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SARTORIUS

Simplifying Progress



Bay Area Odor Assessment Study

May 9-20, 2021





PTR Van at Milpitas, CA Park

BAAQMD Odor Study - Odor Plume Multivariate Data Analysis



What is Multivariate Analysis?.....

.... Multivariate statistics is a subdivision of statistics encompassing the simultaneous observation and analysis of more than one outcome variable. –Wiki

Layperson – Examining relationships between independent variables and how they relate to each other.

How Does it Work?.....

In this case, we are using a class of models, called Principle Component Analysis (PCA) - used to reduce the dimensionality of large data sets, by transforming a large set of variables into a smaller one that still contains most of the information in the large set - Wiki

Layperson - How variables, such as ratio's or specific unique compounds in a group of compounds (plume) correlate to all of the possible compounds in a model (facility plume fingerprint)

How are we applying this to Odor Plume Analysis?...

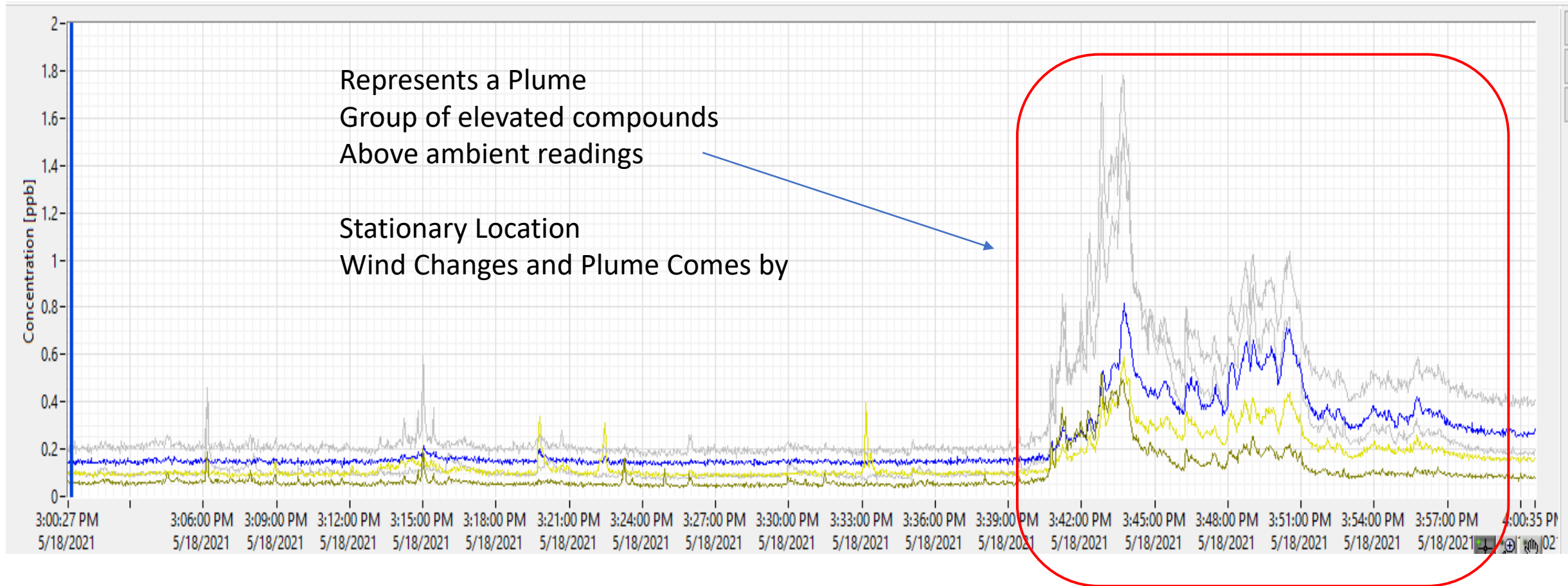
- 1 – Fingerprint each facility and source in facility – generate model to determine if each is unique – develop PCA model
- 2 – Measure plumes found in community – apply PCA – Looks at unique and ratios of compounds and compare to model (facility fingerprint)
- 3 – Bin them into correlations from each data point (air sample) and assign to facility



