Exploring the Latest Advancements in Air Measurement Technologies for Odor Allocation Using Deep Data Collection

MONTROSE ENVIRONMENTAL

SARTORIUS

Dr. Peter G. Zemek
Senior Vice President, Emerging Technology/R&D

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Montrose Continuum of Services

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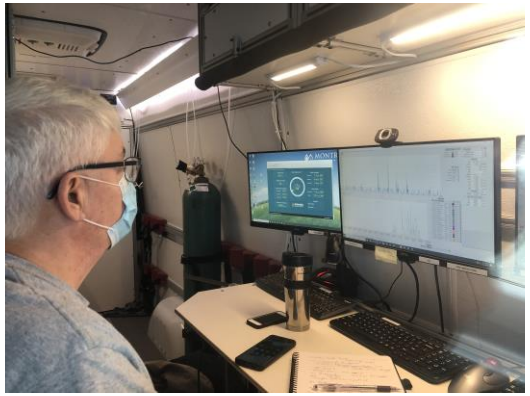
Mobile PTR-TOF-MS Platform

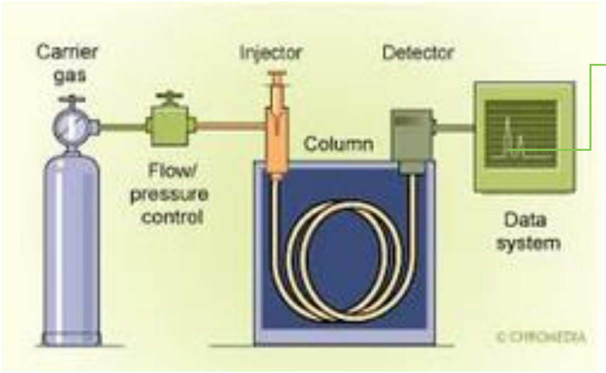
Proton Transfer Reaction Time of Flight Mass Spectrometry – Mobile Real Time Analysis

- BAAQMD Odor Study - Odor Plume 330+ compounds
  - Amines - N
  - Thiols/TRS – S
  - Alcohols – COOH/OH
  - Carbonyls-O/=O (aldehydes/ketones)
- Multivariate Data Analysis
  - Principal Component Analysis

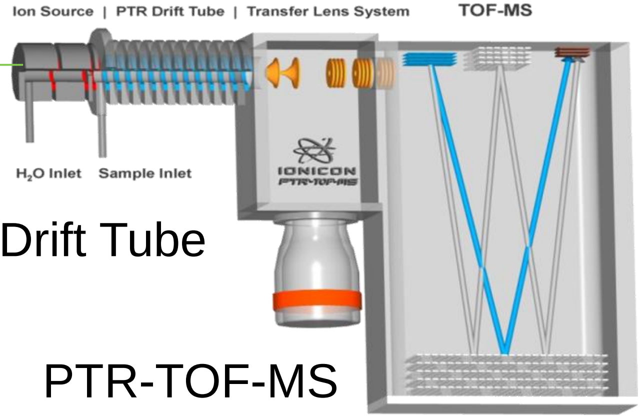


Advantages of PTR-MS

- Mobile Real Time
- Couple to GC for Compliance EPA M18
- Absolute Time and Space
- Real-time, continuous results (1/sec)
- No sample or reagent preparation
- New Reagents all the time
- Single unit can handle multiple sampling ports
- Mobile Platforms and PTR sensitivities



Gas Chromatograph



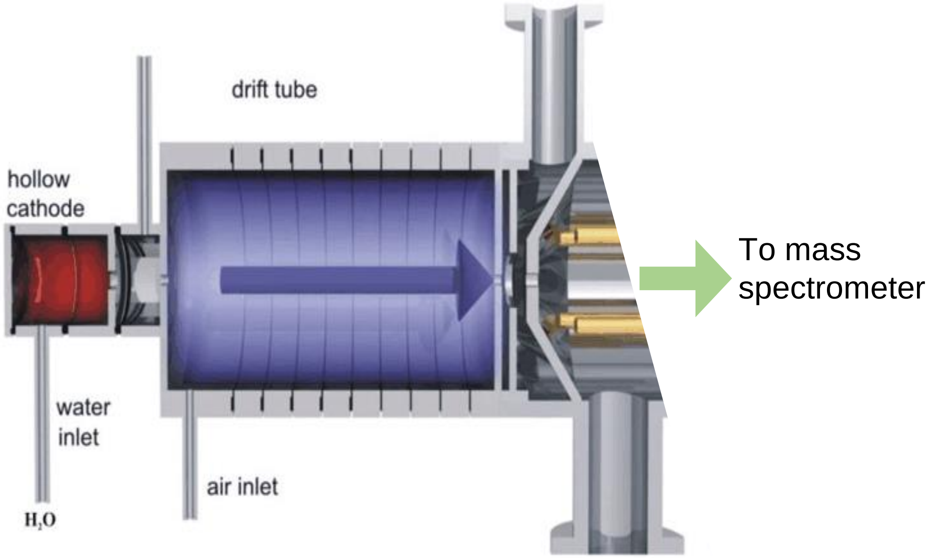
Drift Tube

PTR-TOF-MS

MONTROSE AIR QUALITY SERVICES

Proton Transfer Reaction Time of Flight Mass Spectrometry Mobile Platform (PTR-TOF MS)

- Proton Transfer Reaction Mass Spectrometry for Real Time VOCs and Inorganics
- FTIR Monitoring for Primary Pollutants
- OE-FTIR Analysis of low level OHAPs



Typical Reagent Gases:

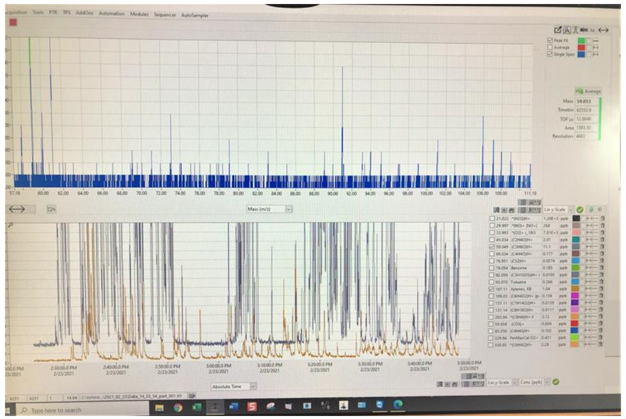
$H_3O^+ + R \rightarrow RH^+ + H_2O$

$O_2^+ + R \rightarrow R^+ + O_2$

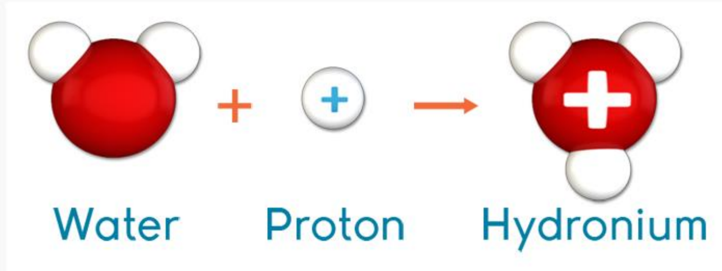
$NO^+ + R \rightarrow R^+ + NO$

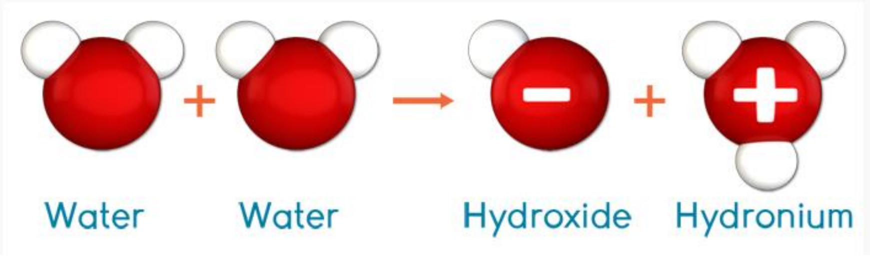
Proton Transfer Reaction Time of Flight Mass Spectrometry Mobile Platform (PTR-TOF MS)

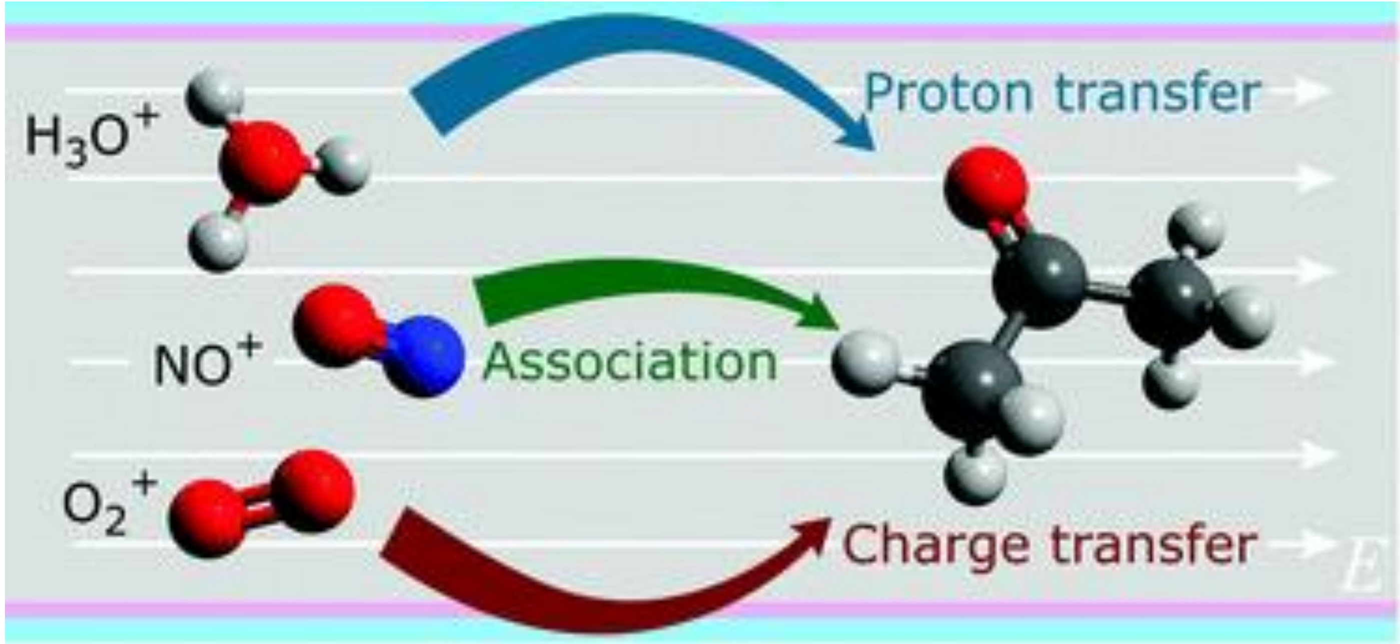
- Optional GC Interface for EPA M18 with pptv MDL for isomers
- Weather Station & GPS
- Real Time 3-D Concentration vs Location Profiling



