ASCEND
PERFORMANCE MATERIALS

September 24, 2010 CERTIFIED MAIL RECEIPT NO. 7004 1350 0002 6049 0775

Mr. Rick Bradburn
Air Program Administrator
Department of Environmental Protection
160 Governmental Center
Pensacola, FL 32502-5794

RE: Proposed Adipic Acid VOC Emission Study

Dear Mr. Bradburn:

As discussed during the September 17, 2010 meeting between Ascend Performance Materials (Ascend) and the Department, the AP-42 Factors used in calculating Adipic Acid VOC emissions are based on limited data, and the AP-42 data has a rating factor of "E" due to the lack of documentation for the testing procedures utilized to develop the emission data. A study has been initiated by Ascend to determine the emission data for the manufacture of Adipic Acid at Ascend's Pensacola site based on actual plant data. Ascend is requesting the Department's approval of the methodology in this study or recommendations to make the methodology suitable prior to the submittal of Ascend's 1080 MAR Adipic Acid rate permit application.

The attached preliminary report is submitted per the Department's request to review Ascend's methodology and data used to calculate VOC emissions in Ascend's Adipic Acid manufacturing process. Ascend will include the final VOC emission data with the permit application for 1080 MAR Adipic Acid rate.

Also, Ascend has scheduled ENTEC Services to perform stack testing to verify current VOC emissions from the TRU and back-up SCR the week of September 27, 2010.

If you have any questions regarding the information provided, please contact Roy Noble at (850) 968-8721 or by electronic mail at rwnobl@AscendMaterials.com.

Sincerely,

Tim Montgomery
Chemicals & Utilities Plant Manager

CC:
Armando Sarasua
Rick Prusa
Debbie Moore

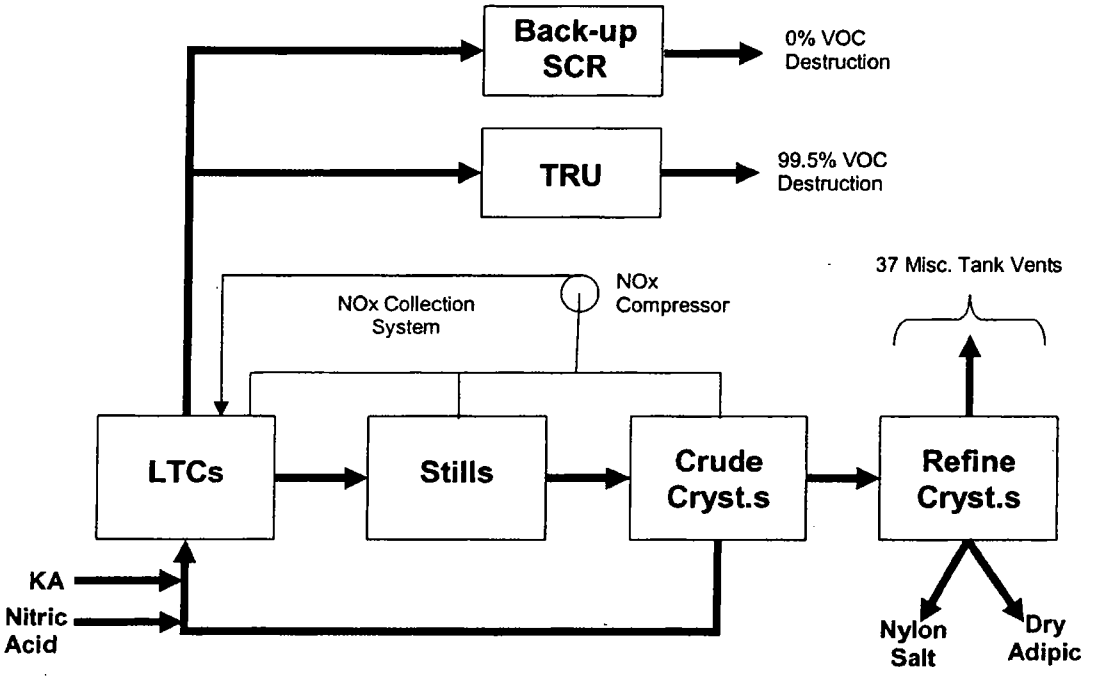
Attachment

This report summarizes the preliminary work and calculations Ascend Performance Materials (Ascend) has completed to date to determine VOC emissions in the manufacture of adipic acid.

Based upon the known testing data and low rating for the EPA's AP-42 emission factor for adipic acid, Ascend wanted to better determine actual emission data for the Pensacola site. This would allow Ascend to re-state baseline emission factors and calculate projected actual emission data associated with Adipic Acid as Ascend moves forward with non-PSD permitting activities.

Process Description:

As shown in the diagram below, the VOC emission streams from Ascend's adipic acid process consist of three components: (1) Thermal Reduction Unit (TRU), (2) Back-Up SCR (Selective Catalytic Reduction) and Refining, which includes crystallization and centrifugation steps.



The Ascend adipic acid production unit has two NOx control devices: (1) the TRU and (2) the Back-Up SCR. The TRU, however, also destroys VOCs in the adipic offgas stream (~99.5%). The Back-Up SCR, in contrast, has 0% VOC destruction. Both control devices are fed offgas from the oxidation reactions occurring in: (a) the Low Temperature Converters ("LTCs"), (b) the Concentrating Stills (which remove water from the process and concentrate the nitric acid for recovery and reuse), and (c) the initial adipic refining step.

The initial refining step is Crude Crystallization and Centrifugation ("Crudes"). Material from the Crude Feed Tank is fed to the Crude Crystallizers/Centrifuges. The vast majority of the nitric acid is separated from the adipic acid in this step and the nitric acid is returned upstream in the process for reuse. The adipic acid from the Crudes is dissolved in water and sent forward to the Refine Feed Tank. There are seven crude crystallizers and seven crude centrifuges along with associated equipment.

The second adipic acid refining step is referred to as Refined Crystallization / Centrifugation ("Refines"). There are 6 crystallizers, 8 centrifuges, and associated equipment in this step. Although the equipment in this second refining step vents to atmosphere, the VOC levels are very low due to the high degree of removal in the previous steps of the process. In the Concentrating Stills, all the process material is distilled under vacuum. In the Crude Crystallizers, the material is put through evaporative crystallization under vacuum. Only the solid adipic crystals are moved forward from the Crudes to the Refine Crystallization step. The product adipic acid from the Refines is then sent to the adipic dryers or to make nylon salt. Water from the Refines is sent to the Crude Crystallization / Centrifugation step for reuse.

Nitric containing tanks and vessels upstream of the second refining step (Refine Crystallization/Centrifugation) are vented to the NOx Collection System. This system uses a compressor to recycle these vents upstream to the LTCs with ultimate disposition in the TRU or Back-Up SCR.

Emission Factor Development:

The table below shows a comparison between the current AP-42 factor methodology and the results of Ascend's recent study on VOC emissions from the Adipic Acid plant.

Sources	Current Method	Calculations Using Plant Data (lb / Ton AA)	Approx. %OST	Act. Emissions (lb/Ton AA)	Basis for Calculations
Adipic Refining (Misc point sources)	AP-42 Factor **0.500** lb / Ton AA (E-Rating due to lack of data)	0.004	100	0.004	- Sample analysis of liquid in each vessel. - VOC emissions calculated using two applications: (1) Water9 (2) Tanks 4.0.9d
TRU (NOx & VOCs)		0.050	80	0.040	- Official stack tests for MON.
Back-Up SCR (Just NOx)		0.460	20	0.092	- Official stack tests for MON.
				0.136	

TRU:

TRU emissions were calculated using an average of 99.5% VOC destruction rate. This rate was determined using VOC measurements on: (a) Adipic offgas to the TRU, (b) Halcon offgas, and (c) the TRU stack. An 80% on-stream time (292 days) is a conservative estimate based upon 2008/2009 average data of 312 days on-line.

Testing on the TRU was conducted three times between 2005 -2008 in support of MON compliance programs. Exit rates by Method 25A were determined to be 2.2 pounds per hour, 0.21 pph and 0.61 pph. For an initial conservative estimate of the TRU emissions, the 2.2 pph value was used. Additionally, the highest single value ever observed for HCN from the testing was used to conservatively estimate emissions. Ascend will conduct additional stack testing as necessary to confirm this data.

Back-up SCR:

Ascend assumes 0% VOC destruction rate for the Back-Up SCR due to the limits of the technology. 20% on-stream time was assumed since this unit must be on-line whenever the TRU is down. 2008/2009 data shows an average of 53 days on-line for the SCR. Therefore, 20 % on-stream time (73 days) is a conservative estimate.

MON testing conducted in 2005 was used to estimate emissions from the Back-up SCR. The VOC's to the TRU were not measured. However, VOC's from the reactors and compressors were measured. Similarly to the TRU exit, the highest single HCN value observed with the TRU offline was used to estimate emissions.

Additional Stack Testing:

Ascend will have ENTEC Services perform stack testing the week of September 27th on both the TRU and Back-Up SCR. This testing will also measure Halcon off-gas to the TRU, the Adipic offgas to the TRU (also the feed to the Back-Up SCR), and the exit of the TRU. All testing will be performed utilizing Method 25A and in addition, HCN testing will be utilized for the Adipic feed to the TRU/SCR and the TRU exit.

Adipic Refining:

Adipic Acid Refining is made up of 37 miscellaneous point source process vessels that vent to atmosphere. The remaining Adipic Acid tanks vent through the NOx collection system which in turn is routed through the TRU and/or Back-up SCR, whichever unit is on-line.

In discussions with Scott Steinsberger, Ph.D. of the testing firm DEECO, Inc., it was determined that the emissions from Adipic Refining are so low that they would not be

able to be confirmed with existing stack testing and analytical methodology. Due to the low emissions, a minimum of 24 hours testing would be required without accounting for the saturated water vapor in the head space of the tank. This additional water would result in samples diluted with condensing water vapor and not allow sufficient sample concentration to be measured in the analytical equipment. Therefore, Ascend calculated the VOC emissions from each point source within Adipic Refining using the following method.

A sample was taken from each of 37 point sources in Adipic Acid Refining. These point sources contain a single phase aqueous solution of various dibasic carboxylic acids (DBA's) and trace quantities of monobasic carboxylic acids (MBA's). The samples were analyzed by STM 01529 to determine the concentration of the DBA's. The MBA's were determined by a modified analysis and a % recovery was calculated. The lab report, Volatile Organic Acid Analysis, and method are included in **Appendices A1 and A2.**

The following table shows an example of the DBA's, MBA's and other constituents in the Refine Feed Tank (RFT):

Water	62.48%
Nitric Acid	0.3%
Adipic Acid	37%
Glutaric Acid	0.12%
Succinic Acid	0.10%
Acetic Acid	Non-detectable
Propanoic (Proponic) Acid	Non-detectable
Butanoic (Butyric) Acid	54 ppm
Pentanoic Acid	83 ppm
Hexanoic Acid	79 ppm
Heptanoic Acid	99 ppm

EPA Modeling software was used to predict the concentration of the vapor space and calculate the VOC emissions at each point source. Calculations have been completed on 32 of the 37 sources and are shown in the table below. (The modeling and calculations are discussed after the table.) The remaining calculations will be performed and will be included in this study.

