FIREX-AQ Chem Otter Science Meeting

Agenda:

1. Important information

Gas

2. Andy Weinheimer: Data update
3. Mike Robinson: NO_x, O3, MCE, and box modeling
4. Paul Van Rooy: GC × GC analysis of VOCs
5. Zach Decker: BBVOCs and $ClNO_2$

Aerosol

6. Ale Franchin and Ann Middlebrook: Aerosol oxidation state and optical properties
7. Rebecca Washenfelder: WSOC concentration and absorption in downwind transects
8. Jay Tomlin and Felipe Rivera: SEM analysis for 8/28 Cow Fire

Other

9. Zach Decker: Go Pro
10. Mike Robinson: Met data

1/31/2020

Where to find flight and fire information?

Flight summary:
https://docs.google.com/spreadsheets/d/1puikxaDmMgNoscQ_-I1vTQKAr1jNtZUYtiOtpqJTifU/edit?usp=sharing

Flight Num	Flight Leg	Start Time (UTC)	Stop Time (UTC)	Duration	Time of Day	Start Airport	Start Code	Stop Airport	Stop Code	Fire Name	Fuel Type	Flight Scientist	Instrument Scientist	Other Details
1	20190729	07/29/2019 17:20:00	07/29/2019 19:25:00	2:05:00	Afternoon	Rocky Mountain Metro	BJC	Rocky Mountain Metr	BJC	Small ag fire	Grass fire	Mike Robinson	Ale Franchin	
2	20190803	08/03/2019 22:08:00	08/04/2019 00:28:00	2:20:00	Afternoon	Boise Airport	BOI	Boise Airport	BOI	None	N/A	Mike Robinson	Rebecca Washenfelde	Calibration of met probes
3	20190805_L1	08/05/2019 21:49:00	08/05/2019 22:33:00	0:44:00	Afternoon	Boise Airport	BOI	Twin Falls Airport	TWF	None (Transit)	N/A	Ale Franchin	Geoff Tyndall	
4	20190805_L2	08/05/2019 23:43:00	08/06/2019 01:44:00	2:01:00	Afternoon	Twin Falls Airport	TWF	Twin Falls Airport	TWF	Goose		Ale Franchin	Geoff Tyndall	
5	20190805_L3	08/06/2019 02:37:00	08/06/2019 03:22:00	0:45:00	Sunset	Twin Falls Airport	TWF	Boise Airport	BOI	None (Transit)	N/A	Ale Franchin	Geoff Tyndall	

RA data status:
https://docs.google.com/spreadsheets/d/1ix1jEWzFsehuB1Ad5lAv-i3uZwD9DZS2olF6nCaj4Cs/edit?usp=sharing

RA and R0 data download:
https://esrl.noaa.gov/csd/groups/csd7/measurements/2019firex-aq/TwinOtter/DataDownload/
Username: firexaq; Password: sm0k3y!

Fire characteristics by Amber Soja and Emily Gargulinski:
https://docs.google.com/spreadsheets/d/1_Jfc3GP9taF8IvP82VHplX1lgsUvvQV7P9CTxrJNRV8/edit#gid=971771572

How to submit final data?

1. The deadline for final data submission for the Chem Twin Otter is February 14, 2020. Please contact Ken Aikin (kenneth.c.aikin@noaa.gov) if you cannot make this deadline.

2. Format for final data:
   - Follow the format of the R0 aircraft met data in submitting a single data file for each flight day rather than each flight leg.
   - Use the time wave provided in the aircraft data for expansion of your data.
   - Fill in the gaps between flight legs with NaNs.
   - We recommend not posting data from the tarmac, so it is best if the valid data from your measurements starts and stops at approximately (or exactly) the same time as the valid data aircraft met data.

3. Submit final data:
   - Log into ftp.al.noaa.gov. Username: firex_aq_otter; Password: sm0k3y!
   - Upload your ICARTT files into the IncomingData folder.
   - Ken will add these files to the data archive.
   - Data will be available at:
     https://esrl.noaa.gov/csd/groups/csd7/measurements/2019firex-aq/TwinOtter/DataDownload/
     Username: firexaq; Password: sm0k3y!

Shared metadata?

Shared, posted “metadata” products would:

- Save time and prevent duplicated efforts among scientists.
- Allow for more consistency between our analyses.

Possibilities:

1. Flag for smoke based on CO and particle mass (e.g. 1 for smoke, -999 otherwise)
2. Transect number (T0, T1, T2, etc)
3. Age of smoke calculated from fire location and instantaneous wind speed
4. Time of smoke emission
5. Location of smoke emission
6. Integrated sunlight exposure, based on smoke age and solar zenith angle.
7. Fire characteristics from Amber and Emily
8. Other suggestions?

Ann Middlebrook will contact Christoph Knote and Chris Holmes to ask about this.
Ken Aikin could be asked to assemble the metadata into posted ICARTT files.

What's next?

1. Complete and post R0 data by February 14, 2020.

2. We will have Chem Otter science telecons in January (today!), February, and possibly March.

3. During February and March: Coordination of Chem Otter scientific analysis and topics.

4. Science meeting for all FIREX-AQ participants in Langley, Virginia during March 17-20, 2020.
   - To register, email your name and group to Caitlin Murphy (caitlin.murphy@nasa.gov) and Bernie Luna (bernadette.luna@nasa.gov).

