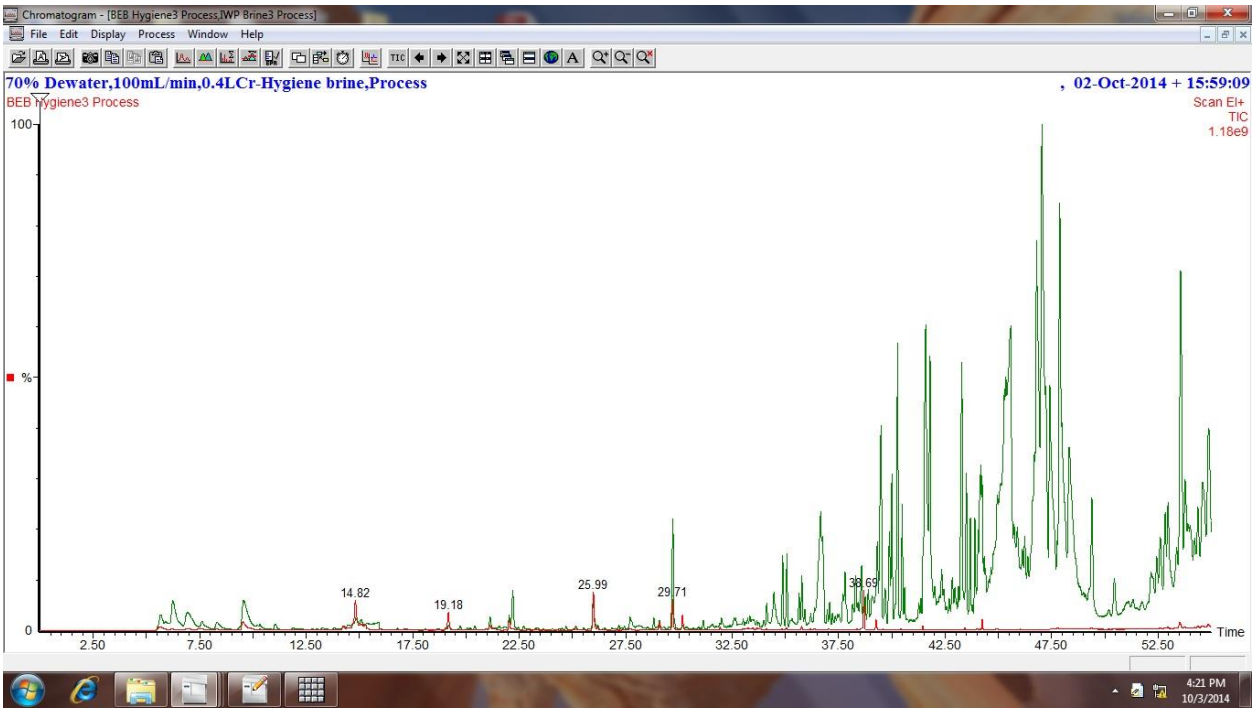

Figure 10. Comparison of an IWP run to a BEB run which had its gas sampling collection rate increased by a factor of 40 so that a direct comparison of the chromatograms could be made between the two systems. The chromatograms show that the BEB (red) produces much less organics than the IWP (green). The chromatogram of the BEB (red) is at the axis, and only the peaks are discernable from the baseline.

Figure 10 clearly shows that the BEB System produces significantly less organics than the IWP process. As stated earlier, this is most likely due to the much smaller volume of air ($1/8000^{th}$) that the BEB System used.

III. Conclusion

The GCMS analysis shows some dramatic differences between the effluent gas obtained from the IWP, UBDS, and BEB systems. These differences include both concentration and also composition. Both the IWP and UBDS produce a substantial quantity of effluent organics compared to the BEB. This is presumably due to the value of purge gas air that each system requires. The hypothesis is that the volatile organics within the brine is removed based upon a Henry's Law process. Thus, the greater the flow of purge gas over the brine, the greater the quantity of organics that will be removed. However, if the effluent gas is recycled in a closed loop, then these organics will not be released from the system.

The composition of the organics observed from the IWP effluent gas consists of aliphatic and aromatic hydrocarbons, which also contain oxygen and sulfur. The effluent gas of the UBDS also contained those species, but included nitrogenous compounds. Those nitrogenous compounds are believed to be formed from the high temperature reaction of the oxygenous species identified from the IWP reacting with ammonia. This reaction results in the nitrogen substitution of the oxygen.