	Vessel ID	Vessel Description	VOC Emissions, lb/yr	
			@ 850 MAR	@ 1080 MAR
1	403TA 20	Absorber Feed Tank	15.5	19.6
2	403TA 50	Utility Tank (WML)	67.6	85.9
3	405TA 001	Refine Feed Tank	229.9	292.1
4	405VE 156A	405A Refine Suspension Tank	7.7	9.8
5	405VE 156B	405B Refine Suspension Tank	7.7	9.8
6	465TA 72	465 Regenerant Tank	13.5	17.2
7	465VE 156A	465A Refine Suspension Tank	7.7	9.8
8	465VE 156B	465B Refine Suspension Tank	7.7	9.8
9	485TA 321	Intermediate Solution Tank	52.2	66.3
10	403TA 136C	Dilution Water Tank (DAML)	2.9	3.68
11	405TA 358	405 Regenerant Tank	13.5	17.2
12	405TA 119	AMLF Tank	3.9	4.9
13	405TA 34A	405A AMLS Tank	<1	<1.2
14	405TA 34B	405B AMLS Tank	<1	<1.2
15	405TA 178B	405 WML Tank	23.2	29.5
16		405 Refine Seal Pot		
17	465VE 41A	465A Crude Soln. Tank	18.4	23.3
18	465VE 41B	465B Crude Soln. Tank	18.4	23.3
19	465TA 178	465 WML Tank	62.8	79.8
20	485VE 41A	485A Crude Soln. Tank	9.7	12.3
21	485VE 41B	485B Crude Soln. Tank	9.7	12.3
22	485VE 41C	485C Crude Soln. Tank	8.69	11.1
23	485TA 126	485 Regenerant Tank		
24	485TA 180	485 WML Tank	53.1	67.5
25	485HE 316	DTB Crystallizer Jet Condenser		
26	485TA 153	Pinch Water Tank		
27	485MS 348	DTB Condenser Seal Pot	<1	<1.2
28	485TA 178	UGA WML Tank	14.5	18.4
29	485TA 120	UGA Feed Tank	25.1	31.9
30	485VE 156C	UGA Suspension Tank	<2	<2.5
31	405SE 177A	405A Refine Centrifuge	<1	<1.2
32	405SE 177B	405B Refine Centrifuge	<1	<1.2
33	465SE 177A	465A Refine Centrifuge	<1	<1.2
34	465SE 177B	465B Refine Centrifuge	<1	<1.2
35	485SC 177C	UGA Centrifuge	<2	<2.5
36	485SC 177A	Intermediate Centrifuge	<2	<2.5
37	485SC 177A	Intermediate IST		
Total Emissions, lbs/year:			**686**	**871**
Total Emissions, lb VOC/ Ton AA:			**0.0016**	

Modeling:

The EPA offers two tank VOC emission prediction tools: TANKS4 and WATER9. Each tool can predict emissions from fixed roof vertical atmospheric storage tanks.

TANKS4 is for concentrated (non-aqueous) organic liquids such as gasoline or concentrated mixtures of other organic liquids. Relative to vapor liquid equilibrium TANKS4 assumes ideal mixture behavior which follows Raoult's Law. The component vapor concentrations are calculated from the component vapor pressure and mole fraction in the liquid phase.

WATER9 was primarily written for wastewater simulation and is for solutions of organic liquids in water. It is best applied to dilute organic solutions. WATER9 predicts vapor concentrations based on Henry's Law using Henry's Law Coefficients. WATER9 also applies a non-ideality term, a UNIFAC activity coefficient, for each organic-water pair. Per the WATER9 manual, "WATER9 provides separate emission estimates for each individual compound that is identified as a constituent of the wastes. The emission estimates are based upon the properties of the compound and its concentration in the wastes. To obtain these emission estimates, the user must identify the compounds of interest and provide their concentrations in the wastes....Estimates of the total air emissions from the wastes are obtained by summing the estimates for the individual compounds."

The aqueous solutions in Ascend's Adipic Acid Refining Tanks best fit the WATER9 VLE model assumptions with the slight exception of the relatively high concentration of adipic acid. Nevertheless, the mixture should fit the WATER9 assumptions better than TANKS4. (A comparison of results from both programs was made and is described in **Appendix B**, along with the physical properties for each component.)

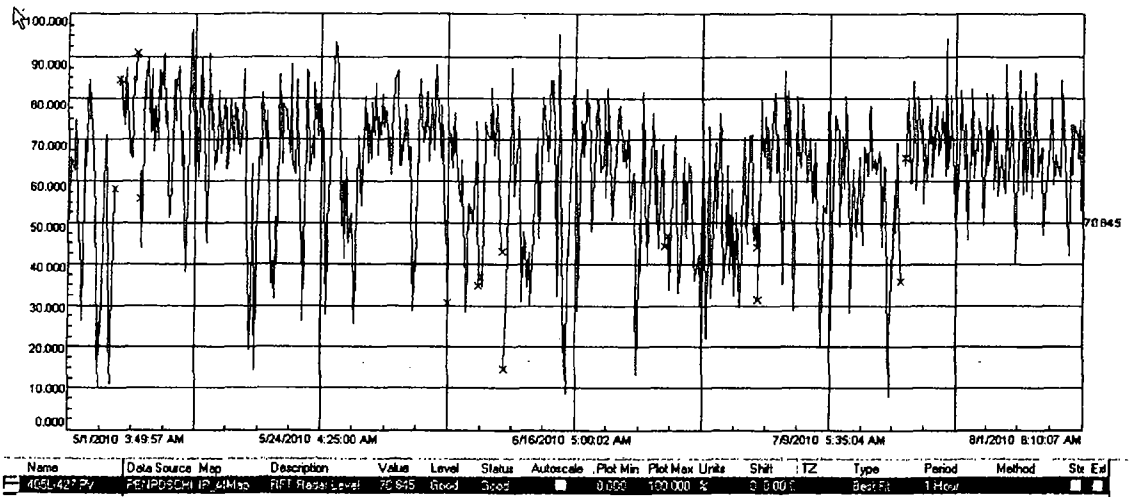
Assume higher for each scenario?

Both programs calculate emission losses from two sources: working induced losses from liquid level swings and breathing/standing losses from vapor expansion due to temperature swings in the vapor space. The two sources of emissions were calculated and combined for the total VOC emission of the vent sources.

Working Loss Calculations:

Ascend analyzed level data for each vent source to model working losses. The level data from Ascend's data historian was downloaded into an Excel spreadsheet as 15 minute average data for a recent three month period. The equivalent change in wall height between each 15 minute data point was calculated and the cumulative change in liquid height for level increases was calculated for the three month period. The EPA emissions software requires that the tank be simulated as operating between two fixed levels. For modeling purposes, calculations were made to determine the average high and low operating levels of each tank.

As an example, the Refine Feed Tank (RFT) level (405LI427) for a three month period is shown here with an assumed average high operating level of 70% and average low operating level of 40%:



Based upon tank dimensions, this correlates to a span of 6.9 ft. (2.1 m) and a working volume of 2.7e+4 gallons.

For the time period and calculated span of 6.9 ft.:
Total number of turnovers = 1502 ft. / 6.9 ft = 220.2
Turnovers per day = 220.2 turnovers / 91 days = 2.42
Average residence/storage time = 1 / 2.42 = 0.413 days

A tank turnover factor is defined and calculated by the program for use in the working loss calculations. The working loss equation in WATER9 is:

$$L_W = 2.40 \times 10^{-5} M_v \cdot P' \cdot V \cdot N \cdot K_n \cdot K_c \qquad (9\text{-}4)$$

where

L_W = working losses, lb/yr

M_v = molecular weight of vapor in storage tank, lb/lb mol

P' = true vapor pressure at bulk liquid conditions, psia

N = number of turnovers per year (dimensionless)

N = $\frac{\text{total throughput per year (gal)}}{\text{tank capacity, } V \text{ (gal)}}$

V = tank capacity, gal

K_n = turnover factor, dimensionless (for turnovers for turnovers > 36, $K_n = \frac{180 + N}{6N}$)

K_c = product factor, dimensionless for crude oil, K_c = 0.84; for all other organic liquids, K_c = 1.

The selection of the level swing span has some effect on the working loss calculation. It appears that greater working capacities (higher spans) result in slightly higher working loss estimates at the same throughputs:

Refine Feed Tank Simulation – Working Loss		
Max Level	70% (16.1 ft)	70% (16.1 ft)
Min Level	40% (9.2 ft)	55% (12.65 ft)
Span	6.9 ft	3.45 ft
Turnovers per day	2.42	4.84
Residence Time	0.413	0.207
Est. VOC Emissions	**140 lb/yr**	**129 lb/yr**

Breathing Loss Calculations:

WATER9 assumes each tank is un-insulated and has no temperature control. It predicts breathing losses based on temperature swings from ambient conditions alone per the following equation:

$$L_b = 2.26 \times 10^{-2} M_v \left(\frac{P'}{P_A - P'}\right)^{0.68} \cdot D^{1.73} H^{0.51} \Delta T^{0.5} F_p C \cdot K_c \quad (5-5)$$

where

L_b = fixed-roof breathing loss, lb/yr

M_v = molecular weight of vapor in tank, lb/lb mol

P' = true vapor pressure at bulk liquid conditions, psia

P_A = average atmospheric pressure at tank location, psia

D = tank diameter, ft

H = average vapor space height, ft (assumed to be one-half of tank height)

ΔT = average ambient diurnal temperature change, °F (20 °F assumed as a typical value)

F_p = paint factor, dimensionless (see Table 5-6)

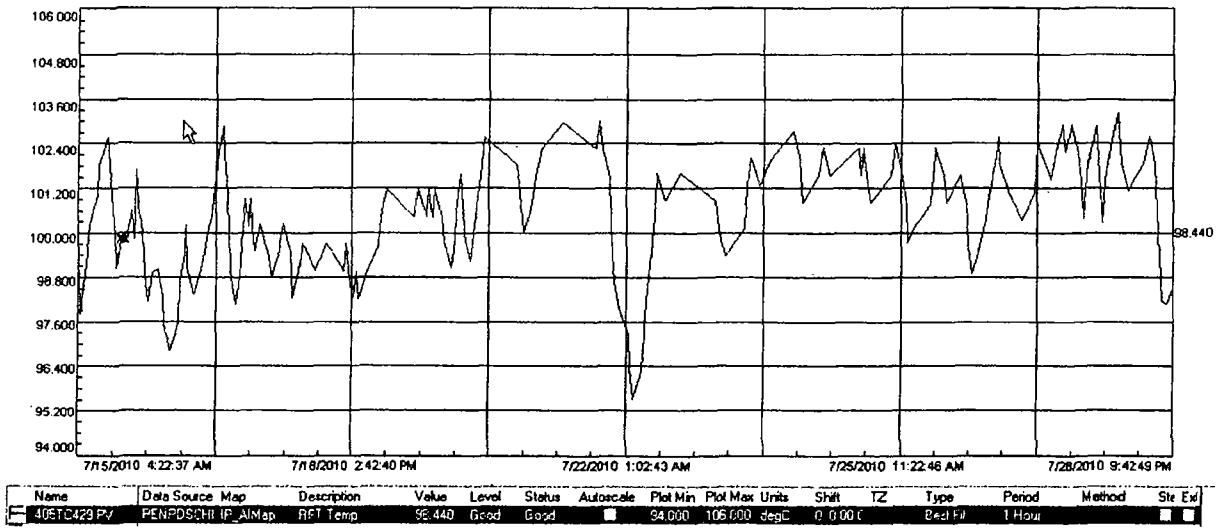
C = adjustment factor for small diameter tanks, dimensionless (for diameter > 30 ft, $C = 1$; for diameter < 30 ft,

$$C = 0.0771 D - 0.0013 D^2 - 0.1334)$$

K_c = product factor, dimensionless (for crude oil, K_c=0.65, for all other organic liquids, K_c = 1.0).