   - NASA will provide travel support for PI+1 attendance for all NASA-funded teams. More than 2 people per group are welcome if you have travel funds and a presentation for each attendee.

   - Presentations will be organized by topic, rather than by platform.

   - Abstracts are due February 21

5. Today: Updates on data and results from each group.

Twin Otter Gas-Phase Instruments

Instrument	Species Measured	Investigators	Institution
Chemiluminescence	NO, NO_2, O_3	Andy Weinheimer, Denise Montzka, Geoff Tyndall, Frank Flocke	NCAR
jNO_2	NO_2 photolysis rate	Mike Robinson	NOAA CSD
Tenax cartridge sampler	Speciated VOCs	Kelley Barsanti, Lindsey Hatch, Avi Lavi, Paul Van Rooy	UC Riverside
I- TOF CIMS	Acids (HNO_3, HONO, Organics), acid gases (N_2O_5, $ClNO_2$), Oxygenated organics, Organic nitrates, Halogens	Joel Thornton, Brett Palm, Carley Fredrickson, Zach Decker	University of Washington NOAA
Picarro CRDS	CO, CO_2, CH_4, H_2O	Colm Sweeney, Mike Robinson	NOAA GMD

NCAR NO, NO_2, O_3

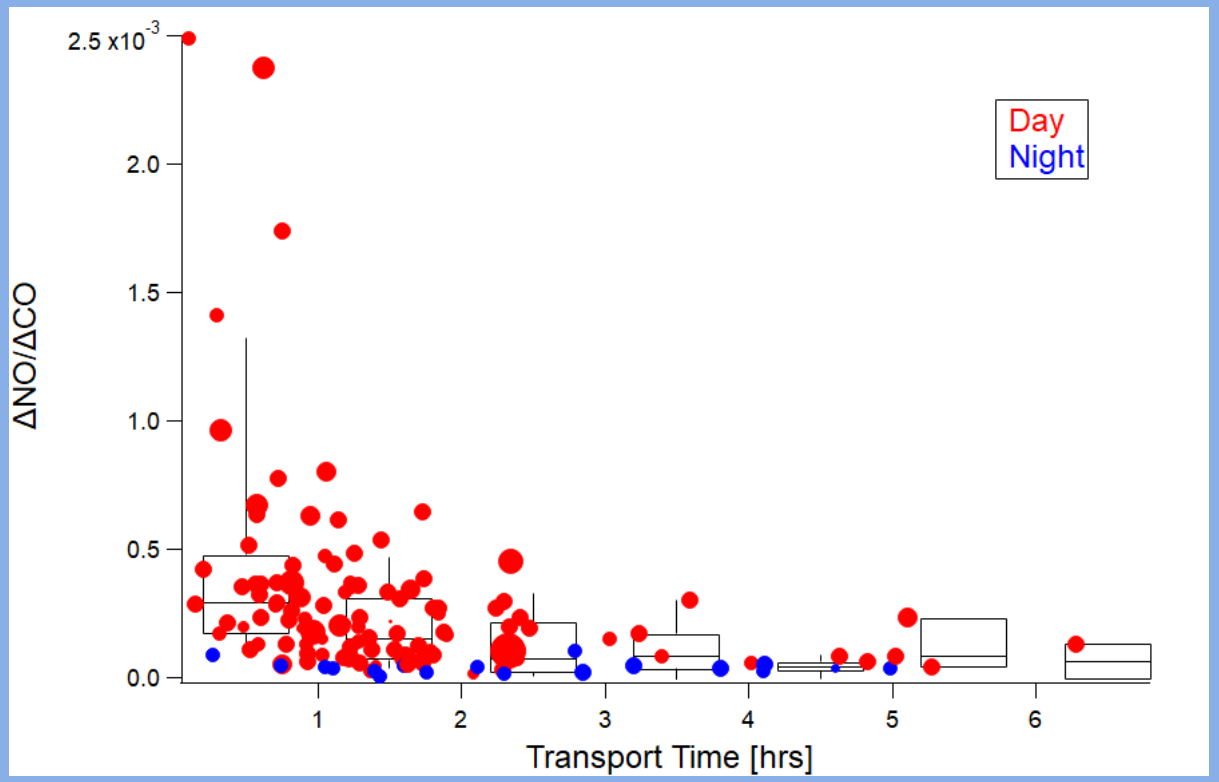
- Reduction is ongoing; not far to go. Plan to make the Feb. 14 deadline.
- Our clock was 30-40 seconds fast throughout, and by an increasing amount. Still need to adjust our time base to synchronize in a manner compatible with others.
- No initial results to present at this time.
- What is plan for merges? NOAA will do?