Acknowledgments

This research was support by the AES Brine Project.

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Appendix A

	IWP - Run 1	
Time	Identification	Area
6.09	Propene	4.1
6.19	Sulfur Dioxide	13.1
6.56	Unknown	4.1
6.94	Methanol	13
7.03	2-methyl-1-propene	10
7.6	Methanthiol	7.4
7.78	Acetaldehyde	2.6
7.91	2-Butene	2.7
8.32	Ethanol	6.2
9.42	2-Propenal	2.1
9.58	acetone	42
9.72	Propanal	15.3
10.21	Unknown	3.7
10.34	acetone	3
10.47	Propanal	0.8
11.08	2-methyl-2-propanol	5.8
11.91	Carbon disulfide	2.2
12.27	Unknown	2
12.8	Unknown	0.7
13.03	2-methyl-propanal	0.8
13.3	tert-butyl methyl ether	3.4
13.8	2,3-dihydro-furan	1.2
14.27	Methyl vinyl ketone	2
14.5	Unknown	3.6
14.74	Pentanal	7
14.87	2-Butanone	10
15.09	Hexane	5
15.38	2-methyl-furan	4.4
15.96	Acetic Acid	20
16.37	Methyl-thiirane	0.2
16.67	Methyl-thiirane	0.1
16.81	2-Pentenal	1.1
17.26	Unknown	0.6
17.7	Unknown	0.2
18.12	2-methyl-2-butanol	0.6
18.7	C6H10O	2.3
18.9	C6H10	0.2
19.1	3-methyl-butanal	1.3
19.21	3-methyl-2-butanone	1.6
19.4	1-hydroxy-2-propanone	0.5
19.65	Benzene	0.4
19.76	2,3-dimethyl-pentanal	1
20.09	2-methyl-4,5-dihydrofuran	0.7
20.2	C5H8O	0.9
20.44	4-penten-2-one + C7H16	0.5
21.16	2-pentanone	9.5
21.58	1-heptene	0.7
21.77	dihydropyrane	0.3
21.88	3-pentanone	1.3
22.06	Pentanal	6.1
22.22	Heptane	3
22.47	3-heptene	0.4
22.74	3-heptene	1.3
22.85	Acetoin	0.2
22.99	C6H12O ketone	1.4
23.2	Unknown	0.3
23.32	C8H16	3.6
23.4	Unknown	1.5
23.96	2,2,4-trimethyl-1,3-dioxolane	0.2
24.08	Formic acid, butyl ester	2.7
24.33	2,4,4-trimethyl-2-pentene	0.4
24.4	C6H10O	0.5
24.55	Unknown	0.3
24.72	2,4-dimethyl-hexane	0.2
25.07	Unknown	0.7
25.2	C6H10O ketone	0.7
25.36	Propylene glycol	12.4
26	dimethyl disulfide	6
26.23	3-methyl-2-pentanone	1.3
26.55	Unknown	0.8
27	Unknown	0.5
27.21	Unknown	0.4
27.34	Unknown	1

27.48	Unknown	2.6
27.73	Toluene	10.6
28.06	6-methyl-3,4-dihydropyran	0.9
28.22	N,N-dimethyl-formamide	5.8
28.42	C7H14O ketone	0.8
28.58	3-hexanone	1.3
28.86	2-hexanone	6.7
29.11	C8H16	2.2
29.32	Unknown	0.5
29.58	Unknown	0.4
29.74	octane	20
29.95	unknown	0.5
30.2	SiO	3.5
31.06	2,3-dihydro-5,6--dimethyl-1,4-dioxene	1.3
31.17	octane	2.5
31.53	Methyl-pyrazine	1.2
32.03	2,5-dimethyl-heptane	2.6
33.04	1-acetyl-2-methyl-1-cyclopentene	3
33.35	Unknown	1.4
33.45	1,2-ethanediol diacetate	2
33.55	Unknown	0.6
34.37	1-hydroxy-2-propaneone	5.5
34.88	5-methyl-3-hexanone	9.3
36.02	2-butoxy-ethanol	1.9
36.41	Acetylfuran	9
36.56	dimethyl pyrazine	42
36.97	Dimethyl sulfone	60
37.08	Methyl-2-propenyl-disulfide	3.7
37.46	Dimethyl-phenol	2.2
37.8	methyl propyl disulfide	4.3
38.05	Unknown	2.2
38.16	methyl-1-propenyl-disulfide	5.2
38.65	Dihydro-5-methyl-2(3H)-furanone	1.5
39.56	phenol	245
39.72	Unknown	3.1
40.03	2-phenyl-propene	81
40.79	2-ethyl-6-methyl-pyrazine	7.4
40.98	Unknown	1.4
41.32	Unknown	1.2
41.55	2-ethyl-hexanol	61.8
41.78	Cymene	21.6