PTR at Don Edwards Estuary Wildlife Refuge

Graphical representation of GPS CMS Map Concentrations – Dixon Landing Park Area

These individual compounds are used in the modeling to determine origin of plume



Fingerprint Models and Sample Bag Analysis

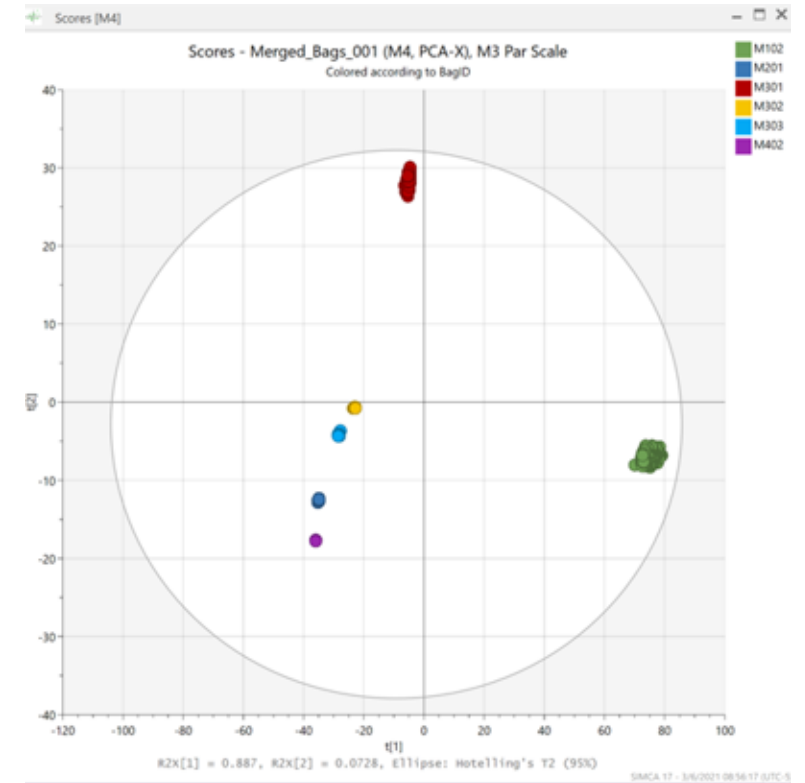
- 15 source bags were measured and identified to be from one of 4 sources
 - WWTP – Wastewater Treatment Plant
 - Newby – Newby landfill
 - ZWED – Zero Waste Energy Development
 - Estuary
- Observations from the Anthony Spangler Middle School were analyzed as the initial test case to start model development
 - Pareto scaling was applied as more populated masses, allowing for a more robust model
 - Several Sensitivity cut offs were explored
 - 0.05 based on the instrument sensitivity
 - 0.10, 0.20, 0.50, and 2.00 to explore if there was a ‘natural noise floor’ in the data



PTR Van at Milpitas, CA Elementary School

Individual bag analysis

- Models for each bag were able to be created
 - Observation distribution is ideal
 - a good model can be built for each bag
 - m21 and m34 were excluded
 - m21's contribution was very high
 - m34's contribution was vary high once m21 was excluded
 - Pareto scaling was applied
 - Enhanced masses with lower concentrations
 - Enhanced separation between bags
 - Enhanced model confidence



7-15 Dimensions examined

Collective bag analysis

- We see nice separation between the bags in the model (circle)
- Loadings, green bars, looks good
 - First loading separates the bags from left to right
 - Second loading separates the bags from bottom to top

Project Window - M5 (PCA-Class)

Number	Model	Type	A	N	R2X(cum)	R2Y(cum)	Q2(cum)	Date	Title	Hierarchical
1	M1	PCA-X	9	3918	1		0.978	3/6/2021		
2	M2	PCA-X	2	3918	0.994		0.848	3/6/2021	Removed m21	
3	M3	PCA-X	2	3918	0.988		0.942	3/6/2021	Removed m34	
4	M4	PCA-X	5	3918	0.991		0.965	3/6/2021	M3 Par Scale	
Class model 1										
5	M5	PCA-Class(M102)	2	653	0.53		0.323	3/6/2021		
6	M6	PCA-Class(M201)	2	627	0.288		-0.21	3/6/2021		
7	M7	PCA-Class(M301)	2	602	0.523		-0.189	3/6/2021		
8	M8	PCA-Class(M302)	2	614	0.625		0.0472	3/6/2021		
9	M9	PCA-Class(M303)	3	743	0.755		0.259	3/6/2021		
10	M10	PCA-Class(M402)	2	679	0.751		-0.161	3/6/2021		