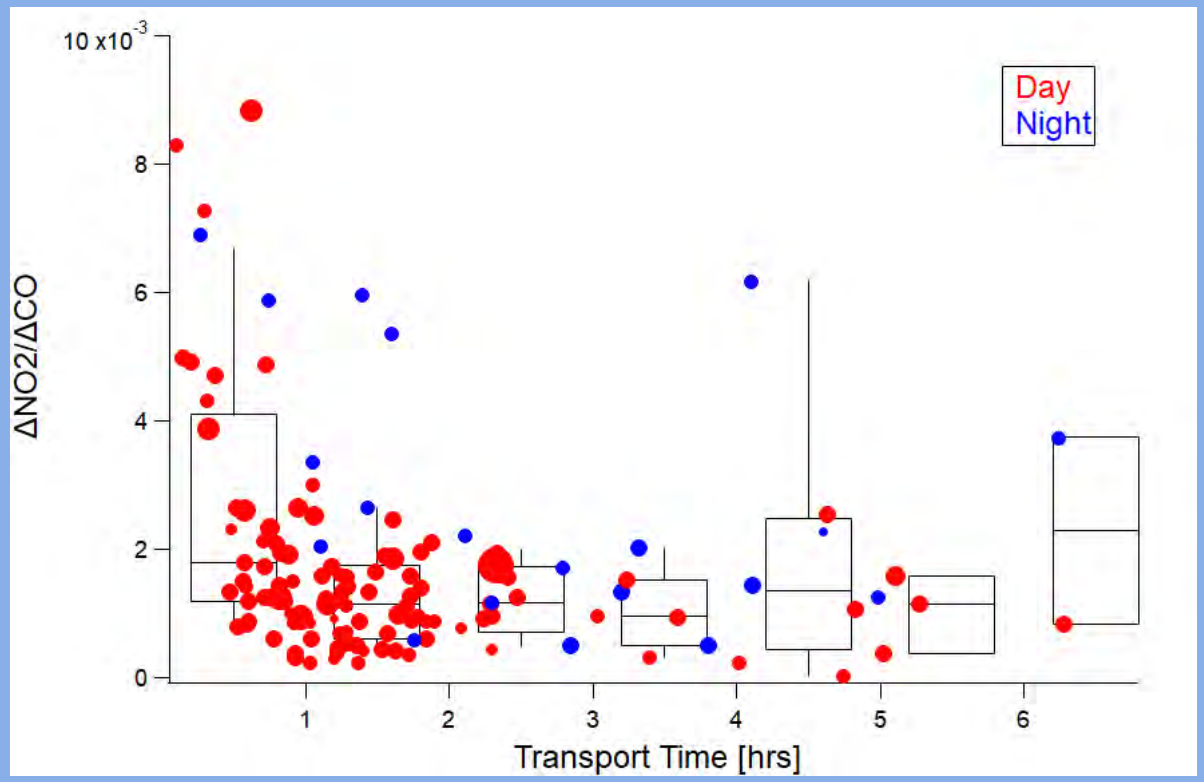
Andy Weinheimer

Jhead team update

Mike Robinson

NOx Enhancement Ratios – Campaign wide

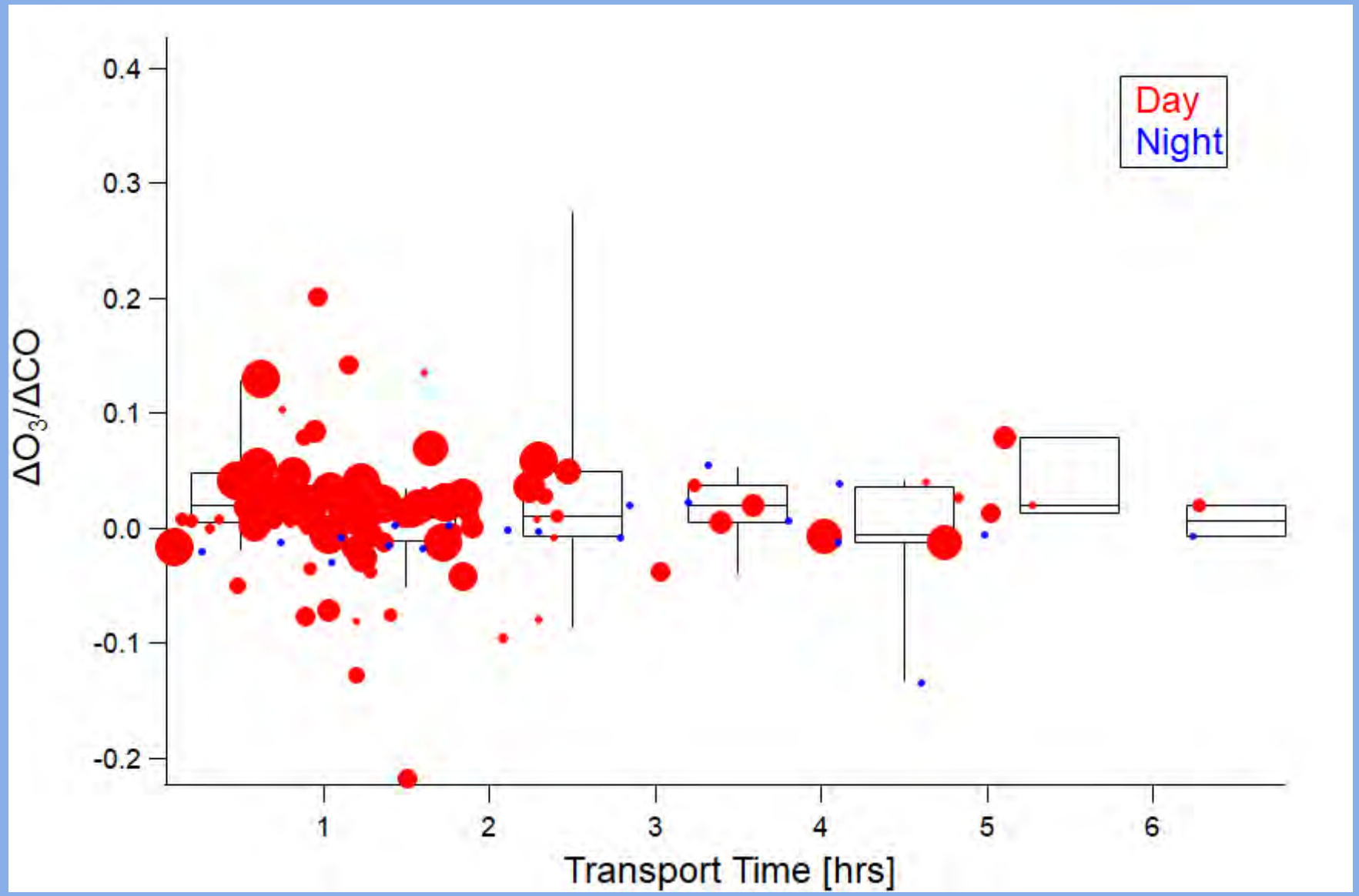