42.03	limonene	2.3
42.11	acetopyridine	2
42.27	2,7-octenedione	1.4
42.36	Unknown	10.5
42.43	Unknown	6
42.48	Unknown	6
42.56	Unknown	6
42.86	Unknown	7.5
42.99	tetrahydropyran-2-one	9.7
43.17	Unknown	5.6
43.37	p-Cresol	170.3
43.72	2-nonanone	9.7
44.08	2-methoxy-phenol	51.5
44.24	Nonanal	76.8
44.45	tetrahydro-6-methyl-2H-pyran-2-one	38.9
44.59	Unknown	2.6
44.68	Unknown	3.8
44.77	Unknown	11.8
44.97	Unknown	14
45.3	Unknown	4
45.37	2-ethyl-hexanoic acid	257
45.59	Unknown	25.7
45.76	Unknown	8.6
45.99	Unknown	1.2
46.16	Unknown	17.5
46.37	1-nonanol	5.7
46.52	Unknown	6.6
46.63	Unknown	21
46.71	Unknown	49.1
46.87	multiple unresolved peaks	300
47.12	multiple unresolved peaks	520
47.43	multiple unresolved peaks	211
47.76	Unknown	10.3
47.9	multiple unresolved peaks	282
48.32	multiple unresolved peaks	225
48.48	multiple unresolved peaks	114
49.83	Benzothiazole	4
51.37	Unknown	9.5
52.2	Unknown	18
52.31	Unknown	13
52.48	Unknown	20

52.64	Unknown	34
52.86	Unknown	32
53	Unknown	10
40-	Raised baseline	1500

55		

	IWP - Run 2	
Time	Identification	Area
5.91	Hydrogen sulfide	1.5
5.91	Formaldehyde	1.6
6.22	Sulfur dioxide	11.1
6.83	Methanol	4.5
7.01	2-methyl-1-propene	4.5
7.61	Methanethiol	4.7
8.33	Ethanol	10.3
9.61	Acetone	121.5
11.9	Carbon disulfide	0.2
13.3	2-methoxy-2-methyl-propane	1
14.28	Methyl vinyl ketone	1.8
20.07	unknown	0.3
20.2	3-methyl-3-buten-2-one	1
20.45	unknown	0.6
20.96	1-chloro-2-propanone	1.2
21.16	2-pentanone	5.1
21.59	1-heptene	1.6
21.84	2,3-dihydro-5-methyl-1,4-dioxin	0.2
22.06	Pentanal	7.3
22.2	Heptane	4.8
22.46	unknown	0.1
22.73	unknown	0.5
22.86	3-hydroxy-2-butanone	0.4
23.37	unknown	0.3
23.66	3-chloro-2-butanone	1.5
23.95	2,2,4-trimethyl-1,3-dioxolane	0.3
24.26	2,4.5-trimethyl-1,3-dioxolane	0.5
24.41	unknown	0.1
24.5	2,5-dimethyl-hexane	0.1
24.72	unknown	0.8
25.07	3-penten-2-one	1.4
25.19	4-methyl-2-pentanone	4
25.56	2-methyl-2-butenal	1.8
26.03	dimethyl disulfide	33
26.22	3-methyl-2-pentanone	5.4
26.4	2-methyl-propanoic acid	5
14.49	2,3-butanedione	2.6
14.71	Butanal	0.5
14.87	2-butanone	4.8
15.09	hexane	2.8
15.7	Acetic acid	41
16.37	Methyl-thiirane	0.3
16.67	Methyl-thiirane	0.1
17.03	C7H16	0.2
17.26	Tetrahydrofuran	0.5
18.1	2-methyl-2-butanol	0.6
19.1	3-methyl-butlanal	0.2
19.21	3-methyl-2-butanone	12.4
19.58	3-methyl-2-butanone	0.1
19.76	2-methyl-hexane	0.9
26.87	2,3-dimethyl-hexane	0.6
26.99	unknown	0.2
27.11	unknown	0.2
27.32	unknown	0.3
27.52	unknown	0.8
27.73	Toluene	3.5
27.85	5-hexen-2-one	4.6
28.18	unknown	0.3
28.42	Hexanoic acid	1.6
28.86	2-Hexanone	6
29.1	2-Octene	1.2
29.23	2,4-dimethyl-3-pentanone	0.8
29.55	C6H10O ketone	1.1
29.75	Hexanal	40
30.69	unknown	0.5
30.93	unknown	1.3
31.05	unknown	0.4
31.17	C8H18	1.5
31.95	Furaldehyde	3.3
32.2	unknown	3.5
32.34	unknown	4.3
32.61	3-methyl-2-hexanone	1.1
32.7	4-methyl-2-hexanone	2.2
33.04	Acetyl-2-methyl-1-cyclopentene	3.5