Properties

Scores

Model: M5

Component: 2

X-axis comp: 1

Color by: BagID

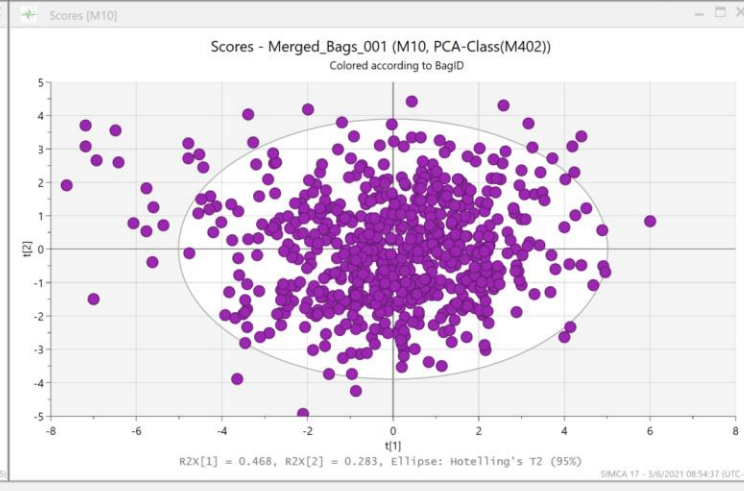
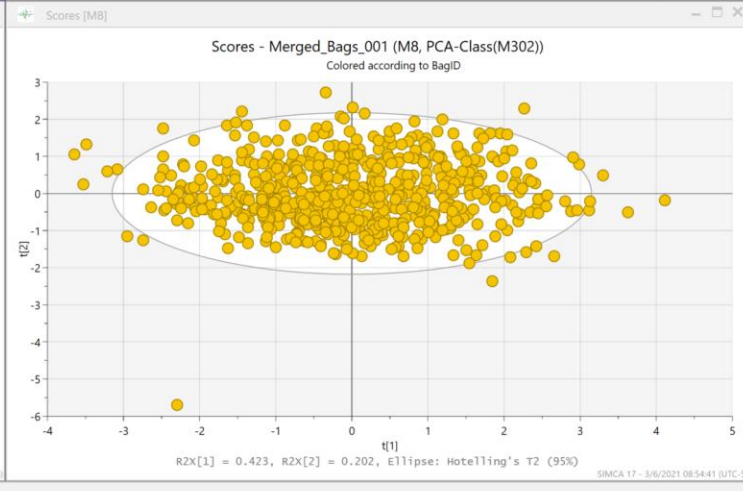
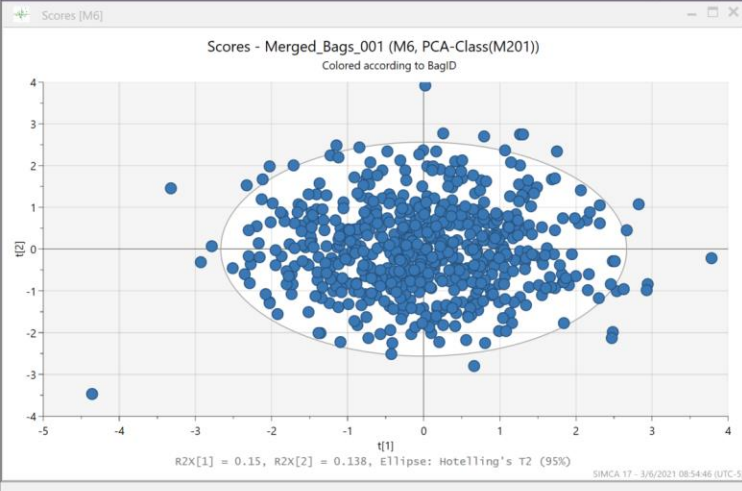