As an example, the RFT is an insulated heated tank. It is not affected by diurnal ambient temperature swings. However, there are process temperature swings which will result in

breathing losses through the tank vent. The temperature for two weeks in July 2010 is shown:



In calculating the breathing losses, assume the typical/average daily temperature variability at the liquid surface is +/- 1.0 deg C. WATER9 is only capable of calculating breathing losses indirectly from diurnal ambient temperature swings. TANKS4 does display the calculated liquid surface temperatures which result from input ambient swings in unheated tanks. To generate a one degree swing in liquid surface temperature in TANKS4, a +/- 1.8 deg C swing in ambient temperature is required.

Simulating the RFT in WATER9 as an un-insulated/unheated storage tank with a +/- 1.8 deg C ambient swing, the program predicts a breathing loss of 69 lb/yr. The total VOC emission loss is therefore working plus breathing losses, 140 + 69 = 209 lbs VOC/year. To be more conservative a +/- 2 deg daily liquid temperature swing was assumed for calculations. This increased the breathing losses in the RFT to 98 and the total VOC emission loss to 238 lbs VOC/year.

TANKS4 loss estimates versus WATER9:

The RFT was simulated in TANKS4 by specifying the water component as an organic liquid with its associated vapor pressure curve. All components were modeled using Raoults Law. The predicted annual VOC emissions were much lower than WATER9:

RFT VOC Losses, lb/year

	WATER9	TANKS4
Working Losses:	140	1.0
Breathing Losses:	98	0.35
Total Losses:	238	1.35

Similarly, TANKS4 was used to calculate emissions from two other tanks with higher emission levels calculated in WATER9. The emissions were once again much lower in TANKS4, therefore the assumption was made that utilizing WATER9 data would be the more conservative approach for calculating the refining VOC emissions.

Tank ID	Tank Description	WATER9, lb/yr	TANKS4, lb/yr
405TA001	Refine Feed Tank	238	1.35
403TA50	Utility Tank (WML)	70	0.11
465TA178	465 WML Tank	65	0.34

Appendix A1

Volatile Organic Acid Analysis

ASCEND
PERFORMANCE MATERIALS

Analytical Sciences Group
Pensacola

Tel: (850) 968-8163
Fax: (850) 968-8441

Date: 07/20/2010
Date Completed: 09/20/2010
From: George Hayman
To: Greg Bush, Amy Dyer, Roy Noble
cc: Patrick O'Neal, Ben Womack
Subject: Volatile Organic Acid Analysis
NBP #:

Background:
This analysis is an attempt to estimate the amount of volatile organic acids which are given off to the atmosphere as a byproduct of Adipic Acid Refining. The current factor being used is 0.5lb / Ton. Monobasic acids (MBA's) from C2 through C7, as well as Dibasic acids (DBA's) from C4 through C6, were analyzed in process stream samples submitted by Michelle Shotts.

Summary & Conclusions:
Recoveries of all analytes were reasonable in all samples. For use in determining concentrations in plant streams I would recommend adjusting results for those compounds which had less than 100% recovery. These results should be useful in estimating VOC emissions due to Volatile Organic Acids.

Experimental:
Samples were collected from various points in the process in 250ml bottles with minimal headspace. Those samples with adipic acid precipitates were placed in a steam bath until the precipitate was in solution. The samples were then analyzed by STM01529 for the DBA's. A 25 ul aliquot of sample was derivatized with the silanizing agent used for the DBA's and analyzed for MBA's by Gas Chromatography. The MBA samples were analyzed neat and a 500ul aliquot was added to 500ul of an MBA standard. A 25ul aliquot of this solution was then derivatized and analyzed and a % recovery calculated for all MBA's.

Calibration:

For the MBA analysis, four levels of standards were prepared as an aqueous solution. A 25ul aliquot of each standard was derivatized and analyzed by GC/FID. All data was collected and analyzed utilizing ATLAS chromatography software. A linear regression was then performed utilizing the ATLAS software. All compounds exhibited reasonably linear behavior. The coefficient of determination (r squared) for the MBA's is as follows. Acetic acid r sq.=0.9997. Propanoic acid r sq.=0.9995. Butanoic acid r sq.=0.9994. Pentanoic acid r sq.=0.9981. Hexanoic acid r sq.=0.9997. Heptanoic acid r sq.=0.9985. For the Dibasic acids a single point calibration was performed per Ascend STM01529, and linearity through the origin was assumed for all compounds. An aliquot of the mid level standard was derivatized and analyzed with each set of samples received to ensure that the initial calibration remained valid. This aliquot was analyzed at the beginning and end of each set of samples as they were run.

Cont. Cal. Ver.

7/22/2010 8:53

Compound	True Value	Calculated Value	% Difference
Acetic acid	642.95	661.10	2.82
Propionic acid	630.50	639.24	1.39
Butanoic acid	584.75	590.70	1.02
Pentanoic acid	573.45	571.75	0.30
Hexanoic acid	557.00	580.92	4.29
Heptanoic acid	600.35	620.55	3.36

7/22/2010 15:48

Compound	True Value	Calculated Value	% Difference
Acetic acid	642.95	634.75	1.28
Propionic acid	630.50	643.22	2.02
Butanoic acid	584.75	592.08	1.25

Pentanoic acid	573.45	572.46	0.17
Hexanoic acid	557.00	568.68	2.10
Heptanoic acid	600.35	599.18	0.19

7/22/2010
23:54

Compound	True Value	Calculated Value	% Difference
Acetic acid	642.95	651.78	1.37
Propionic acid	630.50	643.01	1.98
Butanoic acid	584.75	590.82	1.04
Pentanoic acid	573.45	568.01	0.95
Hexanoic acid	557.00	575.19	3.27
Heptanoic acid	600.35	587.54	2.13

7/23/2010 9:58

Compound	True Value	Calculated Value	% Difference
Acetic acid	642.95	631.85	1.73
Propionic acid	630.50	623.35	1.13
Butanoic acid	584.75	575.51	1.58
Pentanoic acid	573.45	555.36	3.15
Hexanoic acid	557.00	557.35	0.06
Heptanoic acid	600.35	558.34	7.00

7/23/2010
16:55

Compound	True Value	Calculated Value	% Difference
Acetic acid	642.95	610.26	5.09

Propionic acid	630.50	630.33	0.03
Butanoic acid	584.75	583.76	0.17
Pentanoic acid	573.45	557.94	2.70
Hexanoic acid	557.00	555.68	0.24
Heptanoic acid	600.35	566.22	5.69

7/30/2010 8:55

Compound	True Value	Calculated Value	% Difference
Acetic acid	642.95	643.17	0.03
Propionic acid	630.50	628.97	0.24
Butanoic acid	584.75	578.98	0.99
Pentanoic acid	573.45	556.19	3.01
Hexanoic acid	557.00	549.44	1.36
Heptanoic acid	600.35	583.94	2.73

7/30/2010 12:25

Compound	True Value	Calculated Value	% Difference
Acetic acid	642.95	624.05	2.94
Propionic acid	630.50	627.27	0.51
Butanoic acid	584.75	575.28	1.62
Pentanoic acid	573.45	545.78	4.83
Hexanoic acid	557.00	548.12	1.59
Heptanoic acid	600.35	532.16	11.36

Results & Discussion:

See images and table below.

Compound	LPST(ppm)	LPST+STD 1:1 (ppm)	LPST+STD % REC
Acetic acid	284.45	812	103
Propionic acid	421.1	866.38	103
Butanoic acid	1095	1147.46	101
Pentanoic acid	746	978.14	97
Hexanoic acid	134	666.35	107
Heptanoic acid	n.d.	652.36	109

Compound	CAGA(ppm)	CAGA+STD 1:1 (ppm)	CAGA+STD % REC
Acetic acid	48.78	669.74	100.4
Propionic acid	n.d.	637.53	101
Butanoic acid	44.26	596.5	98
Pentanoic acid	81.4	608.24	99
Hexanoic acid	58.77	575.98	98
Heptanoic acid	83.69	649.01	101

Compound	AMLF(ppm)	AMLF+STD 1:1 (ppm)	AMLF+STD % REC
Acetic acid	34.441	831.227	126
Propionic acid	28.016	841.317	130
Butanoic acid	65.725	775.984	126
Pentanoic acid	111.888	782.235	124
Hexanoic acid	58.897	735.475	125
Heptanoic acid	135.49	844.274	126

Compound	AMLF(%)
Succinic	5.86
Glutaric	19.35
Adipic	4.11

Compound	RFD(ppm)	RFD+STD 1:1 (ppm)	RFT+STD %·REC	Compound	RFT(%)
Acetic acid	n.d.	549.964	86	Succinic	0.10
Propionic acid	n.d.	537.583	85	Glutaric	0.12
Butanoic acid	44.58	504.504	83	Adipic	37.24
Pentanoic acid	66.459	482.564	80		
Hexanoic acid	64.604	482.646	82		
Heptanoic acid	80.484	516.432	81		

Compound	405A REF(ppm)	REF+STD 1:1 (ppm)	Ref+STD % REC	Compound	405A REF(%)
Acetic acid	n.d.	561.073	87	Succinic	0.10
Propionic acid	19.991	548.17	86	Glutaric	0.13
Butanoic acid	n.d.	514.036	88	Adipic	36.16
Pentanoic acid	n.d.	498.835	87		
Hexanoic acid	51.977	501.763	86		
Heptanoic acid	81.585	553.187	86		

Compound	403 WML(ppm)	WML+STD 1:1 (ppm)	WML+STD % REC	Compound	403 WML(%)
Acetic acid	n.d.	553.981	86	Succinic	0.08
Propionic acid	24.622	544.19	85	Glutaric	0.08
Butanoic acid	45.192	508.458	84	Adipic	21.11
Pentanoic acid	63.711	486.934	80		
Hexanoic acid	62.756	483.454	82		
Heptanoic acid	80.282	526.713	82		

Compound	403 AFT(ppm)	AFT+STD 1:1 (ppm)	AFT+STD % REC	Compound	403 AFT(%)