33.18	2-methyl-butanoic acid	6.6
33.22	unknown	0.3
33.25	5-methyl-2-hexanone	3.1
34.19	4-heptanone	57.5
34.49	o/p-Xylene	11
34.57	Xylene	2.5
34.63	unknown	1.5
34.75	Pentanoic acid	4
34.89	3-Heptanone	11.7
35.14	2-Heptanone	67
35.23	unknown	0.1
35.32	unknown	0.1
35.59	2,3-dimethyl-3-heptene	1.1
35.66	nonane	6
35.8	1,3-dimethyl-benzene	16
35.95	Cyclohexanone	5
36.01	2-butoxy-ethanol	5
36.23	2-Methyl-2-cyclopenten-1-one	8.2
36.39	acytylfuran	5
36.54	Dimethyl prazine	40
36.68	Dimethyl sulfone	40
36.76	Dihydro-2(3H)-furanone	40
36.88	unknown	0.6
36.98	2,5-Hexanedione	0.6
37.11	Methyl 2-propenyl disulfide	13
37.22	unknown	1.8
37.35	unknown	0.8
37.46	3-Hepten-2-one	4.5
37.57	unknown	1.8
37.7	1-butoxy-2-propanol	6.5
37.82	3-methyl-2-heptanone	22.3
37.9	unknown	2.9
38.05	unknown	0.6
38.17	Methyl 1-propenyl disulfide	9
38.31	6-Methyle-2-heptanone	12.6
38.42	2-Ethyl-hexanal	1.7
38.58	Dihydro-5-methyl-2(3H)-furanone	12.5
38.78	5-methyl-2-heptanone	1
38.84	3-methyl-cyclohexanone	4.2
38.91	Dihydro-4-methyl-2(3H)-furanone	4.2
39.04	Dihydro-2H-pyran-2-carboxaldehyde	2.2
39.07	Methyl-ethyle-benzene	2.2
39.12	4-Octanone	2.2
39.37	Benzaldehyde	68
39.47	Phenol	75
39.66	6-methyl-5-hepten-2-one	3.9
39.72	unknown	3.9
39.89	2-Octanone	12
40.01	2-phenyl-1-propene	29
40.16	Menthene	7
40.28	Decane	58
40.49	Octanal	11.6
40.61	Trimethyl benzene	2.7
40.73	unknown	1.3
40.94	benzofuran	0.8
41.04	4-ethyl-cyclohexanone	1.2
41.18	unknown	0.8
41.29	3,3,4,4-Tetramethyl-2-pentanone	2
41.38	unknown	3.3
41.57	unknown	105
41.76	Benzene complex	31
41.85	unknown	31
42.02	Limonene	4.1
42.33	5-ethenyldihydro-5-methyl-2(3H)-furanone	6.7
42.43	unknown	7
42.62	unknown	1.3
42.68	unknown	3.9
42.85	2-Hydroxy-benzaldehyde	6.1
42.95	unknown	1.2
43.06	4-Nonanone	0.4
43.11	6-Ethyl-2-methyl-6-hepten-2-ol	1.5
43.22	Methyl phenol	33.4
43.37	unknown	3.6
43.48	Acetophenone	18.8
43.68	2-Nonanone	12.6
43.79	Benzene complex	1
43.91	n-Alkane	11.5
44.03	2-Methoxy-phenol	8.3