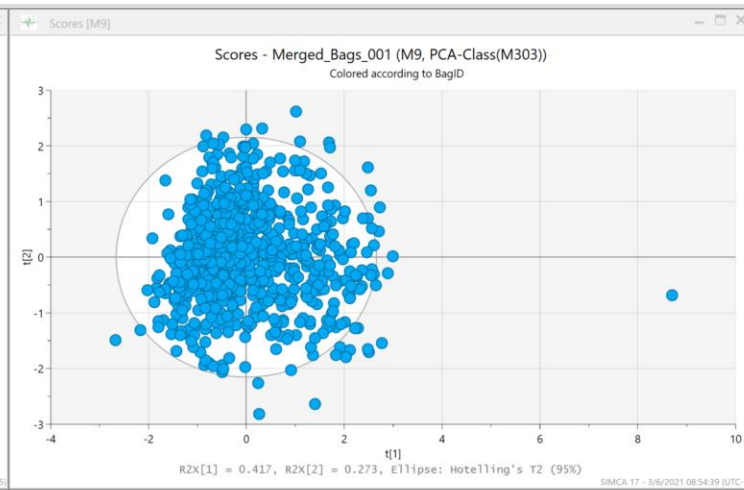
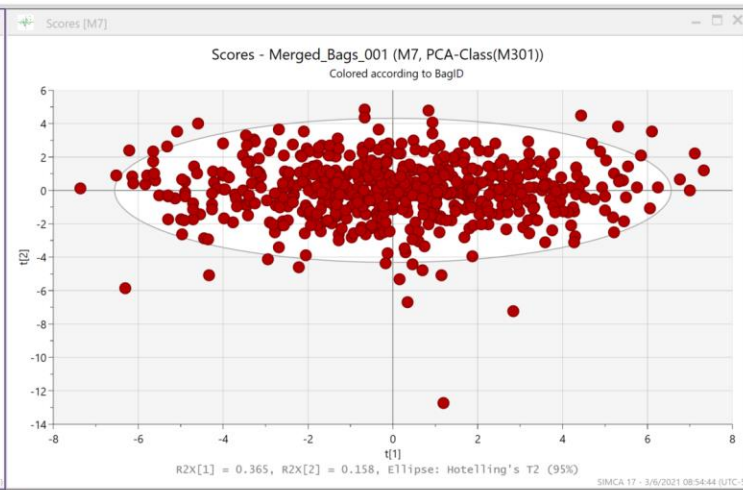
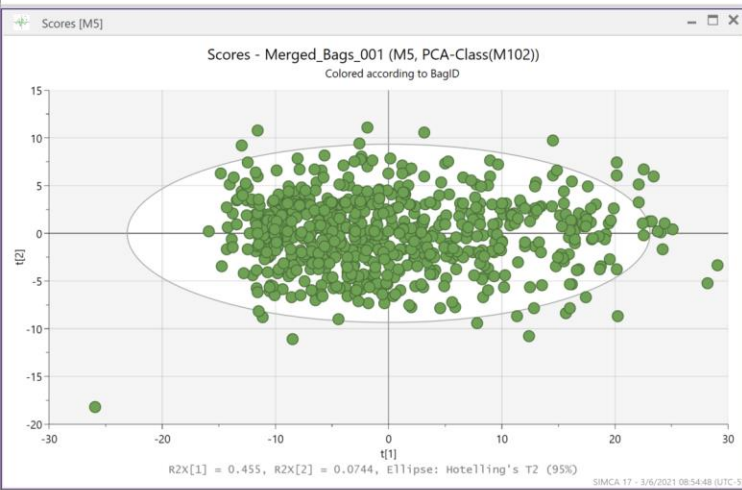
- No ID
- M102
- M201
- M301
- M302
- M303
- M402