Sized by ozone enhancement ratio

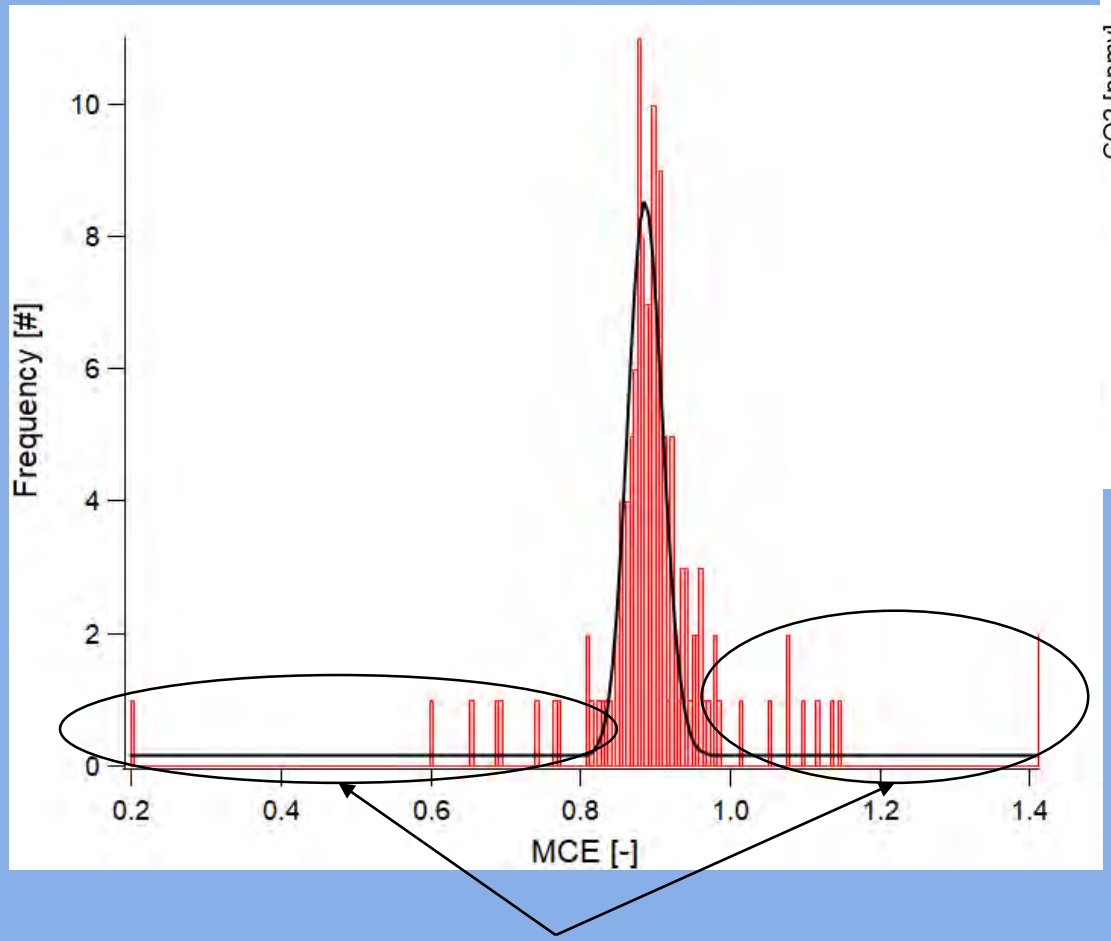
Mike Robinson

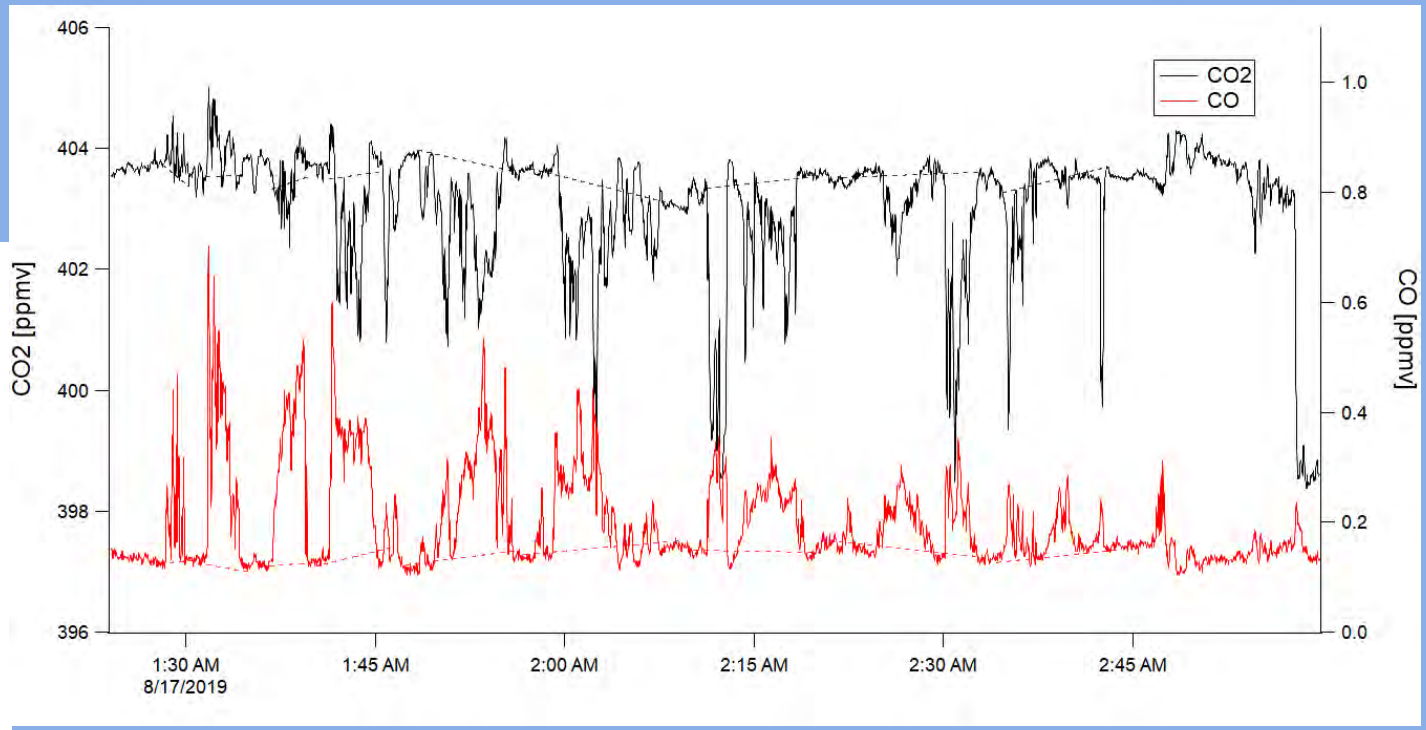