44.13	Benzene complex	26.1
44.18	Nonanal	9.1
44.78	unknown	65
44.95	unknown	4
45.03	unknown	1.5
45.12	unknown	2.5
45.28	unknown	8.4
45.35	unknown	7.2
45.43	unknown	1.4
45.54	Chloro-benzaldehyde	10.6
45.68	4-Isopropenylcyclohexanone	0.8
45.81	unknown	4.1
45.89	unknown	3.2
45.97	unknown	0.6
46.23	unknown	12.6
46.37	unknown	2.2
46.53	Menthone	8
46.6	unknown	15
46.69	unknown	18
46.78	unknown	72
46.87	unknown	29
47.02	unknown	95
47.21	unknown	51
47.41	unknown	38
47.47	unknown	26
47.68	unknown	4
48.83	unknown	55
47.98	unknown	50
48.41	unknown	70
49.02	unknown	6.3
49.28	unknown	4.7
49.4	unknown	15
49.52	unknown	1.3
50-55	multiple bands unknown	150
40-55	Raised baseline	1000

Appendix B

UBDS - Run 1		
Time	Identification	Area
6.01	Propene	5
6.2	Carbonyl sulfide	5
6.36	Difluorodimethyl-silane	6
6.59	Chloromethane	6
6.9	Acetaldehyde	8
7.1	2-methyl-propene	1.6
7.48	Trimethylsilyl fluoride	1
7.61	Methanethiol	4
7.76	Bromomethane	3
8.1	Trimethylamine	18
8.4	Unknown	12
8.67	Acetone	9
918	Tetramethylammonium acetate	6
9.42	Acetonitrile	11
9.62	Acetone	130
10.2	Unknown	3.7
10.37	Unknown	3.8
10.95	Propenenitrile	8
11.53	Unknown	1.3
11.67	2-propenenitrile	1.2
11.85	Carbon disulfide	2.5
12.18	2-propen-1-ol	7
12.5	Unknown	0.6
12.8	2-methyl-propanal	1.3
13.76	Propanenitrile	2.7
14.1	Thiirane	0.4
14.32	Methyl vinyl ketone	1.8
14.55	Unknown	1.4
14.89	2-Butanone	18
15.1	2-Butenenitrile	5.6
15.41	2-methyl-furan	3.4
16.04	Unknown	3.3
16.82	Isobutyronitrile	1
17.2	Tetrahydrofuran	1.3
18	Acetic acid	160
18.26	Unknown	1.5
18.4	C4 Alkene Nitrile	1
18.73	Unknown	1
18.84	Unknown	1
19.12	3-methyl-butanal	1.3
19.26	3-methyl-butanone	5
19.67	Benzene	15
20.05	Unknown	1.8
20.1	Unknown	1
20.28	unknown	6.5
20.44	Unknown	0.6
20.56	2-Chloro-acetonitrile	2.1
20.87	Butenenitrile	0.7
20.97	1-Chloro-2-propanone	0.2
21.22	2-Propanone	11.3
21.6	1-Heptene	1.6
21.94	3-Pentanone	0.8
22.09	Pentanal	2.7
22.2	1-(methylthio)-1-propene	1.5
22.31	2-Ethyl-furan	2
22.42	2-Chloro-2-propenenitrile	0.7
22.74	22,5-dimethyl-furan	0.7
22.85	2-Chloro-pentane	3
23.38	Methyl thiocyanate	120
23.5	Unknown	6
23.75	3-Chloro-2-butanone	10
23.88	1,2-Ethanediol	10
24.05	Unknown	10
24.16	2-Ethenyl-furan	10
24.48	Thiazole	12
24.65	3-methyl-butanenitrile	15
24.84	Unknown	10
25.05	Pyrazine	15
25.22	Thiazole	12
25.37	1-methyl-1H-pyrrole	60
26.09	Dimethyly sulfide	82
26.15	Pyradine	50
26.34	Pyrrole	29
26.48	2-Chloro-2-propenenitrile	10