Acetic acid	365.512	796.195	96	Succinic	0.04
Propionic acid	496.115	839.737	96	Glutaric	0.22
Butanoic acid	1282.811	1192.794	97	Adipic	0.37
Pentanoic acid	1031.167	1048.492	96		
Hexanoic acid	237.171	640.528	95		
Heptanoic acid	81.925	644.255	100		

Compound	IXDAML (ppm)	DAML+STD 1:1 (ppm)	DAML+STD % REC	Compound	1XDAML (%)
Acetic acid	26.145	649.637	99	Succinic	4.37
Propionic acid	24.687	637.778	99	Glutaric	13.63
Butanoic acid	66.652	604	98	Adipic	2.89
Pentanoic acid	92.694	588.271	95		
Hexanoic acid	59.109	577.653	98		
Heptanoic acid	79.764	631.793	99		

Compound	405 REGEN (ppm)	REGN+STD 1:1 (ppm)	REGN+STD % REC	Compound	405 REGEN (%)
Acetic acid	536.629	939.088	103	Succinic	0.08
Propionic acid	544.732	922.399	102	Glutaric	0.09
Butanoic acid	1147.145	1187.939	103	Adipic	0.43
Pentanoic acid	746.964	948.255	100		
Hexanoic acid	129.97	623.416	100		
Heptanoic acid	81.457	619.406	97		

Compound	405 REFINE (ppm)	REFN+STD 1:1 (ppm)	REFN+STD % REC	Compound	405 REFINE (%)
Acetic acid	n.d.	637.925	99	Succinic	0.06

Propionic acid	24.177	624.503	97	Glutaric	0.05
Butanoic acid	45.602	575.342	95	Adipic	0.65
Pentanoic acid	65.272	555.178	92		
Hexanoic acid	64.172	561.645	95		
Heptanoic acid	79.995	557.595	87		

Compound	UGA WML (ppm)	WML+STD 1:1 (ppm)	WML+STD % REC	Compound	UGA WML (%)
Acetic acid	n.d.	655.728	102	Succinic	0.08
Propionic acid	20.947	647.117	101	Glutaric	0.05
Butanoic acid	n.d.	599.033	102	Adipic	12.98
Pentanoic acid	n.d.	573.737	100		
Hexanoic acid	n.d.	575.352	103		
Heptanoic acid	80.788	634.224	99		

Compound	403 REGEN (ppm)* *=Resample	REGN+STD 1:1 (ppm)	REGN+STD % REC	Compound	403 REGEN (%)
Acetic acid	367.616	805.499	97	Succinic	0.03
Propionic acid	486.114	847.913	97	Glutaric	0.11
Butanoic acid	1234.238	1166.012	97	Adipic	0.33
Pentanoic acid	960.515	995.932	95		
Hexanoic acid	210.428	618.988	93		
Heptanoic acid	105.602	598.84	92		

Compound	403 WML (ppm)* *=Resample	AFT+STD 1:1 (ppm)	AFT+STD % REC	Compound	403 WML (%)
Acetic acid	n.d.	649.782	101	Succinic	0.08
Propionic acid	n.d.	640.89	102	Glutaric	0.06
Butanoic acid	n.d.	588.131	101	Adipic	26.09

Pentanoic acid	n.d.	518.021	90
Hexanoic acid	58.233	403.434	69
Heptanoic acid	79.987	408.27	64

Compound	UGAFEED (ppm)	FEED+STD 1:1 (ppm)*	FEED+STD % REC	*dil. 1:1 wth b.s.H2O	Compound	UGAFEED (%)
Acetic acid	n.d.	367.614	114		Succinic	0.08
Propionic acid	n.d.	358.298	114		Glutaric	0.05
Butanoic acid	n.d.	325.723	111		Adipic	57.65
Pentanoic acid	n.d.	280.754	98			
Hexanoic acid	65.227	201.315	68			
Heptanoic acid	86.962	199.812	62			

Compound	UGA SUSP (ppm)	SUSP+STD 1:1 (ppm)*	REGN+STD % REC	*dil. 1:1 wth b.s.H2O	Compound	UGA SUSP %)
Acetic acid	536.629	340.505	75		Succinic	0.08
Propionic acid	19.546	337.969	106		Glutaric	0.04
Butanoic acid	n.d.	314.347	108		Adipic	38.55
Pentanoic acid	n.d.	290.751	101			
Hexanoic acid	n.d.	242.271	87			
Heptanoic acid	n.d.	256.224	85			

Compound	485B CRUDE (ppm)	CRDE+STD 1:1 (ppm)*	CRDE+STD % REC	*dil. 1:1 wth b.s.H2O	Compound	485B CRUDE (%)
Acetic acid	25.408	336.807	103		Succinic	0.07
Propionic acid	n.d.	350.011	111		Glutaric	0.06
Butanoic acid	n.d.	325.825	111		Adipic	47.46
Pentanoic acid	58.759	292.2	97			
Hexanoic acid	59.422	237.188	81			

Heptanoic acid	79.505	226.471	71			
Compound	DTBSLPT (ppm)	DTBSLPT+STD 1:1 (ppm)	FEED+STD % REC		Compound	DTBSLPT (%)
Acetic acid	n.d.	605.993	94			
					Succinic	none detected
Propionic acid	23.378	605.672	94			
					Glutaric	none detected
Butanoic acid	45.99	563.2	93			
					Adipic	0.03
Pentanoic acid	64.465	543.464	90			
Hexanoic acid	66.984	551.6	93			
Heptanoic acid	78.858	546.194	85			
Compound	IUGASOLN (ppm)*	SOLN+STD 1:1 (ppm)	SOLN+STD % REC	*liquid sampled as received		
Acetic acid	n.d.	628.655	98			
Propionic acid	n.d.	618.952	98			
Butanoic acid	n.d.	570.61	98			
Pentanoic acid	n.d.	524.498	91			
Hexanoic acid	53.069	480.906	86			
Heptanoic acid	79.298	490.666	82			
Compound	IUGA IST (ppm)*	IUGA IST+STD 1:1 (ppm)	IUGA IST+STD % REC	*liquid sampled as received		
Acetic acid	n.d.	651.573	101			
Propionic acid	21.204	648.971	101			
Butanoic acid	47.016	599.638	99			
Pentanoic acid	67.244	577.524	95			
Hexanoic acid	66.181	580.979	98			
Heptanoic acid	79.549	613.124	96			
Compound	IUGASOLN	SOLN+STD 1:1	SOLN+STD	*heated until	Compound	IUGASOLN

	(ppm)*	(ppm)	% REC	adipic is in solution		(%)
Acetic acid	n.d.	755.31	117			
					Succinic	none detected
Propionic acid	n.d.	740.982	118			
					Glutaric	none detected
Butanoic acid	n.d.	676.891	116			
					Adipic	49.67
Pentanoic acid	n.d.	617.945	108			
Hexanoic acid	52.108	540.379	97			
Heptanoic acid	81.924	563.161	94			

Compound	IUGA 1st (ppm)*	IUGA 1ST+STD 1:1 (ppm)	IUGA 1ST+STD % REC	*heated until adipic is in solution	Compound	IUGA 1st (%)
Acetic acid	n.d.	795.136	124			
					Succinic	none detected
Propionic acid	24.523	781.862	124			
					Glutaric	none detected
Butanoic acid	46.771	708.381	121			
					Adipic	60.49
Pentanoic acid	68.025	645.212	113			
Hexanoic acid	66.997	572.397	103			
Heptanoic acid	82.3	594.864	99			

Compound	AMLS 1st (ppm)	AMLS 1ST+STD 1:1 (ppm)	AMLS 1ST+STD % REC		Compound	AMLS 1st (%)
Acetic acid	n.d.	646.442	100.1			
					Succinic	13.97
Propionic acid	46.953	645.226	99			
					Glutaric	17.32
Butanoic acid	201.931	672.701	98			
					Adipic	4.01
Pentanoic acid	314.576	704.28	96			
Hexanoic acid	119.879	619.393	100			
Heptanoic acid	n.d.	634.948	106			

STM-01529 as written incorporates the use of an internal standard for use in compensating for matrix effects on the derivatization and subsequent

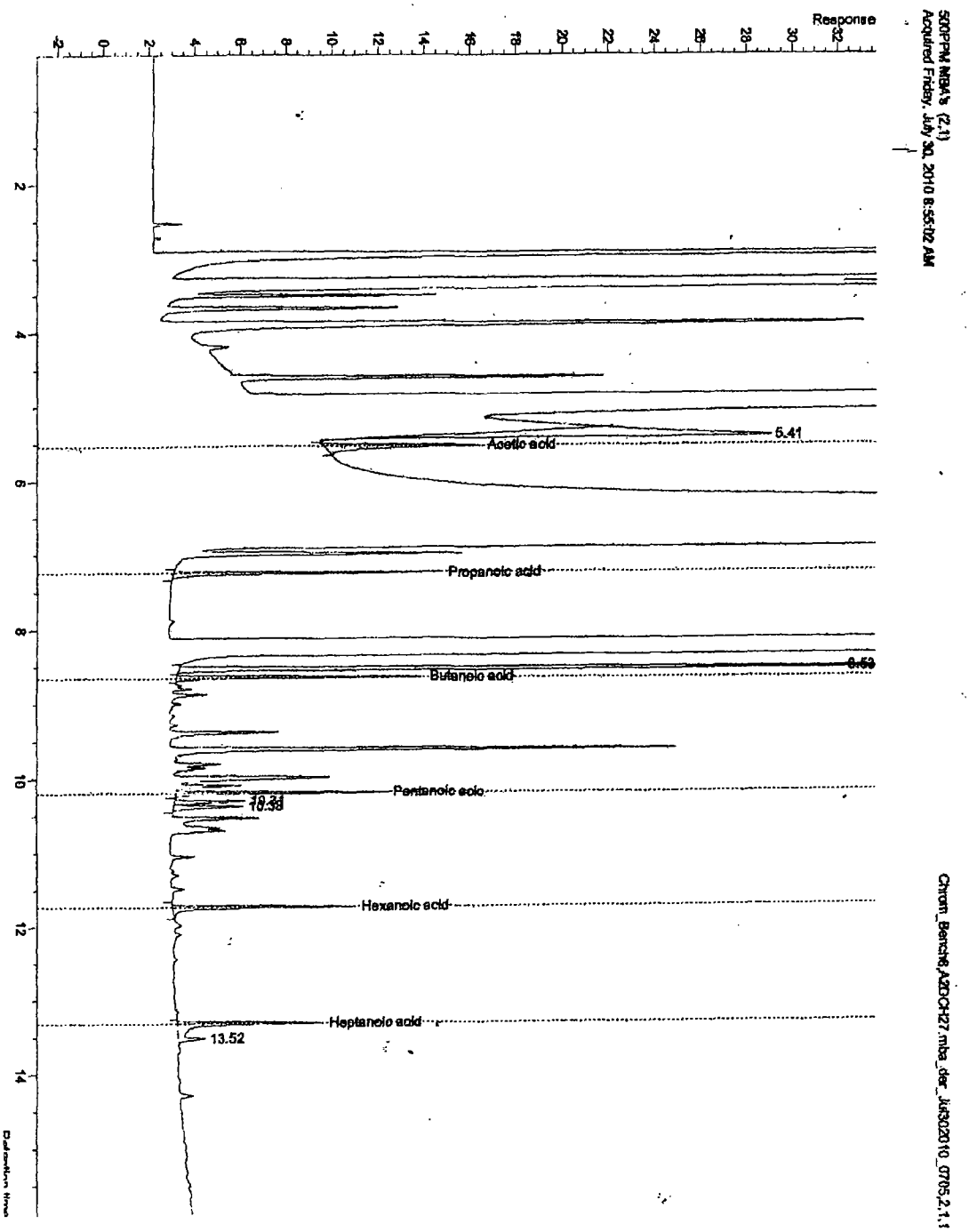
quantitation of the dibasic acids, which are typically present at percent levels. The mono basic acids were expected to be present at ppm levels. This precluded diluting the samples with an internal standard solution prior to derivatization and analysis. To compensate for matrix effects on derivatization and analysis, all samples prepared for the analysis of mono basic acids were analyzed neat and spiked with the compounds of interest. Where the recovery was less than 100%, it was assumed that this was due to incomplete derivatization and the results were adjusted by dividing the result for that analyte by the decimal percent recovery. Where the result was greater than 100% it was decided to use the result from the neat sample with no adjustment. All spiked samples were prepared by diluting 500ul of sample with 500ul of standard. The standard had the following concentrations of analytes:

Acetic acid:1285.9ppm
Propanoic acid:1261.0ppm
Butanoic acid:1169.5ppm
Pentanoic acid: 1146.9ppm
Hexanoic acid:1114.0ppm
Heptanoic acid: 1200.7ppm

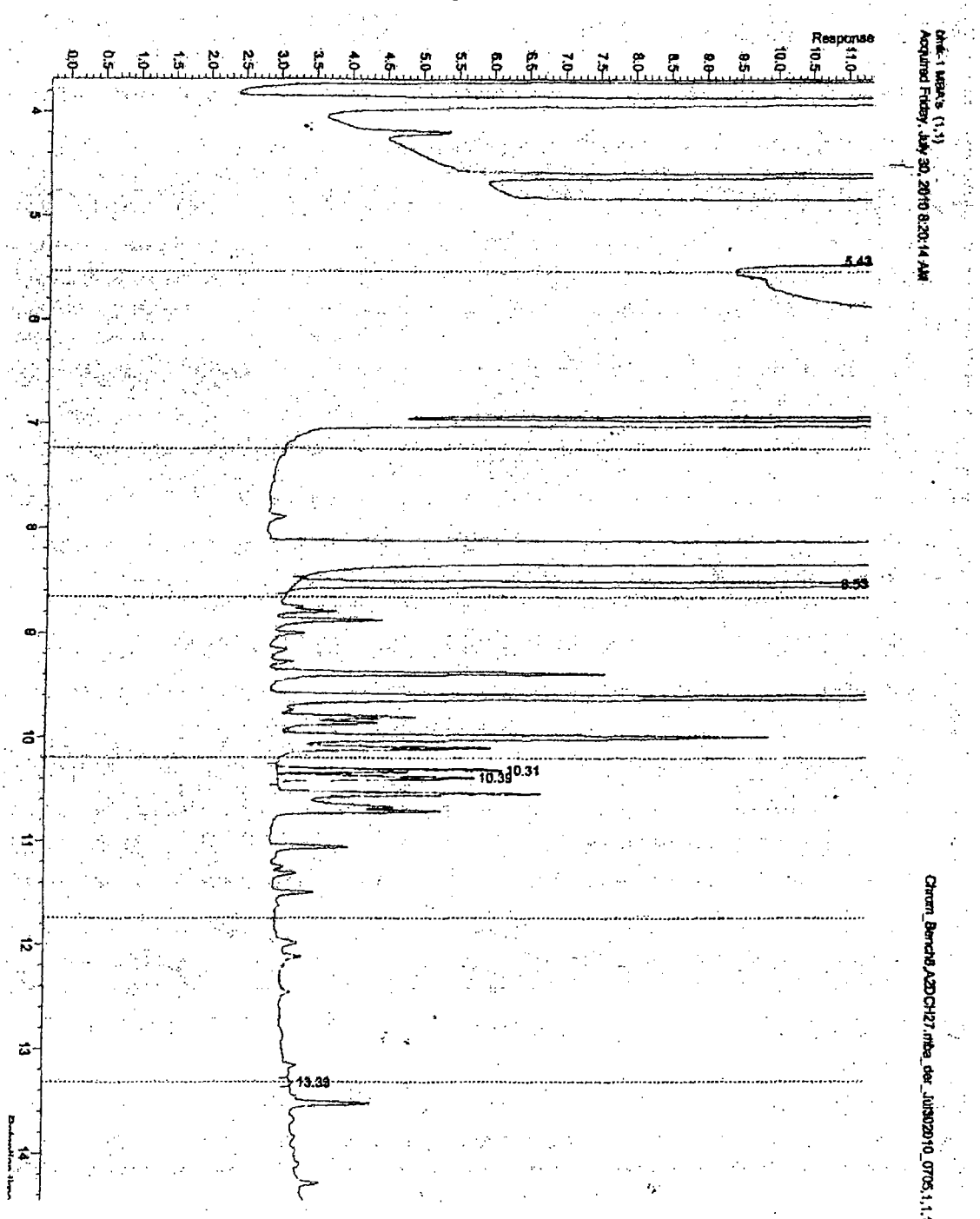
The calculation for % recovery is: $\% = \frac{\text{spike sample result} \times 100}{(0.5 \times \text{neat result}) + (0.5 \times \text{standard conc})}$