Size by: No sizing | Dcrit | Vector...

Labels: Primary ID

More properties...

Quick Info Properties What-If Data Explorer



Project Window - M4 (PCA-X) - M3 Par Scale

Number	Model	Type	A	N	R2X(cum)	R2Y(cum)	Q2(cum)	Date	Title	Hierarchical
1	M1	PCA-X	9	3918	1		0.978	3/6/2021		
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Class model 1										
5	M5	PCA-Class(M102)	2	653	0.53		0.323	3/6/2021		
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8	M8	PCA-Class(M302)	2	614	0.625		0.0472	3/6/2021		
9	M9	PCA-Class(M303)	3	743	0.755		0.259	3/6/2021		
10	M10	PCA-Class(M402)	2	679	0.751		-0.161	3/6/2021		

Properties

Scores

Model: M4

Component: 2

X-axis comp: 1

Color by: BagID

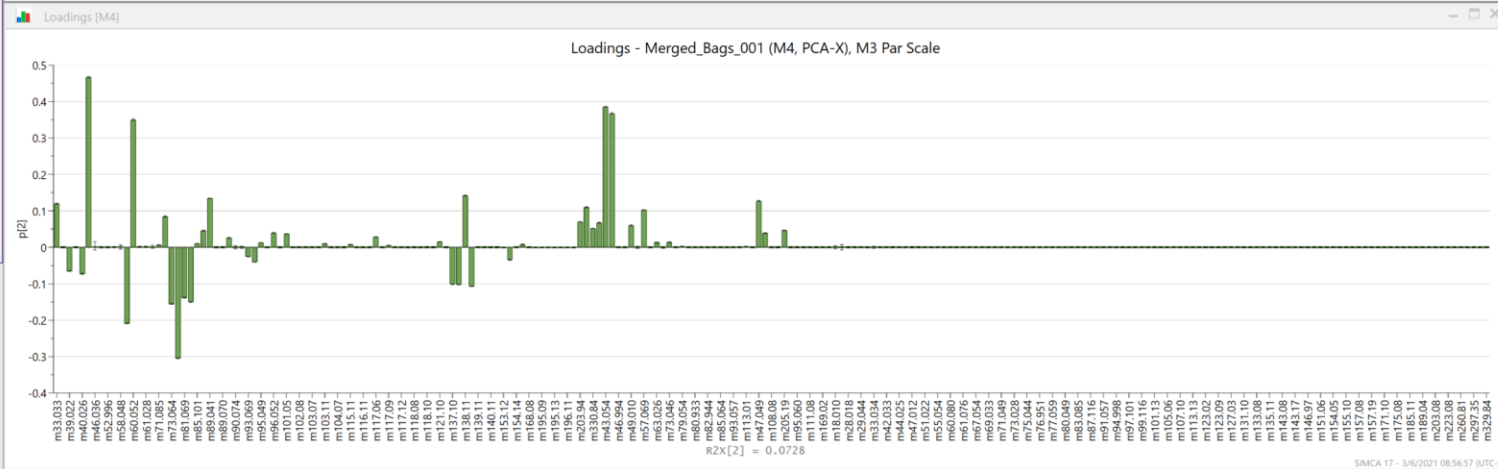
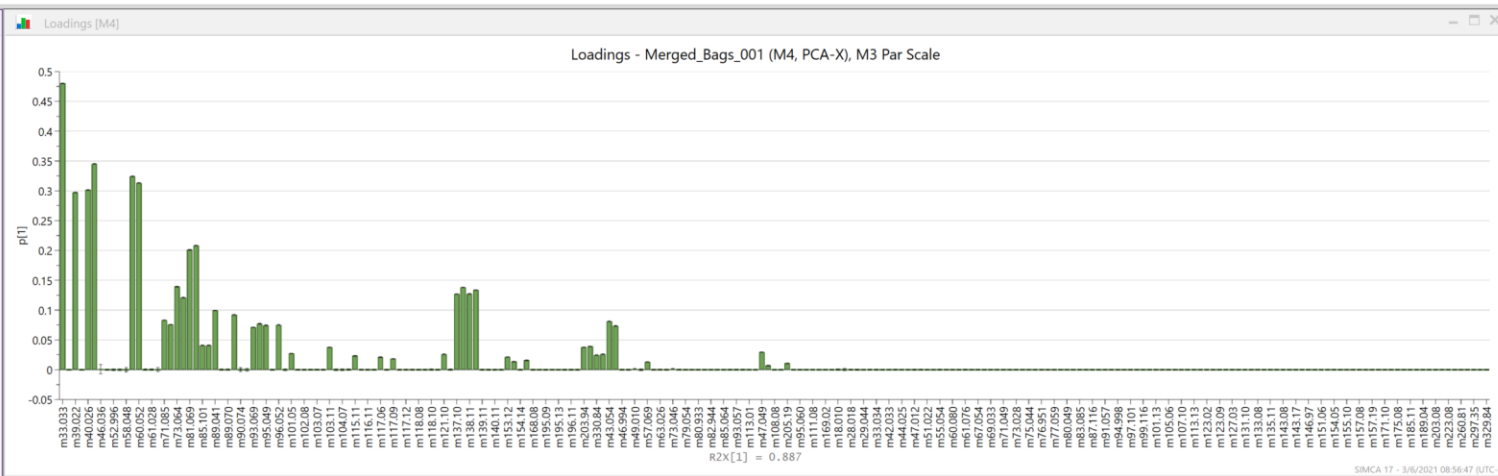
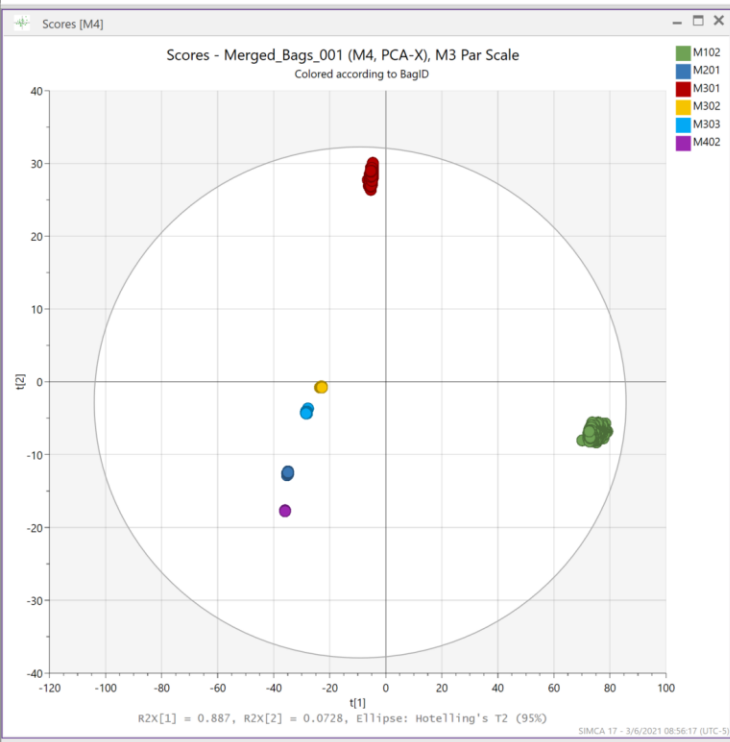
- No ID
- M102
- M201
- M301
- M302
- M303
- M402