O3 Enhancement Ratios – Campaign wide

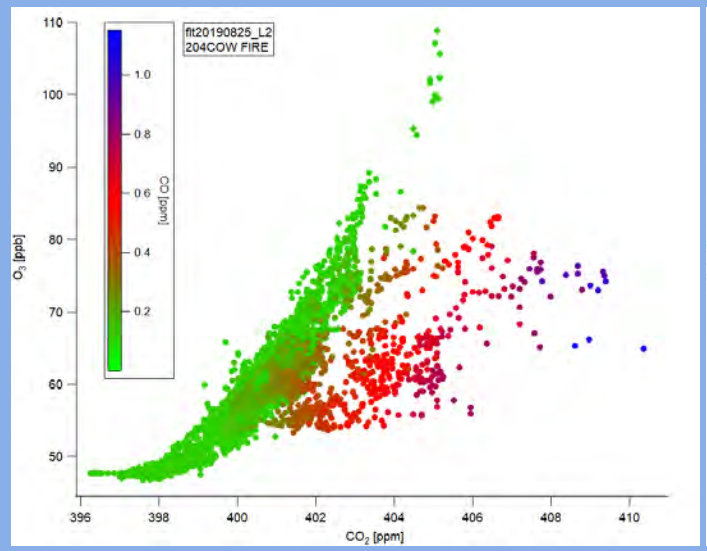


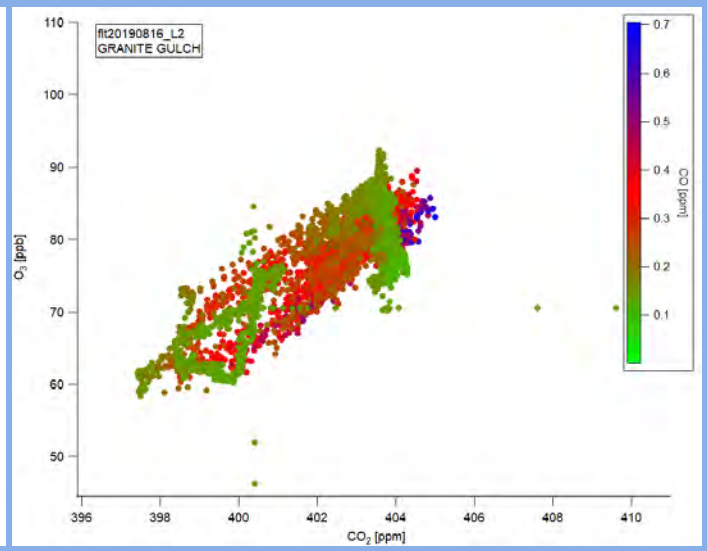
Mike Robinson

Issues w/MCE @GG (8/16 – 8/17)