Chromatograms

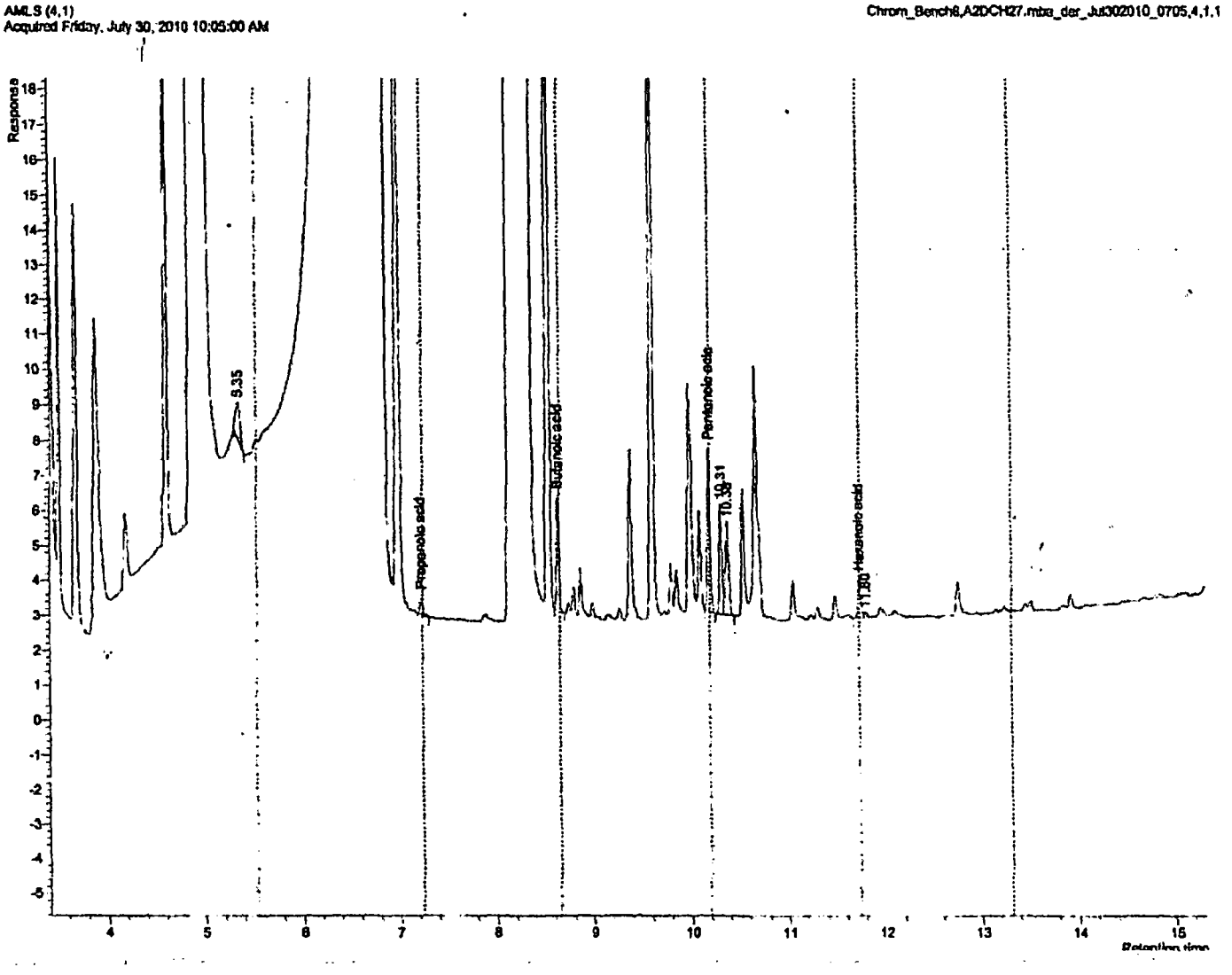
~500ppm Continuing Calibration Standard



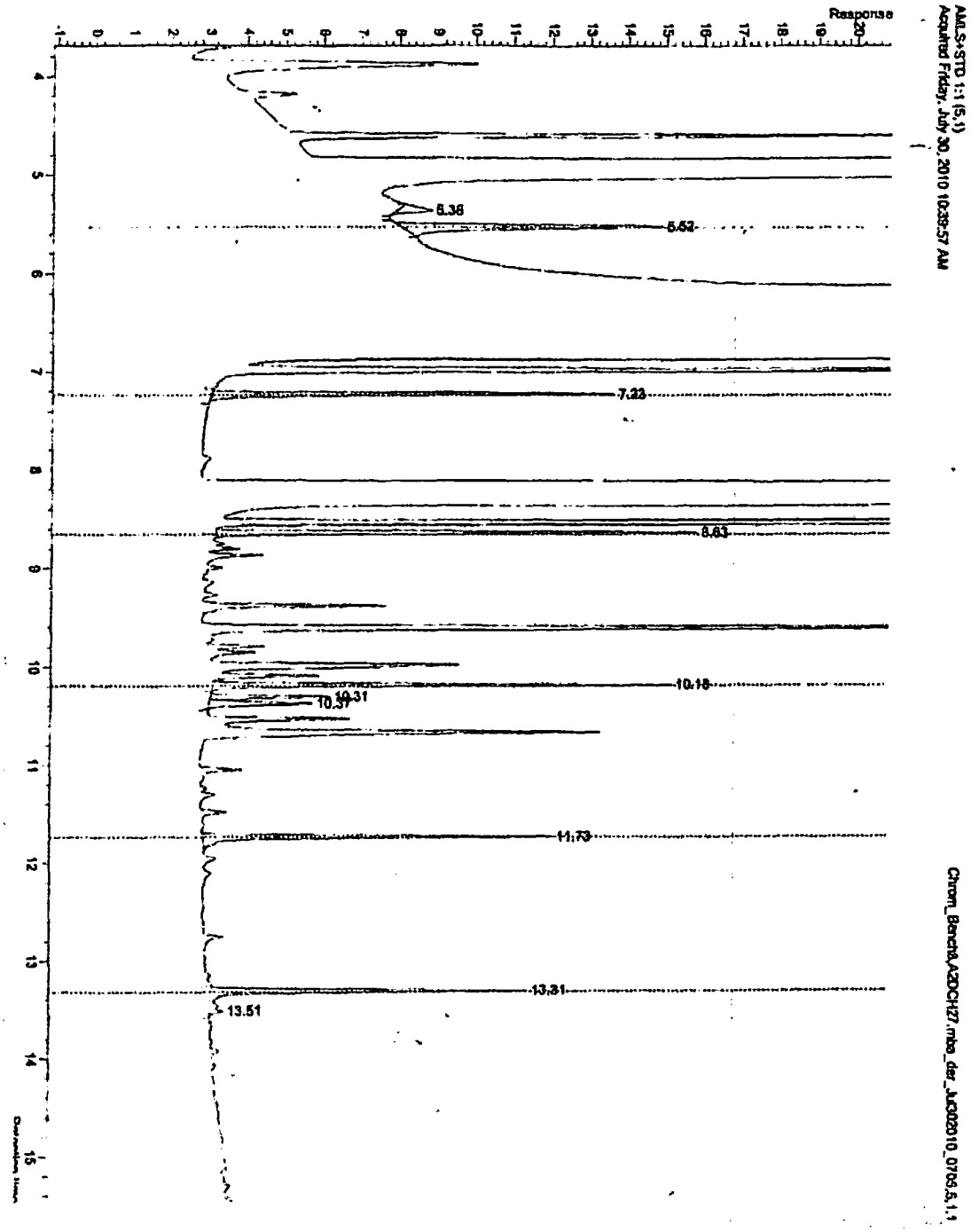
Reagent Blank



Typical Sample (AMLS)



Sample +
Standard(Spike)



Appendix B

WATER9 Summary of Adipic Refine Feed Tank VOC Emissions

WASTEWATER TREATMENT SUMMARY I 09-23-2010 11:53:27

Project C:\Program Files\Wastewater treatment models\refinefeedtank 7/29/2010 2:51:16 PM

COMPOUND	RATE (g/s)	Fraction Air	Removal	Exit	Adsorb	error	emissions
ACETIC ACID	2.88E-23	.99	.	.0003	0.0000	0.0000	(9.07E-22 Mg/yr)
HEXANEDIOIC ACID (adipic acid)	1.61E-04	.	.	1.	0.0000	0.0000	(5.09E-03 Mg/yr)
BUTYRIC ACID	1.06E-04	.00	.	.9993	0.0000	0.0000	(3.36E-03 Mg/yr)
PENTANEDIOIC ACID (glutaric acid)	1.21E-06	.	.	1.	0.0000	0.0000	(3.83E-05 Mg/yr)
HEXANOIC ACID	3.34E-04	.00	.	.9985	0.0000	0.0000	(1.05E-02 Mg/yr)
PROPANOIC ACID	2.88E-23	.99	.	.0004	0.0000	0.0000	(9.07E-22 Mg/yr)
BUTANDIOIC ACIC (succinic acid)	4.78E-07	.	.	1.	0.0000	0.0000	(1.51E-05 Mg/yr)
PENTANOIC ACID	6.00E-04	.00	.	.9975	0.0000	0.0000	(1.89E-02 Mg/yr)
HEPTANOIC ACID	2.22E-03	.00	.	.9922	0.0000	0.0000	(6.99E-02 Mg/yr)
TOTAL ALL COMPOUNDS	3.42E-03 g/s air emissions						
TOTAL ALL COMPOUNDS	1.08E-01 Mg/yr air emissions						

WATER9 Detailed Output of Adipic Acid in Refine Feed Tank

```
 DETAILED CALCULATIONS at Unit 1 def.storage tank
Type: storage tank
  Project C:\Program Files\Wastewater treatment models\refinefeedtank
  7/29/2010 2:51:16 PM  11:58:32
COMPOUND: HEXANEDIOIC ACID (adipic acid)

Type of unit is storage tank
1 Description of unit                          1     def.storage tank
2 Wastewater temperature   (C)                       98.5
3 Open surface area of tank  (m2)                    0
4 Density of liquid in tank (g/cc)                   1.07
5 tank waste Mwt, water=18                           18
6 unit storage time (days)                           0.41
7 tank paint factor                                  1
8 tank diameter (m)                                  7.86
9 tank vapor space height (m)                        4
10 diurnal temp. change (deg.C)                      7.2
11 tank height (m)                                   2.1
12 oil in composite wastewater (wt. %)               0
19 pH                                                0

Properties of HEXANEDIOIC ACID (adipic acid) at 98.5 deg.C (209.3 deg.F)
   hl= 2.558e-08 atm-m3/mol      vp= 0.014274 mmHg (2.761e-04 psia)
       0.001421 y/x
       8.393e-07 g/L gas per g/L liquid
   kl= 0. L/g-hr          dl= 8.526e-06 cm2/s  dv= 0.096907 cm2/s
The oil corrected aqueous HL is 1.421e-03 (y/x)
The concentration in the tank inlet is 3.7e+05 ppmw
The flowrate of liquid is 2.876e-03 M3/s
liquid flowrate (from tank holding) is 2.876e-03 M3/s
The total loading of the compound is 3.59e+10 g/yr.
The working volume is 1.019e+02 m3 (2.692e+04  gal)
The mass lost per turnover is 2.372e-06 Mg/turnover
The vapor pressure of the compound in solution is .000276 psia.
MWT = 146.1    dia= 25.8  ft.
Breathing:  Lb = 0.0000102 * MWT * (p / (14.7 - p)) ^ 0.68 * dia ^ 1.73
mass emissions= Lb * h ^ 0.51 * dt ^ 0.5 * Fp * c   Mg/yr
c = .99    h= 13.1  ft.
dt = 12.96 deg.F    Fp= 1.
mass emissions= 33.36E-04   Mg/yr
The temperature in the tank is 98.5 deg.C
The type of liquid is  Aqueous matrix
The concentration in the liquid waste is 3.7e+05 g/m3
The fraction in the oil is .
The vapor pressure (p) is 2.761e-04  psia(1.427e-02  mmHg)
The fraction of the compound in the oil phase is ..
The residence time in the tank is .41 days.
   unit storage time (days)                  0.41
   Tank turnover factor                      0.20037
   Tank working loss (fraction)              5.88e-08
   Tank breathing loss  (fraction)           9.29e-08
   Open tank volatilization loss             0.
   concentration in headspace (ppmv)         1.878e-05
   fraction of compound in oil phase         0.
   TOTAL FRACTION VOLATILIZED                1.517e-07
   FRACTION BIOLOGICALLY REMOVED             0.
   TOTAL AIR EMISSIONS  (g/s)                1.615e-04
                        (Mg/year)            0.005092
   EMISSION FACTOR  (g/cm2-s)                3.327e-10
   UNIT EXIT CONCENTRATION (ppmw)            3.7e+05
```

TANKS 4.0.9d
Emissions Report - Detail Format
Tank Indentification and Physical Characteristics

Identification		
User Identification:	Area II Refine Feed Tank	
City:	Pensacola	
State:	Florida	
Company:	Ascend	
Type of Tank:	Vertical Fixed Roof Tank	
Description:		
Tank Dimensions		
Shell Height (ft):		20.00
Diameter (ft):		25.79
Liquid Height (ft) :		6.90
Avg. Liquid Height (ft):		6.90
Volume (gallons):		26,963.41
Turnovers:		883.00
Net Throughput(gal/yr):		23,808,693.06
Is Tank Heated (y/n):	Y	
Paint Characteristics		
Shell Color/Shade:	White/White	
Shell Condition	Good	
Roof Color/Shade:	White/White	
Roof Condition:	Good	
Roof Characteristics		
Type:	Dome	
Height (ft)		0.00
Radius (ft) (Dome Roof)		31.00
Breather Vent Settings		
Vacuum Settings (psig):		0.00
Pressure Settings (psig)		0.00

Meterological Data used in Emissions Calculations: Pensacola, Florida (Avg Atmospheric Pressure = 14.73 psia)

TANKS 4.0.9d
Emissions Report - Detail Format
Liquid Contents of Storage Tank

Area II Refine Feed Tank - Vertical Fixed Roof Tank
Pensacola, Florida

Mixture/Component	Month	Daily Liquid Surf. Temperature (deg F) Avg.	Min.	Max.	Liquid Bulk Temp (deg F)	Vapor Pressure (psia) Avg.	Min.	Max.	Vapor Mol. Weight.	Liquid Mass Fract.	Vapor Mass Fract.	Mol. Weight	Basis for Vapor Pressure Calculations
Aqueous Adipic Solution	All	209.30	205.70	212.90	209.30	13.0263	12.1104	13.9993	18.0006			26.81	
Adipic Acid						0.0003	0.0002	0.0003	146.1400	0.3724	0.0000	146.14	Option 2: A=8.358, B=2813.07, C=177.2
Butanoic Acid						1.8215	1.6885	1.9635	88.0000	0.0001	0.0000	88.00	Option 2: A=8.064, B=2263.39, C=273.16
Glutaric Acid						0.0037	0.0033	0.0042	132.0000	0.0012	0.0000	132.00	Option 2: A=6.9478, B=2093.11, C=174.66
Heptanoic Acid						0.0815	0.0716	0.0926	130.0000	0.0001	0.0000	130.00	Option 2: A=7.175, B=1536, C=136
Hexanoic Acid						0.1838	0.1654	0.2041	116.0000	0.0001	0.0000	116.00	Option 2: A=9.4775, B=3158.9, C=273.16
Pentanoic Acid						0.8961	0.8083	0.9915	102.0000	0.0001	0.0000	102.00	Option 2: A=6.0825, B=879.77, C=100.7
Succinic Acid						0.0265	0.0234	0.0301	118.0000	0.0010	0.0000	118.00	Option 2: A=10.35, B=3794, C=273
Water						13.9897	13.0061	15.0347	18.0000	0.6251	1.0000	18.00	Option 2: A=8.1077, B=1750.3, C=235

TANKS 4.0.9d
Emissions Report - Detail Format
Detail Calculations (AP-42)