Labels: Primary ID

Size by: No sizing | Dcrit | Vector...

More properties...

Quick Info Properties What-If Data Explorer



Initial Classification by Source Principle Component Analysis

	1	2	3	4	5	6	7	8
1 M9, M10, M11, M12	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)	
2 WWTP	0	0%	0	0	0	0	0	0
3 Newby	0	0%	0	0	0	0	0	0
4 ZWED	0	0%	0	0	0	0	0	0
5 Estuary	0	0%	0	0	0	0	0	0
6 No class	3356		1656	1049	0	0	651	2.00
7 Total	3356	0%	1656	1049	0	0	651	

	1	2	3	4	5	6	7	8
1 M17, M18, M19, M20	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)	
2 WWTP	0	0%	0	0	0	0	0	0
3 Newby	0	0%	0	0	0	0	0	0
4 ZWED	0	0%	0	0	0	0	0	0
5 Estuary	0	0%	0	0	0	0	0	0
6 No class	3356		2	2234	687	81	352	0.20
7 Total	3356	0%	2	2234	687	81	352	

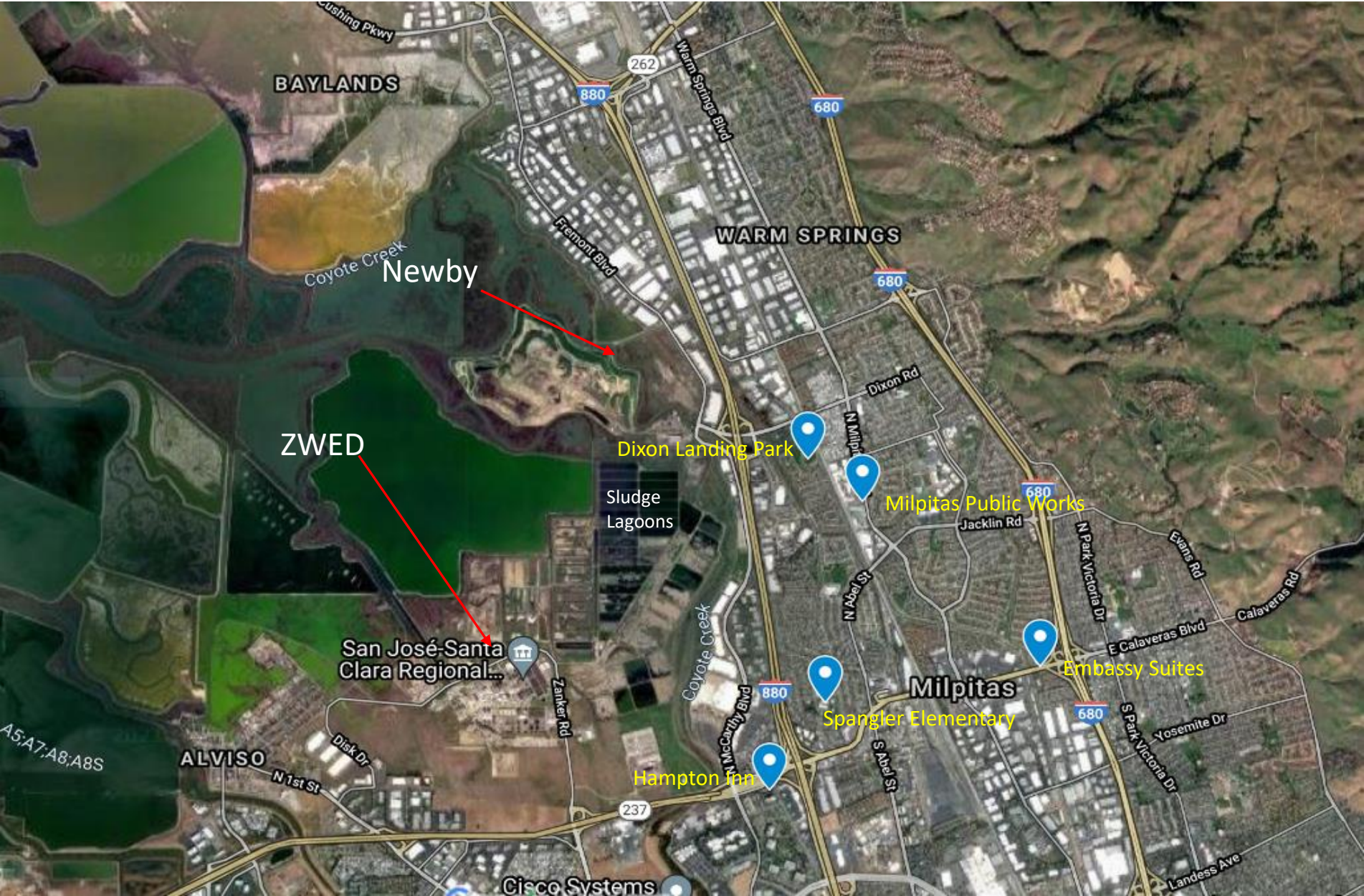
	1	2	3	4	5	6	7	8
1 M13, M14, M15, M16	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)	
2 WWTP	0	0%	0	0	0	0	0	0
3 Newby	0	0%	0	0	0	0	0	0
4 ZWED	0	0%	0	0	0	0	0	0
5 Estuary	0	0%	0	0	0	0	0	0
6 No class	3356		3	2680	51	98	524	0.50
7 Total	3356	0%	3	2680	51	98	524	

	1	2	3	4	5	6	7	8
1 M21, M22, M23, M24	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)	
2 WWTP	0	0%	0	0	0	0	0	0
3 Newby	0	0%	0	0	0	0	0	0
4 ZWED	0	0%	0	0	0	0	0	0
5 Estuary	0	0%	0	0	0	0	0	0
6 No class	3356		201	1522	1483	138	12	0.10
7 Total	3356	0%	201	1522	1483	138	12	

	1	2	3	4	5	6	7	8
1 M25, M26, M27, M28	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)	
2 WWTP	0	0%	0	0	0	0	0	0
3 Newby	0	0%	0	0	0	0	0	0
4 ZWED	0	0%	0	0	0	0	0	0
5 Estuary	0	0%	0	0	0	0	0	0
6 No class	3356		241	1698	1222	184	11	0.05
7 Total	3356	0%	241	1698	1222	184	11	

- 3356 samples from the Anthony Spangler School were compared to the 4 Source Models
- Cutoff is noted in each frame
 - 0.05 and 0.10 had the lowest number not classified
 - 2.00 was the ‘cleanest’
 - Is this the right metric?
 - What is an acceptable percentage for No Class?