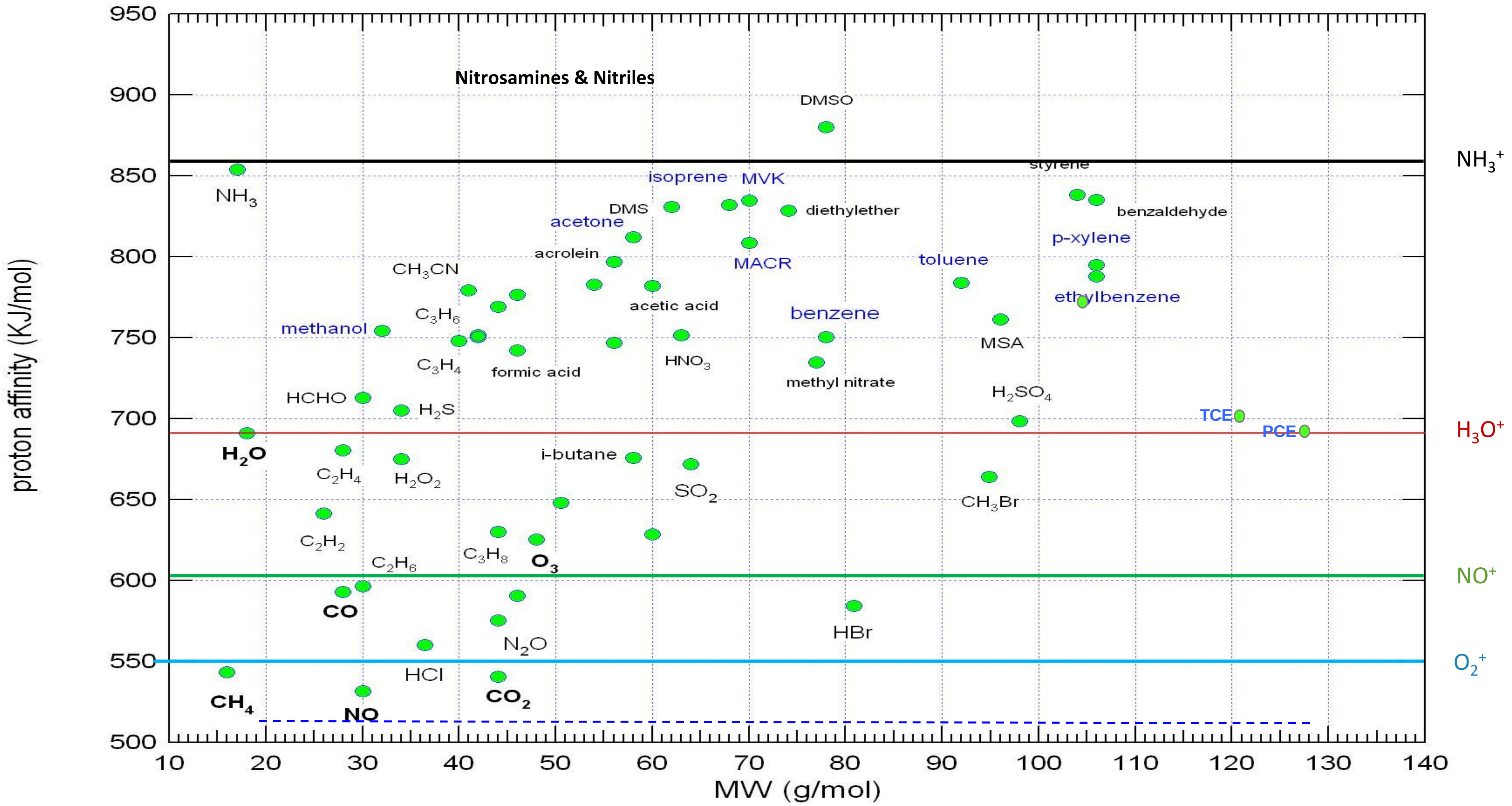
Reagents and Molecular Interactions







Speciation with Selective Ionization Reagents



Anything above the green line with NO^+

Anything above the blue line with O_2^+

Anything above the red line with H_3O^+

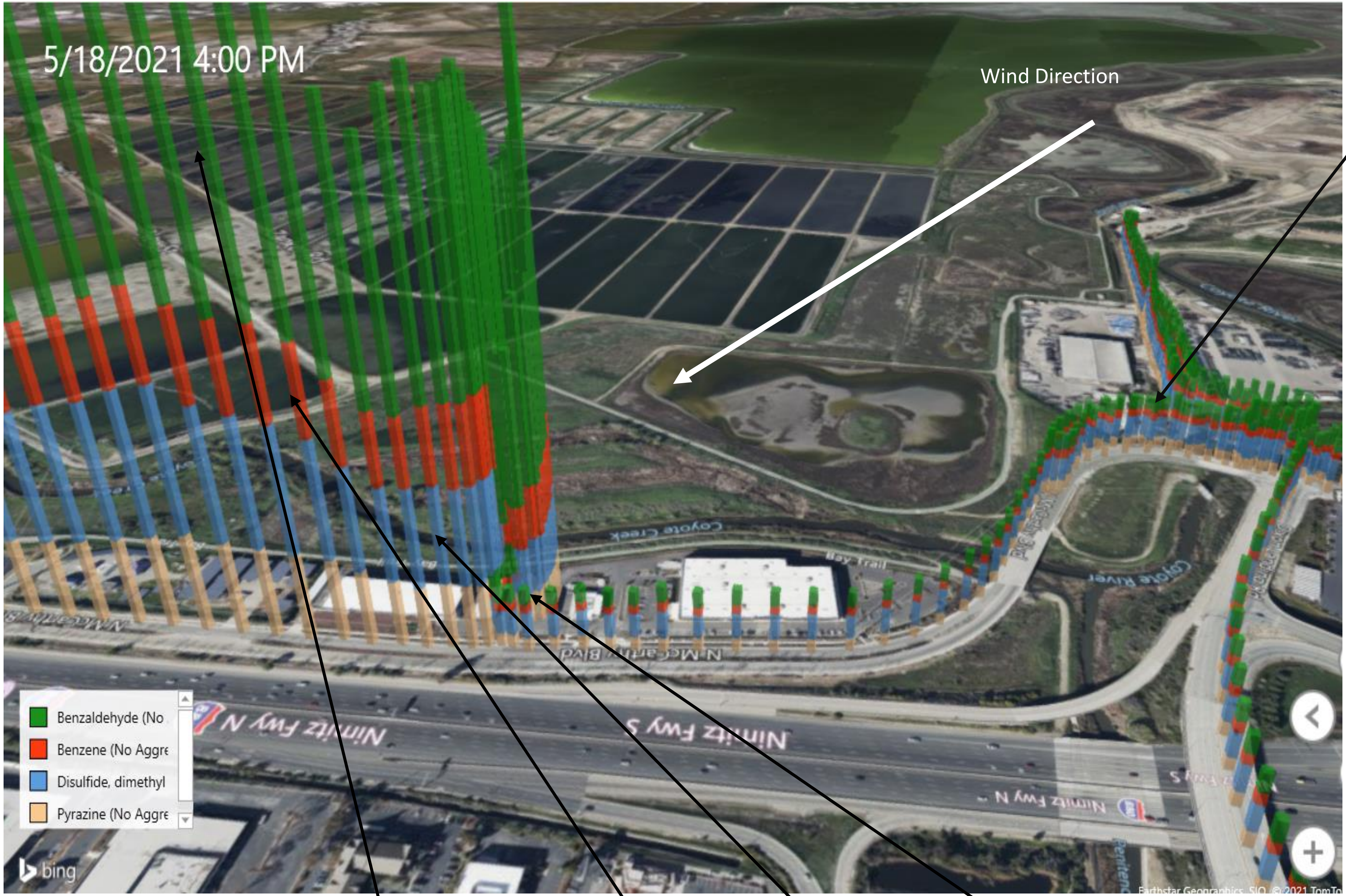
Anything above the black line with NH_3^+