Area II Refine Feed Tank - Vertical Fixed Roof Tank
Pensacola, Florida

Annual Emission Calcaulations	
Standing Losses (lb):	9,172.6604
Vapor Space Volume (cu ft):	7,588.6366
Vapor Density (lb/cu ft):	0.0327
Vapor Space Expansion Factor:	1.1182
Vented Vapor Saturation Factor:	0.0907
Tank Vapor Space Volume:	
Vapor Space Volume (cu ft):	7,588.6366
Tank Diameter (ft):	25.7900
Vapor Space Outage (ft):	14.5268
Tank Shell Height (ft):	20.0000
Average Liquid Height (ft):	6.9000
Roof Outage (ft):	1.4268
Roof Outage (Dome Roof)	
Roof Outage (ft):	1.4268
Dome Radius (ft):	31.0000
Shell Radius (ft):	12.8950
Vapor Density	
Vapor Density (lb/cu ft):	0.0327
Vapor Molecular Weight (lb/lb-mole):	18.0006
Vapor Pressure at Daily Average Liquid Surface Temperature (psia):	13.0263
Daily Avg. Liquid Surface Temp. (deg. R):	668.9700
Daily Average Ambient Temp. (deg. F):	67.6708
Ideal Gas Constant R (psia cuft / (lb-mol-deg R)):	10.731
Liquid Bulk Temperature (deg. R):	668.9700
Tank Paint Solar Absorptance (Shell):	0.1700
Tank Paint Solar Absorptance (Roof):	0.1700
Daily Total Solar Insulation Factor (Btu/sqft day):	1,384.3333
Vapor Space Expansion Factor	
Vapor Space Expansion Factor:	1.1182
Daily Vapor Temperature Range (deg. R):	7.2000
Daily Vapor Pressure Range (psia):	1.8890
Breather Vent Press. Setting Range(psia):	0.0000
Vapor Pressure at Daily Average Liquid Surface Temperature (psia):	13.0263
Vapor Pressure at Daily Minimum Liquid Surface Temperature (psia):	12.1104
Vapor Pressure at Daily Maximum Liquid Surface Temperature (psia):	13.9993
Daily Avg. Liquid Surface Temp. (deg R):	668.9700
Daily Min. Liquid Surface Temp. (deg R):	665.3700
Daily Max. Liquid Surface Temp. (deg R):	672.5700
Daily Ambient Temp. Range (deg. R):	17.6917
Vented Vapor Saturation Factor	
Vented Vapor Saturation Factor:	0.0907
Vapor Pressure at Daily Average Liquid: Surface Temperature (psia):	13.0263
Vapor Space Outage (ft):	14.5268
Working Losses (lb):	26,669.4981
Vapor Molecular Weight (lb/lb-mole):	18.0006
Vapor Pressure at Daily Average Liquid Surface Temperature (psia):	13.0263
Annual Net Throughput (gal/yr.):	23,808,693.0644
Annual Turnovers:	883.0000
Turnover Factor:	0.2006
Maximum Liquid Volume (gal):	26,963.4123
Maximum Liquid Height (ft):	6.9000
Tank Diameter (ft):	25.7900
Working Loss Product Factor:	1.0000
Total Losses (lb):	35,842.1584

TANKS 4.0.9d
Emissions Report - Detail Format
Individual Tank Emission Totals

Emissions Report for: Annual

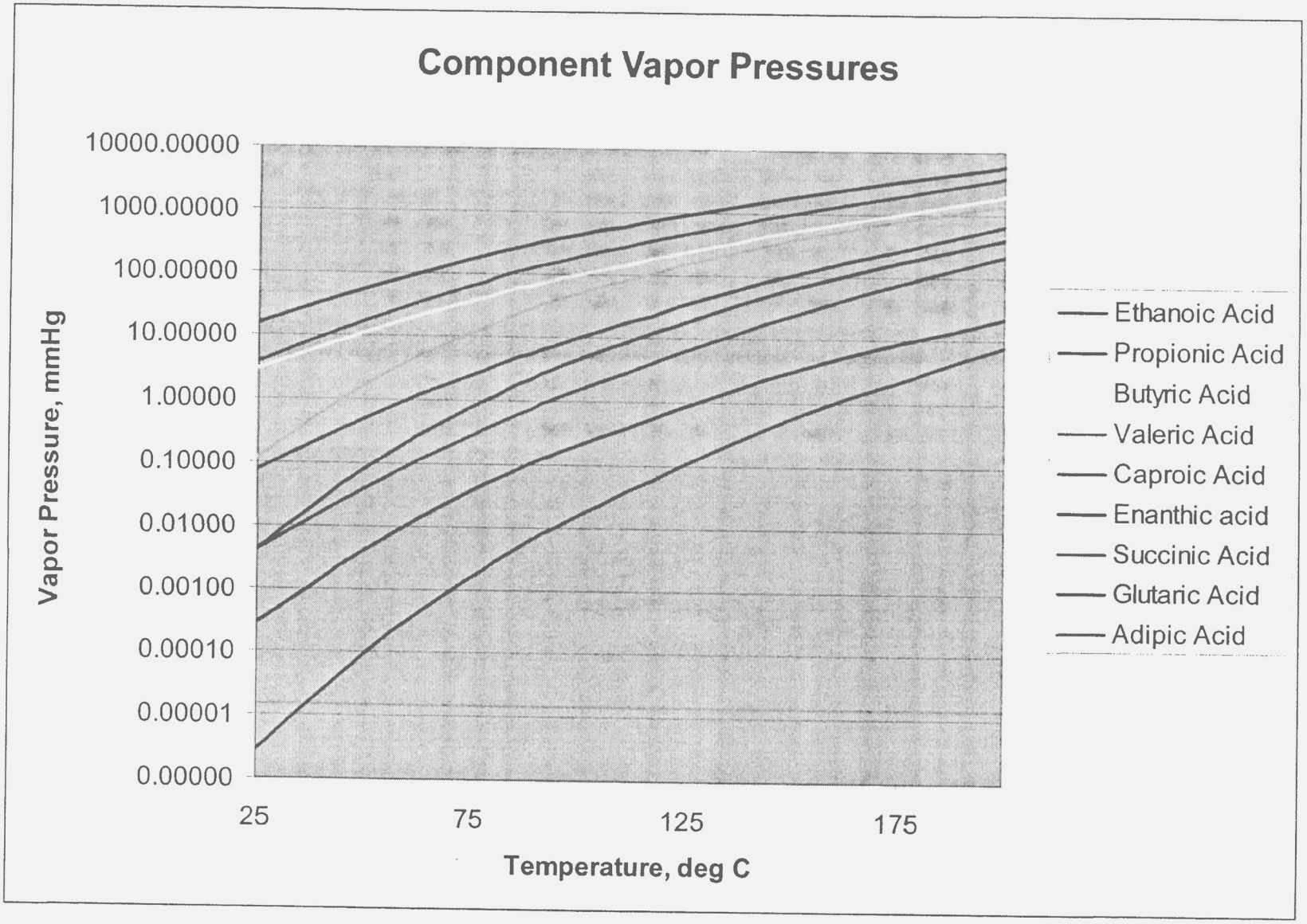
Area II Refine Feed Tank - Vertical Fixed Roof Tank
Pensacola, Florida

	Losses(lbs)		
Components	Working Loss	Breathing Loss	Total Emissions
Aqueous Adipic Solution	26,669.50	9,172.66	35,842.16
Adipic Acid	0.31	0.11	0.42
Water	26,668.50	9,172.32	35,840.81
Glutaric Acid	0.01	0.00	0.02
Succinic Acid	0.08	0.03	0.11
Heptanoic Acid	0.02	0.01	0.03
Hexanoic Acid	0.04	0.02	0.06
Pentanoic Acid	0.23	0.08	0.31
Butanoic Acid	0.30	0.10	0.40

Adipic VOC Emission Simulation Physical Property Data

	IUPAC Name	Common Name	MW	Henry's Law Constant HI (atm*m3/mol)	Henry's Law Constant K (y/x) @25C	UNIFAC Activity Coeff.in Water
C2	Acetic Acid	Ethanoic Acid	60	1.19E-06	0.06609	3.5
C3	Propanoic Acid	Propionic Acid	74	4.59E-07	0.0255	9.1
C4	Butanoic Acid	Butyric Acid	88	1.08E-06	0.06	24.7
C5	Pentanoic Acid	Valeric Acid	102	4.54E-07	0.02525	68.5
C6	Hexanoic Acid	Caproic Acid	116	7.14E-07	0.03968	192.5
C7	Heptanoic Acid	Enanthic acid	130	6.48E-07	0.036	545
C4	Butanedioic Acid	Succinic Acid	118	3.33E-12	1.85E-07	3.25
C5	Pentanedioic Acid	Glutaric Acid	132	5.00E-12	2.78E-07	6.78
C6	Hexanedioic Acid	Adipic Acid	146	5.00E-12	2.78E-07	15.1

	IUPAC Name	Common Name	MW	VP@25C mm Hg	Antoine Coeff.'s: (P=mmHg, T=C) A	B	C
C2	Acetic Acid	Ethanoic Acid	60	15.4	7.387	1533.3	222.3
C3	Propanoic Acid	Propionic Acid	74	3.5	7.6258	1678.86	213.328
C4	Butanoic Acid	Butyric Acid	88	0.84	8.064204	2263.39	273.16
C5	Pentanoic Acid	Valeric Acid	102	0.196	6.0825	879.77	100.7
C6	Hexanoic Acid	Caproic Acid	116	0.044	9.4775	3158.9	273.16
C7	Heptanoic Acid	Enanthic acid	130	0.0107	7.175	1536	136
C4	Butanedioic Acid	Succinic Acid	118	0.00418	10.35	3794	273
C5	Pentanedioic Acid	Glutaric Acid	132	0.000291359	6.9478	2093.11	174.66
C6	Hexanedioic Acid	Adipic Acid	146	2.79E-06	8.358	2813.066	177.2


Component Vapor Pressures
Vapor Pressure, mmHg
10000.00000
1000.00000
100.00000
10.00000
1.00000
0.10000
0.01000
0.00100
0.00010
0.00001
0.00000
25
75
125
175
Temperature, deg C
Ethanoic Acid
Propionic Acid
Butyric Acid
Valeric Acid
Caproic Acid
Enanthic acid
Succinic Acid
Glutaric Acid
Adipic Acid

Detailed Component Physical Property Summary for WATER9:

PROPERTIES OF ACETIC ACID at 25 deg.C

The following compound properties are estimated.

```
Type of compound        O
density  (g/cc)                                1.05
molecular weight                                60.05
diffusion coef. water (cm2/s)                   1.2e-05
diffusion coef. air  (cm2/s)                    0.113
vapor pressure (mm Hg)                          15.4
Henry's law constant (atm-m3/mol)               1.19e-06   y/x= 0.06609
   Reference for Henry's law: DIPPR911
vapor pressure temp. coefficients               7.387    1533.313    222.309
The enthalpy of vaporization 177.146 cal/cc.
zero order biorate constant (mg/g-hr)           14.
first order biorate constant (l/g-hr)           0.98
octanol water partition coefficient             -0.31
solubility ppmw 1.e+06
the UNIFAC activity coef. in water at 25 deg. C is 3.50551
The water solubility estimated from the activity coefficient (25 C) is
8.161e+05
The activity coefficient in octanol at 25 deg. C is 0.88639
UNIFAC code     2111[000000000
CAS code     64-19-7
          The estimated vapor pressure is  15.352 mm Hg.
```

PROPERTIES OF PROPANOIC ACID at 25 deg.C

The following compound properties are estimated.

```
The density is estimated from the default values.
The octanol water partition coef. is estimated from the UNIFAC method.
The biorate Kmax is estimated from the default.
The liquid diffusion coef. is estimated from the correlation.
The vapor diffusion coef. is estimated from the correlation.
Type of compound        O
density  (g/cc)                                0.97
molecular weight                                74.08
diffusion coef. water (cm2/s)                   1.12e-05
diffusion coef. air  (cm2/s)                    0.0973
vapor pressure (mm Hg)                          3.53
Henry's law constant (atm-m3/mol)               4.59e-07   y/x= 0.0255
   Reference for Henry's law: Servant (1991)
vapor pressure temp. coefficients               7.6258    1678.86    213.328


The enthalpy of vaporization 156.171 cal/cc.
zero order biorate constant (mg/g-hr)           17.56
first order biorate constant (l/g-hr)           0.17394
octanol water partition coefficient             0.28965
solubility ppmw 3.7e+05
the UNIFAC activity coef. in water at 25 deg. C is 9.115
```

The water solubility estimated from the activity coefficient (25 C) is 5.287e+05
The activity coefficient in octanol at 25 deg. C is 0.82387
UNIFAC code 311121[0000000
CAS code 79-09-4
The estimated vapor pressure is 3.8076 mm Hg.