27	2-methylene-butanenitrile	1.3
27.24	Unknown	0.4
2.3	Unknown	2.3
27.79	Toluene	40
27.91	Pentanenitrile	4
28.12	3-Methyl-thiophene	2
28.18	2,4-Pentadienenitrile	2
28.55	N,N-dimethyl-formamide	20
28.63	3-Hexanone	2
28.76	2-Methyl-thiophene	3
28.93	2-Hexanone	5
29.38	Acetamide	30
29.55	Butanoic Acid	1.5
29.81	2-Furancarbonitrile	25
30.01	S-Methyl 2-Propenethioate	1
30.2	Matrix	60
30.45	2-Methyl-thiazole	10
30.56	2-Butenedinitrile	5
30.69	Tetrachloroethylene	5
31	3-Methyl-pyrimidine	1.5
31.22	2-Methyl-pyrimidine	8
31.35	N-formyl-N-methyl-formamide	4
31.61	Methyl-pyrazine	7
31.78	3-Methyl-phenol	1
32.02	Furaldehyde	8
32.2	Unknown	1
32.4	4-Methyl-3-hexanone	1
32.49	3-Methyl-butanoic acid	2
32.77	Monoacetate-1,2-ethanediol	25
32.98	2-Methyl-Butanoic acid	1
33.07	Unknown	1
33.2	2-Furanmethanol	7
33.31	Chlorobenzene	10
33.5	1-Chloro-hexane	2
33.6	Unknown	3
33.66	Unknown	2
33.79	Diallyl sulfide	2
33.92	N-Methyl-N-nitro-methanamine	5
34.09	N,N-Dimethylacetamide	7
34.18	3-Heptanone	12
34.51	Unknown	5
34.88	3-Isothiocyanato-1-propene	6
35.08	4-Cyclopentene-1,3-dione	60
35.23	Unknown	0.6
35.41	Fumaronitrile	2
35.58	Unknown	0.5
35.68	Unknown	0.4
35.77	1,3,5,7-cyclooctatetraene	2
35.78	Chloro-pyridine	2
35.86	Xylene	0.4
35.96	Unknown	0.7
36.04	2-Butoxy-ethanol	6
36.25	2-Ethyl-pyriine	1
36.46	Matrix	50
36.53	Dimethyl sufone	15
36.58	2(5H)-furanone	10
36.67	Butyrolactone	12
37.11	Dimethyl sufone	100
37.23	unknown	1
37.36	Unknown	25
37.48	Dimethyl sufone	5
37.61	N-Methyl-1H-pyrrole-2,5-dione	4
37.72	5-Methyle-2(5H)-Furanone	3
37.84	Methyl propyl disulfide	2
37.9	Unknown	1
38.18	Methyl Propenyl disulfide	0.6
38.25	Unknown	4
38.31	6-Methyl-2-heptanone	4
38.52	Dihydro-5-methyl-2(3H)-Furanone	4
38.77	Matrix	121
38.91	5-Methyl-2-Furfural	4
39.11	1-Heptanol	9
39.32	Benzaldehyde	7
39.44	Phenol	20
39.55	Diacetate-1,2-ethanediol	8
39.74	Matrix	6
39.91	2-Octanone	4
39.98	Dimethyl trisulfide	3
40.05	2-Pentyl-Furan	2
40.17	1-methyl-4-(1-	2.5

	methylethylidene)-cyclohexane	
40.32	Benzonitrile	65
40.51	2-Propyl-Pyridine	1
40.64	Unknown	1.3
40.75	Unknown	1.8
40.95	Benzamidine	4
41.04	Unknown	1.4
41.25	Unknown	1
41.39	Unknown	2
41.48	Matrix	4
41.65	Unknown	9
41.78	Cymene	9
42.09	Unknown	7
42.28	Dihydro-5-methyl-5-vinyl-2(3H)-furanone	5.5
42.45	Unknown	3.5
42.58	Unknown	3
42.78	Unknown	2.5
42.89	Matrix	3
43.02	Unknown	2
43.21	Matrix	25
43.48	Unknown	9
43.68	N,a-dimethyl-benzeneethanamine	1.3
43.8	Unknown	0.5
43.96	Matrix	1.6
44.06	Unknown	3.2
44.15	Unknown	1.2
44.31	Matrix	100
40-55	Raised baseline and unknown bands	150

Appendix C

BEB - Run 1		
Time	Identification	Area
6.92	Acetaldehyde	2
9.51	Acetone	2
25.18	4-Methyl-2-pentanone	0.1
25.98	Dimethyl sulfide	0.7

BEB - Run 2		
Time	Identification	Area
6.91	Acetaldehyde	1.5
8.3	Ethanol	0.15
9.52	Acetone	2
10.41	Dimethyl diazene	0.05
26	Dimethyl disulfide	0.3
39.27	Benzaldehyde	0.3
43.44	Acetophenone	0.3

BEB - Run 3		
Time	Identification	Area
6.91	Acetaldehyde	1.7
8.3	Ethanol	0.3
9.39	Aminoacetonitrile	0.04
9.51	Acetone	2.2
14.84	2-Butanone	0.1
25.19	4-Methyl-2-pentanone	0.05
25.98	Dimethyl sulfide	0.5
39.27	Benzaldehyde	0.15
43.44	Acetophenone	0.4