5/18/2021 3:00 PM
Nimitz Fwy N
Nimitz Fwy S
N McCarthy Blvd
Bay Trail
Coyote Creek
Coyote River
Zanker Rd
Penitencia Creek Lower
Berryessa Creek
N Abel St
N Milpitas Blvd
Jacklin Rd
Fairmeadow Way
Edgewater Dr
Folsom Circle
Superior Rd
Ontario Rd
Erie Circle
Coventry Way
Hanson Ct
Summerwind Way
Milmont Dr
Sunnyhills Ave
Railroad Ct
Railroad Ave
Winsor St
N Main St
Cadillac Ct
Fairview Way
Abbott Ave
Heath St
Smithwood St
Silvera St
Easter Ave
Walnut Dr
Elm Ave
Willow Ave
Chestnut Ave
Maple Ave
Coyote St
Vasona St
Calero St
Berryessa St
Oregon Way
Sudbury Dr
Berrendo Dr
Kovanda Way
Belbrook Way
Benzaldehyde (No
Benzene (No Aggre
Disulfide, dimethyl
Pyrazine (No Aggre

Ambient Concentrations:

Benzaldehyde 75 ppt
Benzene 60 ppt
DMDS 102 ppt
Pyrazine 87 ppt

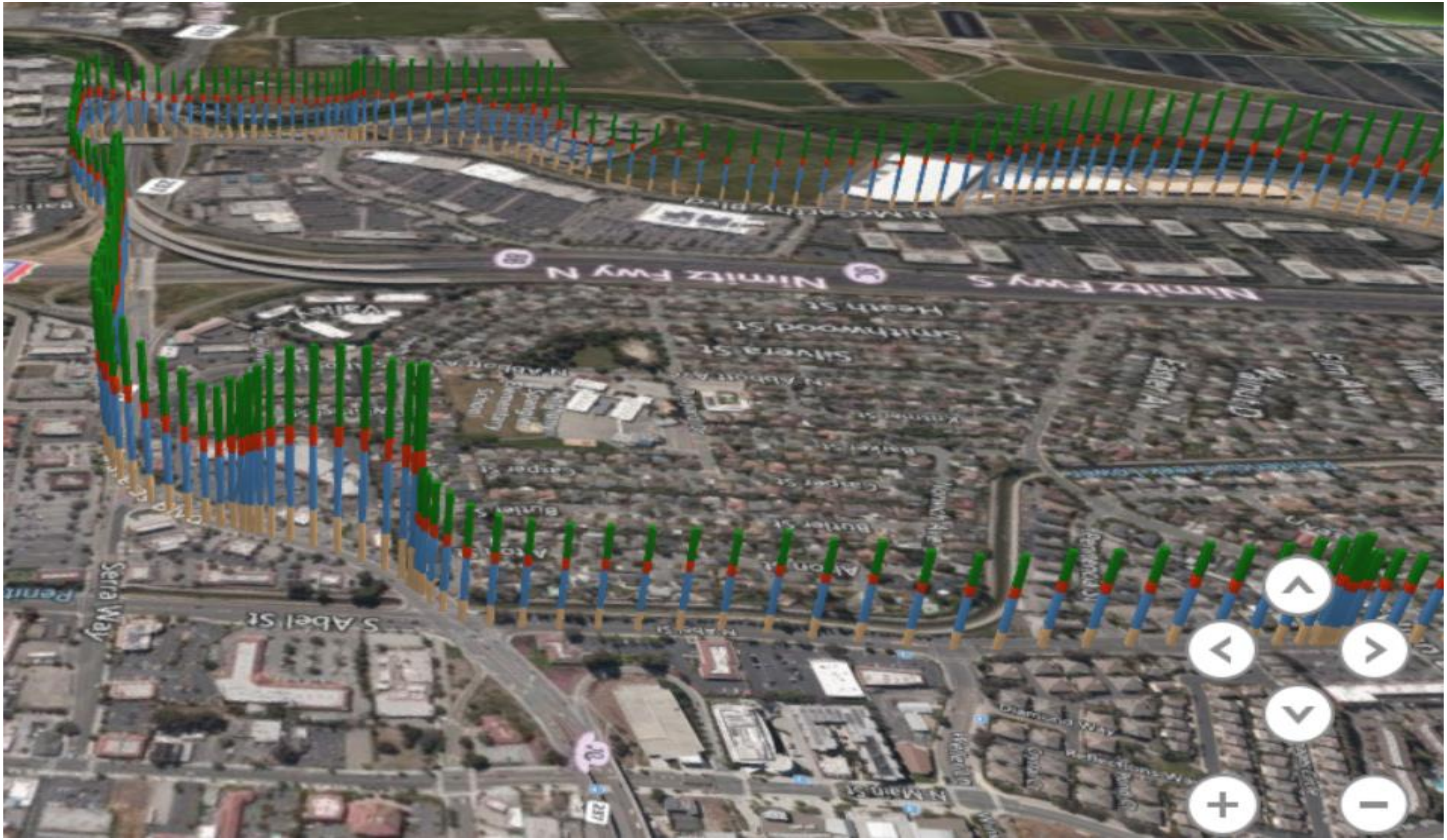
North of sources – very low background readings



Interim Concentrations:

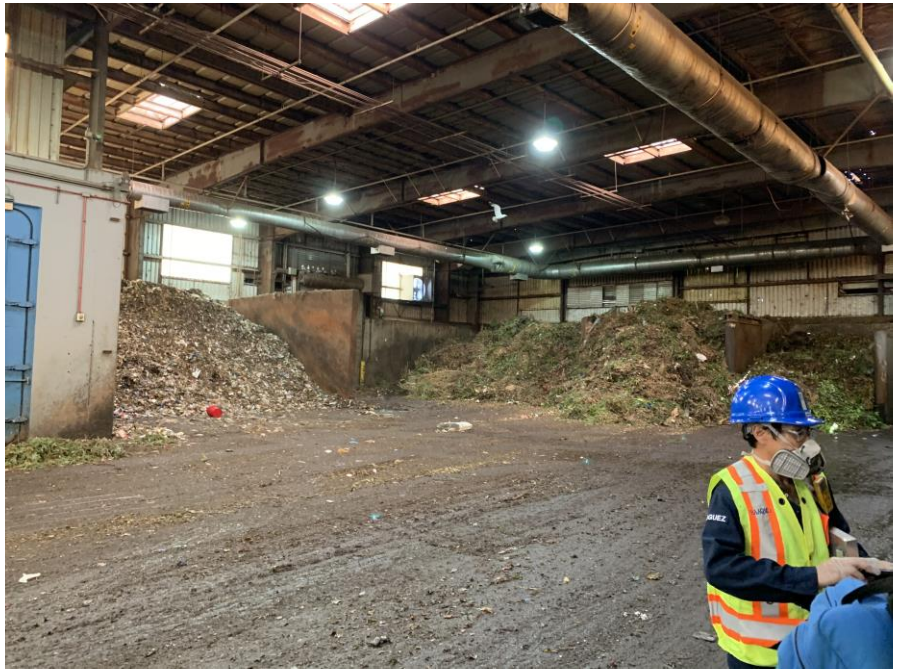
Benzaldehyde 106 ppt
Benzene 62 ppt
DMDS 151 ppt
Pyrazine 116 ppt