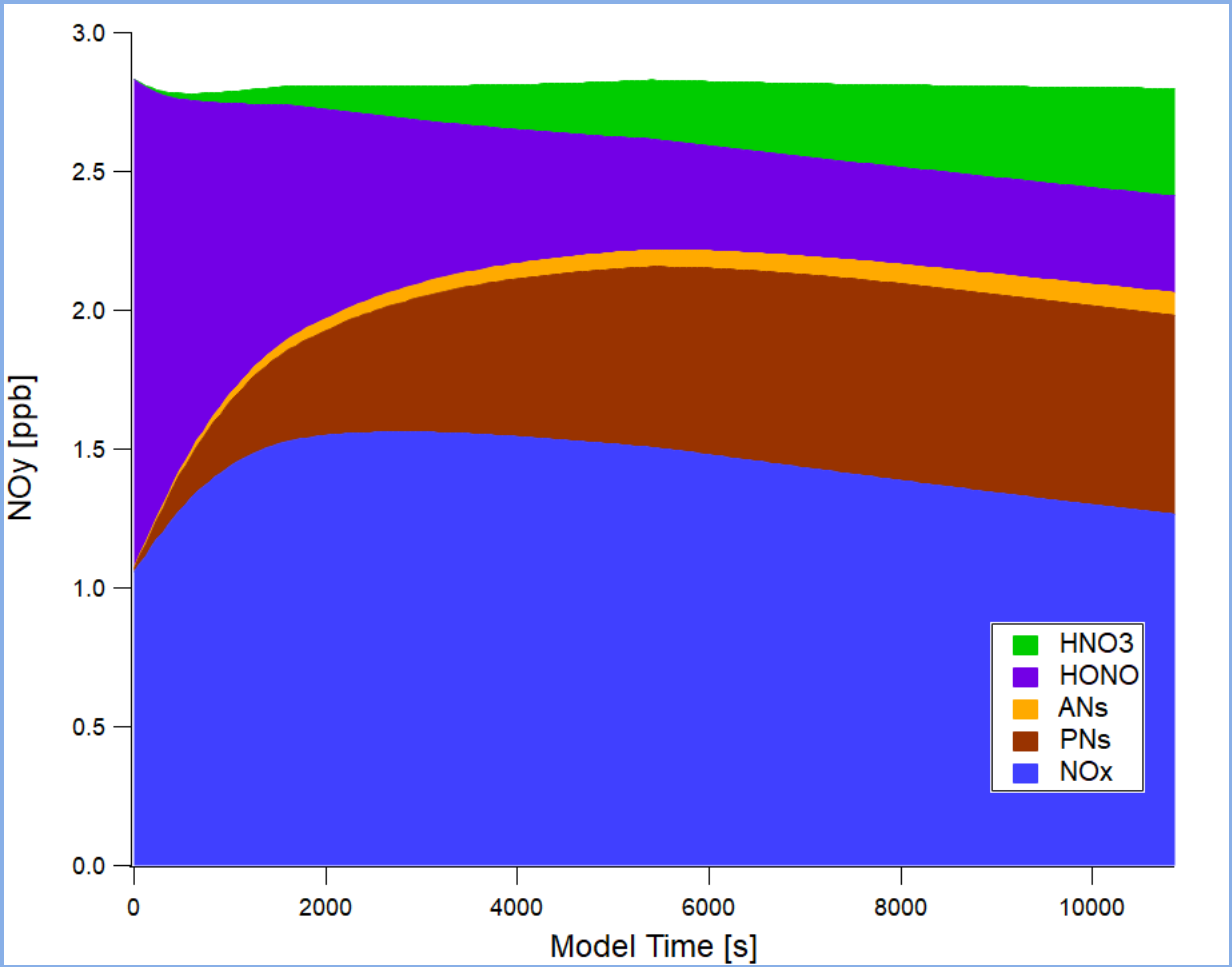


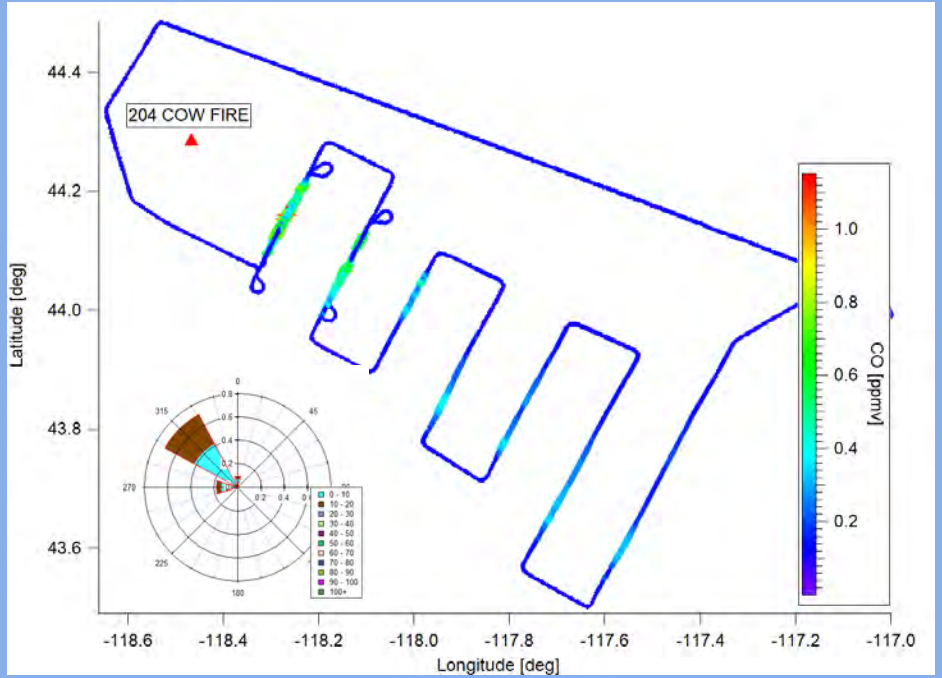


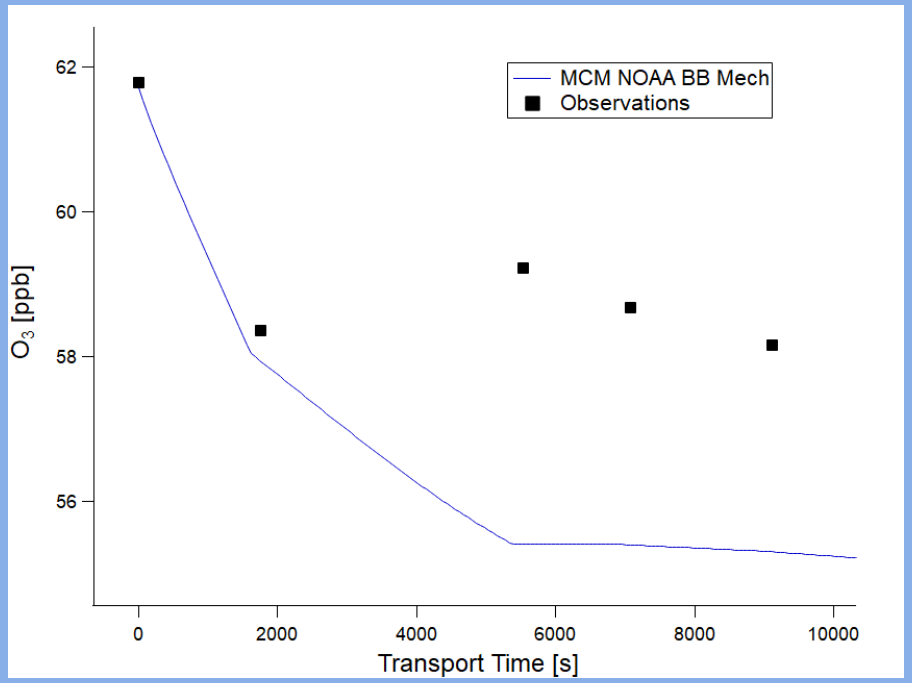
- Numerous outliers in MCE, warrant investigation
- 80% of these come from Granite Gulch on 8/16 or 8/17