Public Odor Complaint Areas - Various Plume Sampling Locations



Classification of Sources - Various Plume Samples - PCA Results

Spangler Middle	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)
WWTP	0	0%	0	0	0	0	0
Newby	0	0%	0	0	0	0	0
ZWED	0	0%	0	0	0	0	0
Estuary	0	0%	0	0	0	0	0
No class	2173		0	1286	841	46	0
Total	2173	0%	0	1286	841	46	0
			0%	59%	39%	2%	0%

Dixon Landing	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)
WWTP	0	0%	0	0	0	0	0
Newby	0	0%	0	0	0	0	0
ZWED	0	0%	0	0	0	0	0
Estuary	0	0%	0	0	0	0	0
No class	3939		0	3886	17	0	36
Total	3939	0%	0	3886	17	0	36
			0%	99%	0%	0%	1%

Embassy Suites	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)
WWTP	0	0%	0	0	0	0	0
Newby	0	0%	0	0	0	0	0
ZWED	0	0%	0	0	0	0	0
Estuary	0	0%	0	0	0	0	0
No class	16701		0	16289	151	0	261
Total	16701	0%	0	16289	151	0	261
			0%	98%	1%	0%	2%

Milpitas PW	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)
WWTP	0	0%	0	0	0	0	0
Newby	0	0%	0	0	0	0	0
ZWED	0	0%	0	0	0	0	0
Estuary	0	0%	0	0	0	0	0
No class	15736		0	14998	0	0	738
Total	15736	0%	0	14998	0	0	738
			0%	95%	0%	0%	5%

Samples from Various locations were compared to the 4 Source Models, comprised of Primary and Secondary fingerprint constituents 0.05 Cutoff

- The model determines the ratios of the components present, and then scores those ratios to identify the source

Plume Analysis Details – Hampton Inn Overnight Sampling Location – Wind Vectors



Hampton Inn Overnight Plume Monitoring

Attempts to catch plume when wind is out of Northwest

Possible Odor Sources

Hampton Inn Sampling Location

21 Hour Plume Analysis - Hampton Inn Monitoring Location

5/14-5/15/2021

5/14/21

Hampton Inn 1430-2030	Samples	WWTP	Newby	ZWED	Estuary	No class
Total	10802	0	9652	1103	28	19
		0%	89%	10%	0%	0%

5/14 - 5/15/21

Hampton Inn 2030-0230	Samples	WWTP	Newby	ZWED	Estuary	No class
Total	10803	0	9701	995	0	107
		0%	90%	9%	0%	1%

5/15/21

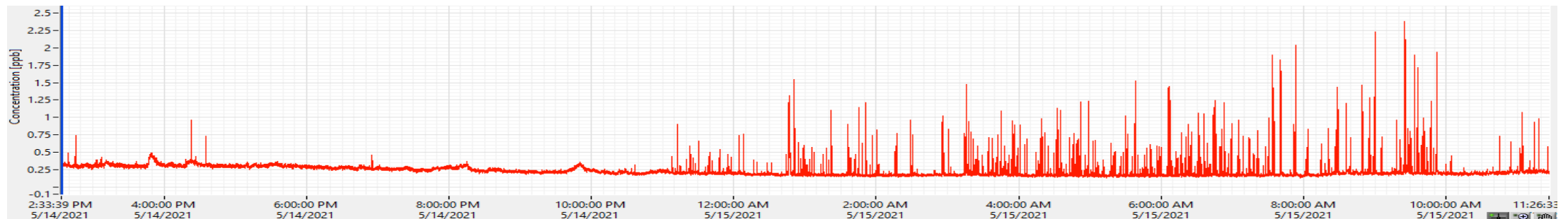
Hampton Inn 0230-0830	Samples	WWTP	Newby	ZWED	Estuary	No class
Total	10803	0	10783	6	0	14
		0%	100%	0%	0%	0%

5/15/21

Hampton Inn 0830-1130	Samples	WWTP	Newby	ZWED	Estuary	No class
Total	5180	0	5067	93	0	20
		0%	98%	2%	0%	0%

Primary Component Analysis Model Results

Individual Component Analysis
Graphical Result for Acetaldehyde



Results and Future Work....

1. These results confirm that Primary Component Analysis Modeling is a valid technique for classification of odor plumes present in the South Bay Area
2. Refinement of Preprocessing Methods and Models with the goal to remove known and unknown bias with the end goal to provide a robust model for the prediction of the odor source
3. Non-Odororous plumes captured during this event does NOT identify the facility from which odor complaints are arising. Capturing plumes while they are odorous will identify which facility(ies) the odors are originating. Sampling during odor complaints are warranted