Downwind Concentrations: Benzaldehyde 1750 ppt Benzene 480 ppt DMDS 816 ppt Pyrazine 589 ppt



West Calaveras Blvd 1.3 miles downwind

Pictures of Possible Sources



Unknown Odor Source Outfall Pipe During Low Tide

What is Multivariate Analysis?

Deep Data- 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)

What is Multivariate Analysis?

Applications for Odor Plume Analysis

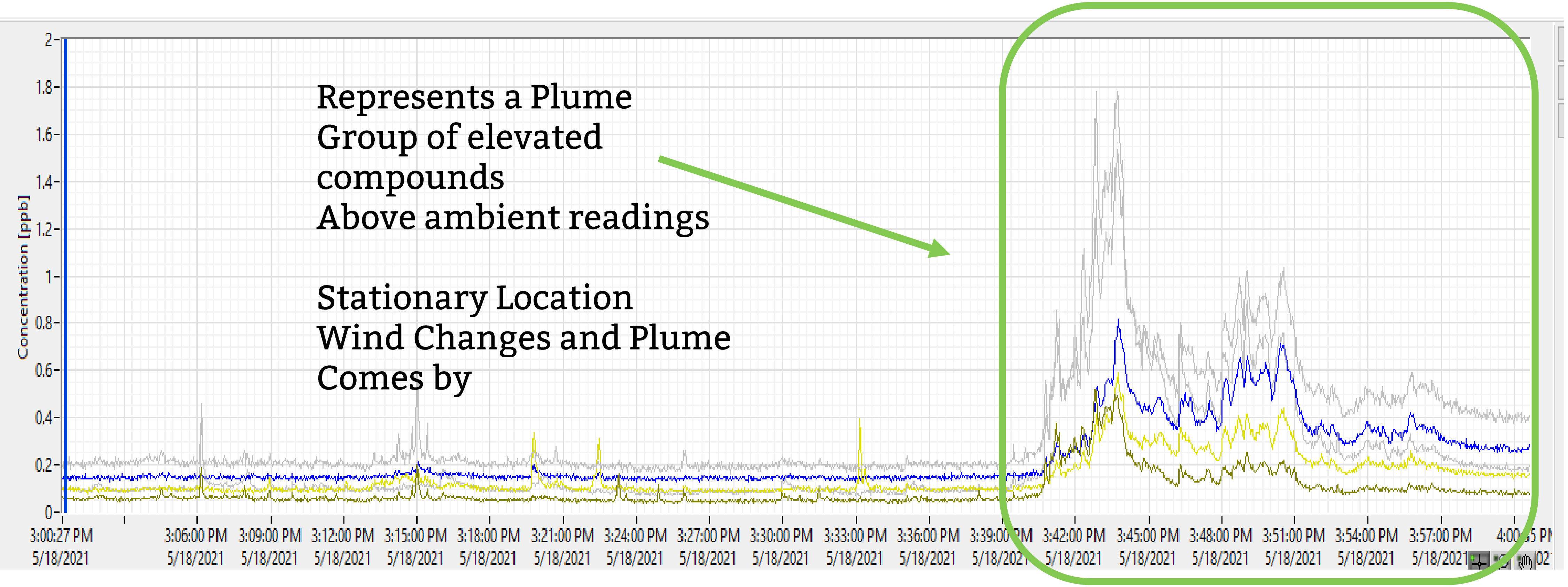
1. Fingerprint each facility and source in facility – generate model to determine if each is unique – develop PCA model

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

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

These individual compounds are used in the modeling to determine origin of plume
Example showing only 4 compounds



Fingerprint Models and Sample Bag Analysis

15 source bags were measured and identified to be from one of 4 sources

- WWTP – 110 MGD Wastewater Treatment Plant
- MSW landfill
- Wet Fermentation Food Compost
- Estuary

Fingerprint Models and Sample Bag Analysis

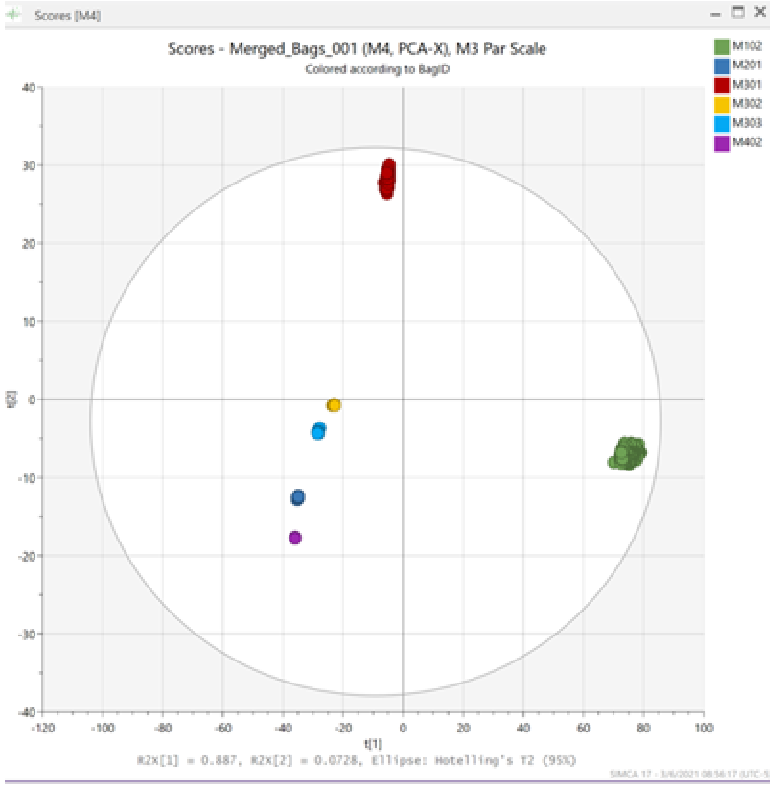
Observations from the Anthony Spangler Middle School were analyzed as the initial test case to start model development