PROPERTIES OF BUTYRIC ACID at 25 deg.C

The following compound properties are estimated.

The octanol water partition coef. is estimated from the UNIFAC method.
The biorate Kmax is estimated from the default.
The liquid diffusion coef. is estimated from the correlation.
The vapor diffusion coef. is estimated from the correlation.

Type of compound	O		
density (g/cc)	0.958		
molecular weight	88.1		
diffusion coef. water (cm2/s)	1.e-05		
diffusion coef. air (cm2/s)	0.0845		
vapor pressure (mm Hg)	0.84		
Henry's law constant (atm-m3/mol)	1.08e-06	y/x= 0.06	
Reference for Henry's law: DIPPR911			
vapor pressure temp. coefficients	8.0642	2263.39	273.16

The enthalpy of vaporization 112.627 cal/cc.

zero order biorate constant (mg/g-hr)	17.56
first order biorate constant (l/g-hr)	0.25431
octanol water partition coefficient	0.72377

solubility ppmw 5.62e+04
the UNIFAC activity coef. in water at 25 deg. C is 24.723
The water solubility estimated from the activity coefficient (25 C) is 2.72e+05
The activity coefficient in octanol at 25 deg. C is 0.79874
UNIFAC code 311221[0000000
CAS code 107-92-6
The estimated vapor pressure is 2.9716 mm Hg.

PROPERTIES OF PENTANOIC ACID at 25 deg.C

The following compound properties are estimated.

The octanol water partition coef. is estimated from the UNIFAC method.
The biorate Kmax is estimated from the default.
The liquid diffusion coef. is estimated from the correlation.
The vapor diffusion coef. is estimated from the correlation.
The solubility is estimated from the vapor pressure and Henry's law.

Type of compound		
density (g/cc)	0.939	
molecular weight	102.14	
diffusion coef. water (cm2/s)	9.1e-06	
diffusion coef. air (cm2/s)	0.0737	
vapor pressure (mm Hg)	0.196	
Henry's law constant (atm-m3/mol)	4.545e-07	y/x= 0.02525
Reference for Henry's law: Khan 1995 M S		

vapor pressure temp. coefficients 6.0825 879.77 100.7
The enthalpy of vaporization 199.361 cal/cc.
zero order biorate constant (mg/g-hr) 15.3
first order biorate constant (1/g-hr) 0.37182
octanol water partition coefficient 1.15789
solubility ppmw 5.796e+04
the UNIFAC activity coef. in water at 25 deg. C is 68.539
The water solubility estimated from the activity coefficient (25 C) is 1.097e+05
The activity coefficient in octanol at 25 deg. C is 0.79155
UNIFAC code 311321[0000000
CAS code 109-52-4
The estimated vapor pressure is .12084 mm Hg.

PROPERTIES OF HEXANOIC ACID at 25 deg.C

The following compound properties are estimated.

The biorate Kmax is estimated from the default.
The liquid diffusion coef. is estimated from the correlation.
The vapor diffusion coef. is estimated from the correlation.
Type of compound O
density (g/cc) 0.9265
molecular weight 116.06
diffusion coef. water (cm2/s) 8.36e-06
diffusion coef. air (cm2/s) 0.0646
vapor pressure (mm Hg) 0.0435
Henry's law constant (atm-m3/mol) 7.142e-07 y/x= 0.03968
Reference for Henry's law: Khan 1995 M S
vapor pressure temp. coefficients 9.478 3158.9 273.16
The enthalpy of vaporization 115.396 cal/cc.

zero order biorate constant (mg/g-hr) 17.56
first order biorate constant (1/g-hr) 0.72433
octanol water partition coefficient 1.92
solubility ppmw 1.1e+04
the UNIFAC activity coef. in water at 25 deg. C is 192.476
The water solubility estimated from the activity coefficient (25 C) is 3.993e+04
The activity coefficient in octanol at 25 deg. C is 0.7946
UNIFAC code 311421[0000000
CAS code 142-62-1
The estimated vapor pressure is .076 mm Hg.

PROPERTIES OF HEPTANOIC ACID at 25 deg.C

The following compound properties are estimated.

The biorate Kmax is estimated from the default.
The liquid diffusion coef. is estimated from the correlation.
The vapor diffusion coef. is estimated from the correlation.
Type of compound
density (g/cc) 0.918

molecular weight 130.2
diffusion coef. water (cm2/s) 7.76e-06
diffusion coef. air (cm2/s) 0.0564
vapor pressure (mm Hg) 0.0107
Henry's law constant (atm-m3/mol) 6.48e-07 y/x= 0.036
Reference for Henry's law: SRC estimated 2000
vapor pressure temp. coefficients 7.175 1536. 136.
The enthalpy of vaporization 165.394 cal/cc.
zero order biorate constant (mg/g-hr) 15.3
first order biorate constant (1/g-hr) 1.12186
octanol water partition coefficient 2.42
solubility ppmw 2820.
the UNIFAC activity coef. in water at 25 deg. C is 544.948
The water solubility estimated from the activity coefficient (25 C) is 1.455e+04
The activity coefficient in octanol at 25 deg. C is 0.80419
UNIFAC code 311521[0000000
CAS code 111-14-8
The estimated vapor pressure is .0043092 mm Hg.

PROPERTIES OF BUTANDIOIC ACIC (succinic acid) at 25 deg.C

The following compound properties are estimated.

The biorate Kmax is estimated from the default.
The liquid diffusion coef. is estimated from the correlation.
The vapor diffusion coef. is estimated from the correlation.
Type of compound O
density (g/cc) 1.552
molecular weight 118.09
diffusion coef. water (cm2/s) 1.12e-05
diffusion coef. air (cm2/s) 0.0794
vapor pressure (mm Hg) 0.00418
Henry's law constant (atm-m3/mol) 3.334e-12 y/x= 1.852e-07
Reference for Henry's law: Saxena 1996 E S
vapor pressure temp. coefficients 10.348 3794. 273.
The enthalpy of vaporization 228.416 cal/cc.
zero order biorate constant (mg/g-hr) 17.56
first order biorate constant (1/g-hr) 0.0805
octanol water partition coefficient -0.59
solubility ppmw 8.32e+04
the UNIFAC activity coef. in water at 25 deg. C is 3.25264
The water solubility estimated from the activity coefficient (25 C) is 9.932e+05
The activity coefficient in octanol at 25 deg. C is 2.36042
UNIFAC code 2222[000000000
CAS code 110-15-6
The estimated vapor pressure is .0041268 mm Hg.

PROPERTIES OF PENTANEDIOIC ACID (glutaric acid) at 25 deg.C

The following compound properties are estimated.

```
 The density is estimated from the default values.
 The octanol water partition coef. is estimated from the UNIFAC method.
 The biorate Kmax is estimated from the default.
 The liquid diffusion coef. is estimated from the correlation.
 The vapor diffusion coef. is estimated from the correlation.
Type of compound       O
density  (g/cc)                              0.97
molecular weight                             132.13
diffusion coef. water (cm2/s)                7.95e-06
diffusion coef. air  (cm2/s)                 0.0568
vapor pressure (mm Hg)                       2.9e-04
Henry's law constant (atm-m3/mol)            5.e-12    y/x= 2.778e-07
   Reference for Henry's law: Saxena 1996 E S
vapor pressure temp. coefficients            6.94783    2093.118    174.66
The enthalpy of vaporization 154.339 cal/cc.
zero order biorate constant (mg/g-hr)        17.56
first order biorate constant (l/g-hr)        0.13763
octanol water partition coefficient          0.022041
solubility ppmw 6.4e+05
the UNIFAC activity coef. in water at 25 deg. C is 6.77828
The water solubility estimated from the activity coefficient (25 C) is
8.883e+05
The activity coefficient in octanol at 25 deg. C is 1.75829
UNIFAC code    2322[000000000
CAS code    110-94-1
          The estimated vapor pressure is  .00029108 mm Hg.
```

PROPERTIES OF HEXANEDIOIC ACID (adipic acid) at 25 deg.C

```
 The following compound properties are estimated.

 The biorate Kmax is estimated from the default.
Type of compound       O
density  (g/cc)                              1.37
molecular weight                             146.14
diffusion coef. water (cm2/s)                6.84e-06
diffusion coef. air  (cm2/s)                 0.0659
vapor pressure (mm Hg)                       2.79e-06
Henry's law constant (atm-m3/mol)            5.e-12    y/x= 2.778e-07
   Reference for Henry's law: Saxena 1996 E S
vapor pressure temp. coefficients            8.358    2813.066    177.2
The enthalpy of vaporization 258.418 cal/cc.
zero order biorate constant (mg/g-hr)        17.56
first order biorate constant (l/g-hr)        0.14479
octanol water partition coefficient          0.08
solubility ppmw 3.08e+04
the UNIFAC activity coef. in water at 25 deg. C is 15.143
The water solubility estimated from the activity coefficient (25 C) is
6.771e+05
The activity coefficient in octanol at 25 deg. C is 1.40414
UNIFAC code    2422[000000000
CAS code    124-04-9
          The estimated vapor diffusion coefficient is .0578 cm2/s
          The estimated vapor pressure is  .0000027892 mm Hg.
```

Tank Details:

Vessel ID	405TA 001
Vessel Description	Refine Feed Tank
Height	25' 0"
Diameter	25' 9 9/16"
Fluid Density	66.765
Horizontal/Vertical	Vertical
Roof Type	Fixed
Roof Height	31' spherical radius
Bottom Head	Flat
100% Liquid Height on vessel	22.4'
0% Liquid Height on Vessel	0"
Level Tag	405LI432.PV
Average Tank Throughput (kpph)	400
Insulated?	Yes
Shell Color	
Temperature Controlled?	Yes
Heated/Cooled	Heated
Temperature Range (°C)	94 - 103
Temperature Tag	405TC429.PV
Atmospheric/Pressurized	Atmospheric
Operating Pressure	Atmospheric
Conservation Vent Setting	None