- 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

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

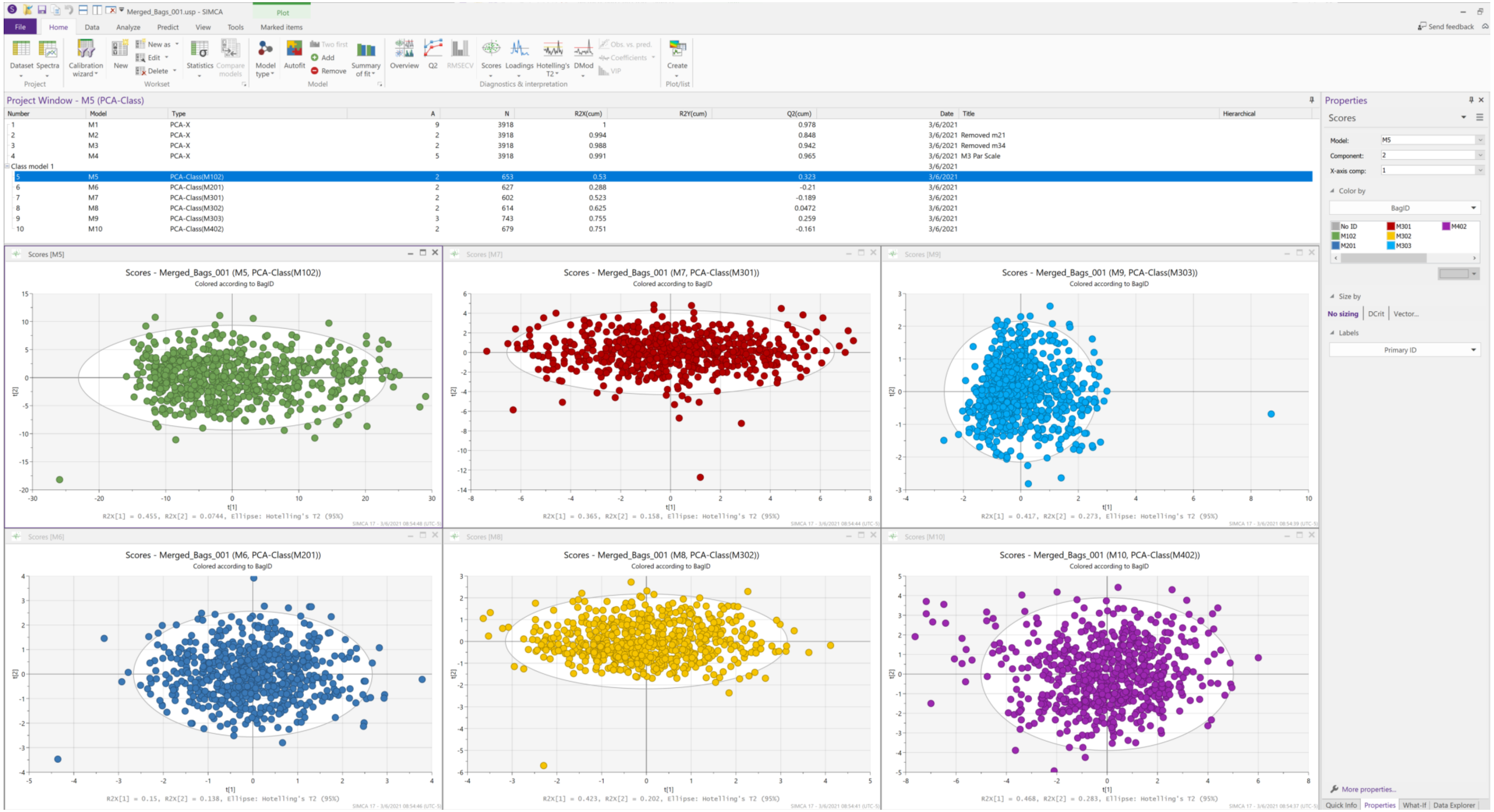


7-15 Dimensions examined

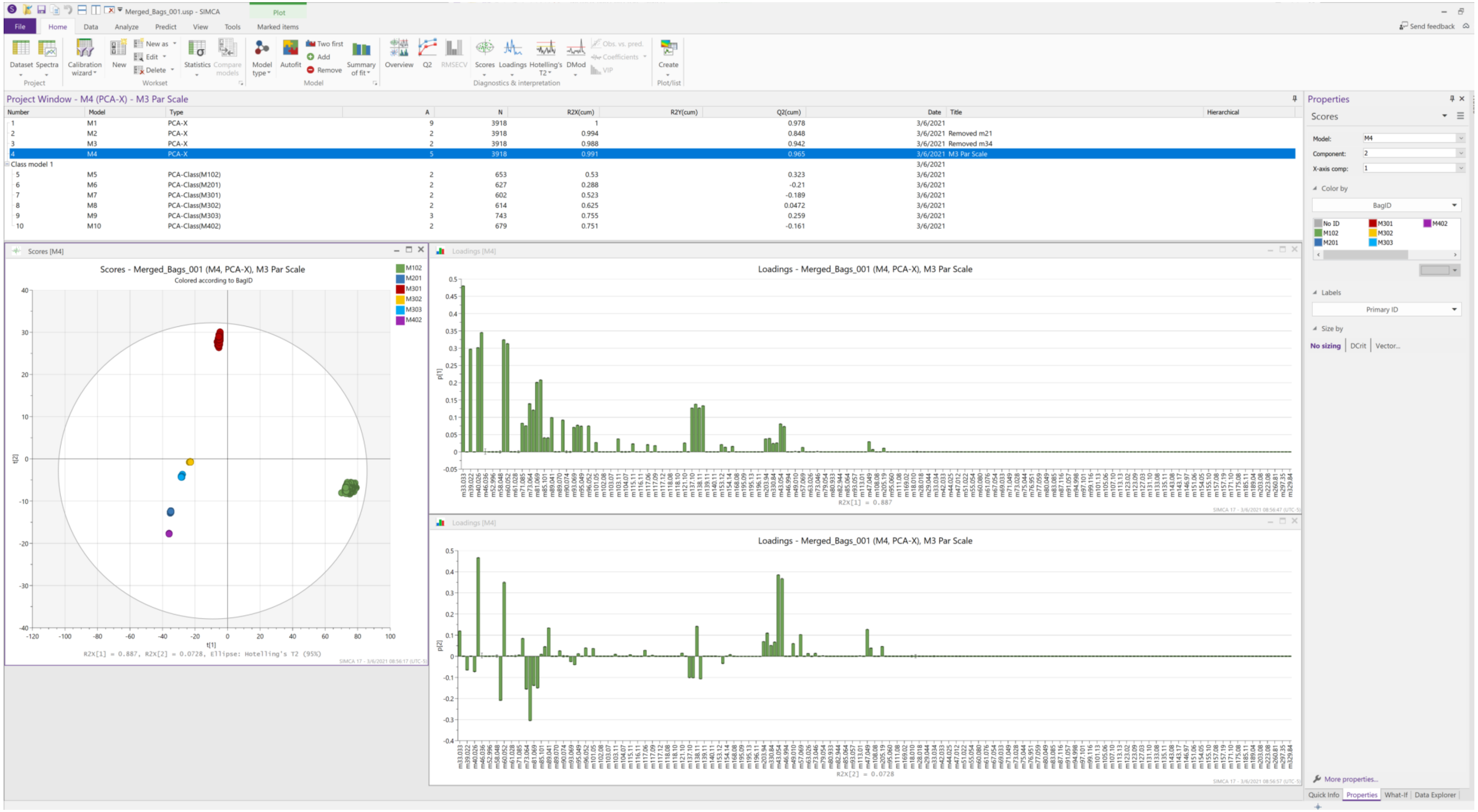
Collective Bag Analysis

- 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

PCA Results of Individual Bag Analysis Showing Unique Compound Ratios/Individuals



PCA -How the Model Works - Unique Sector Analysis Right to Left and Top to Bottom



Initial Classification by Source Principle Component Analysis

- 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?

Misclassification Table for Model 9, 10, 11, 12

2.00

	1							8
1	M9, M10, M11, M12			Facility A	Facility B	Facility C	Facility D	ass (PModX+ <= 0)
2	Facility A	0	0%	0	0	0	0	0
3	Facility B	0	0%	0	0	0	0	0
4	Facility C	0	0%	0	0	0	0	0
5	Facility D	0	0%	0	0	0	0	0
6	No class	3356		0	1656	1049	0	651
7	Total	3356	0%	0	1656	1049	0	651

Misclassification Table for Model 17, 18, 19, 20

0.20

	1							8
1	M17, M18, M19, M20			Facility A	Facility B	Facility C	Facility D	ass (PModX+ <= 0)
2	Facility A	0	0%	0	0	0	0	0
3	Facility B	0	0%	0	0	0	0	0
4	Facility C	0	0%	0	0	0	0	0
5	Facility D	0	0%	0	0	0	0	0
6	No class	3356		2	2234	687	81	352
7	Total	3356	0%	2	2234	687	81	352

Misclassification Table for Model 13, 14, 15, 16

0.50

	1							8
1	M13, M14, M15, M16			Facility A	Facility B	Facility C	Facility D	ass (PModX+ <= 0)
2	Facility A	0	0%	0	0	0	0	0
3	Facility B	0	0%	0	0	0	0	0
4	Facility C	0	0%	0	0	0	0	0
5	Facility D	0	0%	0	0	0	0	0
6	No class	3356		3	2680	51	98	524
7	Total	3356	0%	3	2680	51	98	524

Misclassification Table for Model 21, 22, 23, 24

0.10

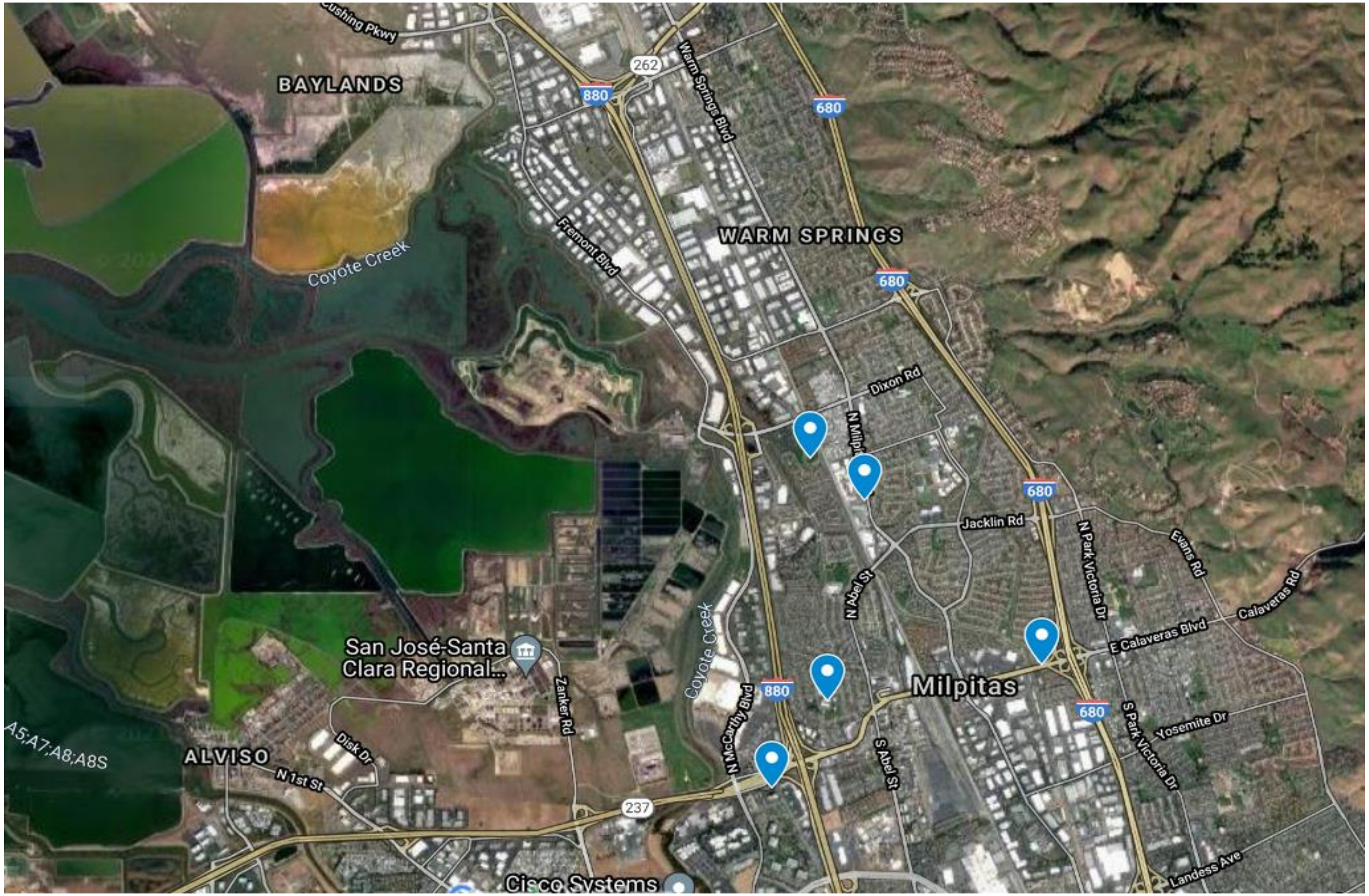
	1							8
1	M21, M22, M23, M24			Facility A	Facility B	Facility C	Facility D	ass (PModX+ <= 0)
2	Facility A	0	0%	0	0	0	0	0
3	Facility B	0	0%	0	0	0	0	0
4	Facility C	0	0%	0	0	0	0	0
5	Facility D	0	0%	0	0	0	0	0
6	No class	3356		201	1522	1483	138	12
7	Total	3356	0%	201	1522	1483	138	12

Misclassification Table for Model 25, 26, 27, 28

0.05

	1							8
1	M25, M26, M27, M28			Facility A	Facility B	Facility C	Facility D	ass (PModX+ <= 0)
2	Facility A	0	0%	0	0	0	0	0
3	Facility B	0	0%	0	0	0	0	0
4	Facility C	0	0%	0	0	0	0	0
5	Facility D	0	0%	0	0	0	0	0
6	No class	3356		241	1698	1222	184	11
7	Total	3356	0%	241	1698	1222	184	11

Public Odor Complaint Areas - Various Plume Sampling Locations



Classification of Sources - Various Plume Samples - PCA Results

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

Spangler Middle	Members	Correct	WWTP	Newby	ZWED	Estuary	No class (PModX+ <= 0)
Facility A	0	0%	0	0	0	0	0
Facility B	0	0%	0	0	0	0	0
Facility C	0	0%	0	0	0	0	0
Facility D	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)
Facility A	0	0%	0	0	0	0	0
Facility B	0	0%	0	0	0	0	0
Facility C	0	0%	0	0	0	0	0
Facility D	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)
Facility A	0	0%	0	0	0	0	0
Facility B	0	0%	0	0	0	0	0
Facility C	0	0%	0	0	0	0	0
Facility D	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)
Facility A	0	0%	0	0	0	0	0
Facility B	0	0%	0	0	0	0	0
Facility C	0	0%	0	0	0	0	0
Facility D	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%

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

Primary Component Analysis Model Results: **5/14-5/15/2021**

5/14/21

Hampton Inn 1430-2030	Samples	Facility A	Facility B	Facility C	Facility D	No class
Total	10802	0	9652	1103	28	19
		0%	89%	10%	0%	0%

5/14 – 5/15/21

Hampton Inn 2030-0230	Samples	Facility A	Facility B	Facility C	Facility D	No class
Total	10803	0	9701	995	0	107
		0%	90%	9%	0%	1%

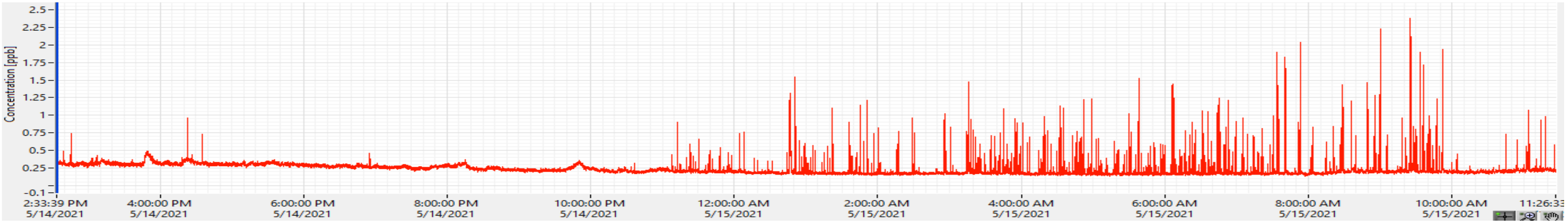
5/15/21

Hampton Inn 0230-0830	Samples	Facility A	Facility B	Facility C	Facility D	No class
Total	10803	0	10783	6	0	14
		0%	100%	0%	0%	0%

5/15/21

Hampton Inn 0830-1130	Samples	Facility A	Facility B	Facility C	Facility D	No class
Total	5180	0	5067	93	0	20
		0%	98%	2%	0%	0%

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-Odorous plumes captured during this event does <u>NOT</u> identify the facility from which odor complaints are arising. Capturing plumes while they are odorous <u>will</u> identify which facility(ies) the odors are originating. Sampling during odor complaints are warranted

Recommendations – Montrose Options

- Model is Developed (initial data inputs)
  - Can collect Summa Canisters or Mylar/Tedlar Bags (10L) during odor complaints for shipping to Houston for PTR analysis
- Summer Months - Secure PTR Van to come to site of odor complaints over a period of time to capture odorous plumes for identification by PCA and/or MET triangulation Software "Bloodhound" (May make model more robust with more fenceline fingerprinting – diff compounds in Summer Months?)
- Lease PTR Instrument in a stationary location near most complaints and set up MET station to pinpoint source (Likely take 2-3 months)
- Purchase PTR mobile Platform (~$850K) to respond to odor complaints and other applications

Questions?

Peter G. Zemek, Ph.D.
Senior Vice President, Emerging Technology
pzemek@montrose-env.com