Mike Robinson

Box modeling – 8/25/19 Leg 2



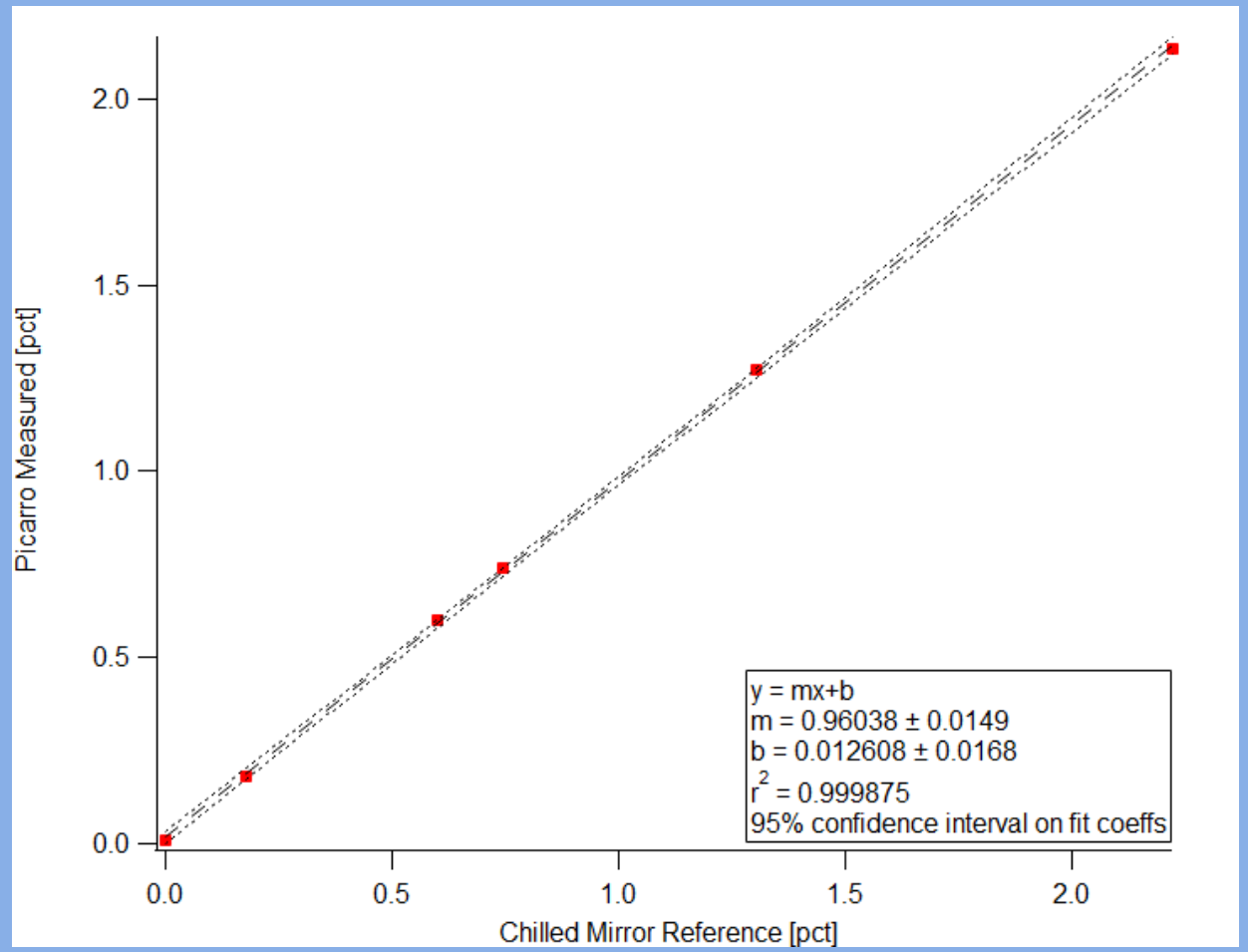




MCMv331 w/NOAA BB Mech (Coggon et al)
f0am interface (Wolfe et al.)

Mike Robinson

Update on CO/CO2/CH4/H2O R0 data

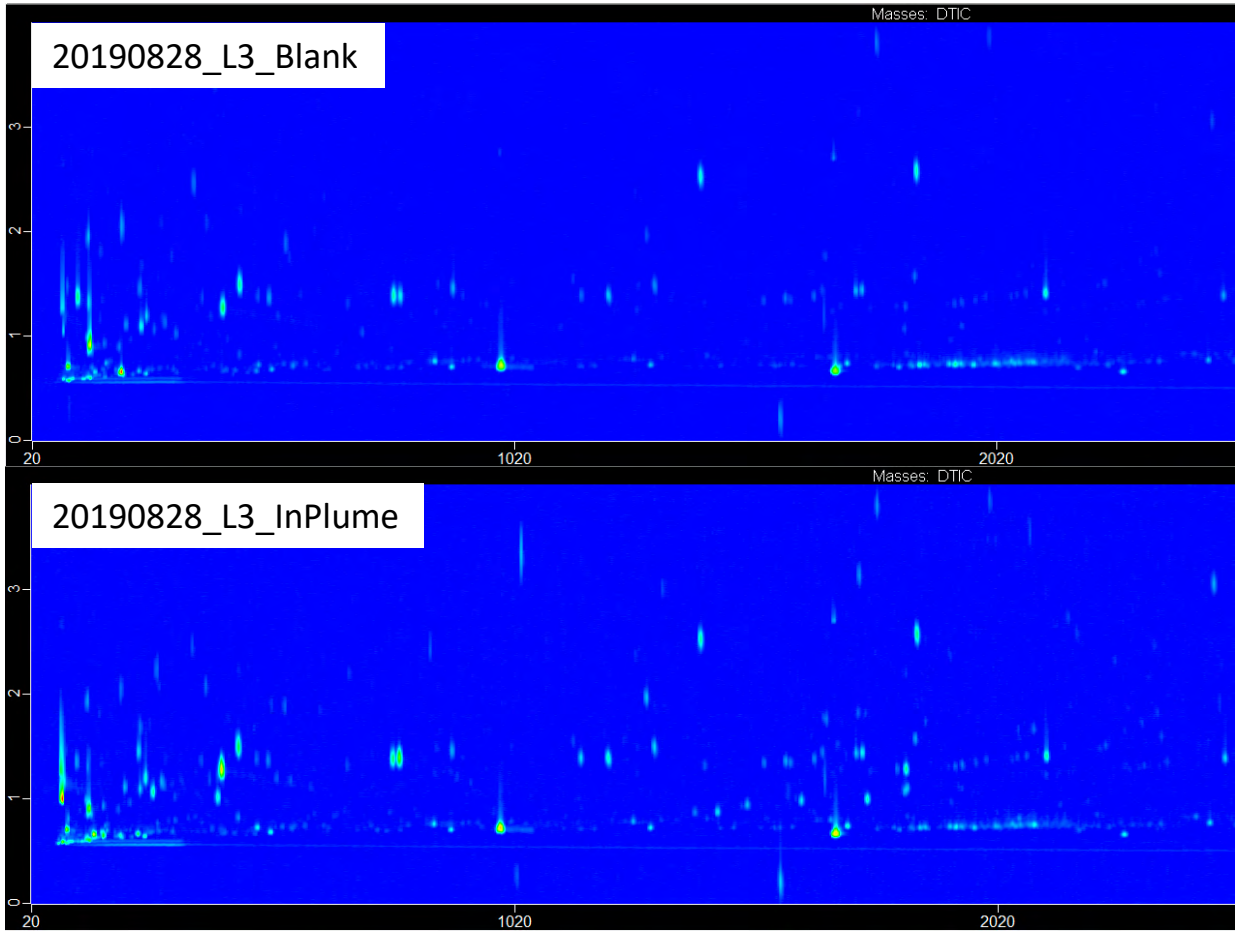


Final data will be up next week!

Contact me for time aligned CO data if you can't wait that long…

Mike Robinson

GCxGC analysis (Barsanti Group)

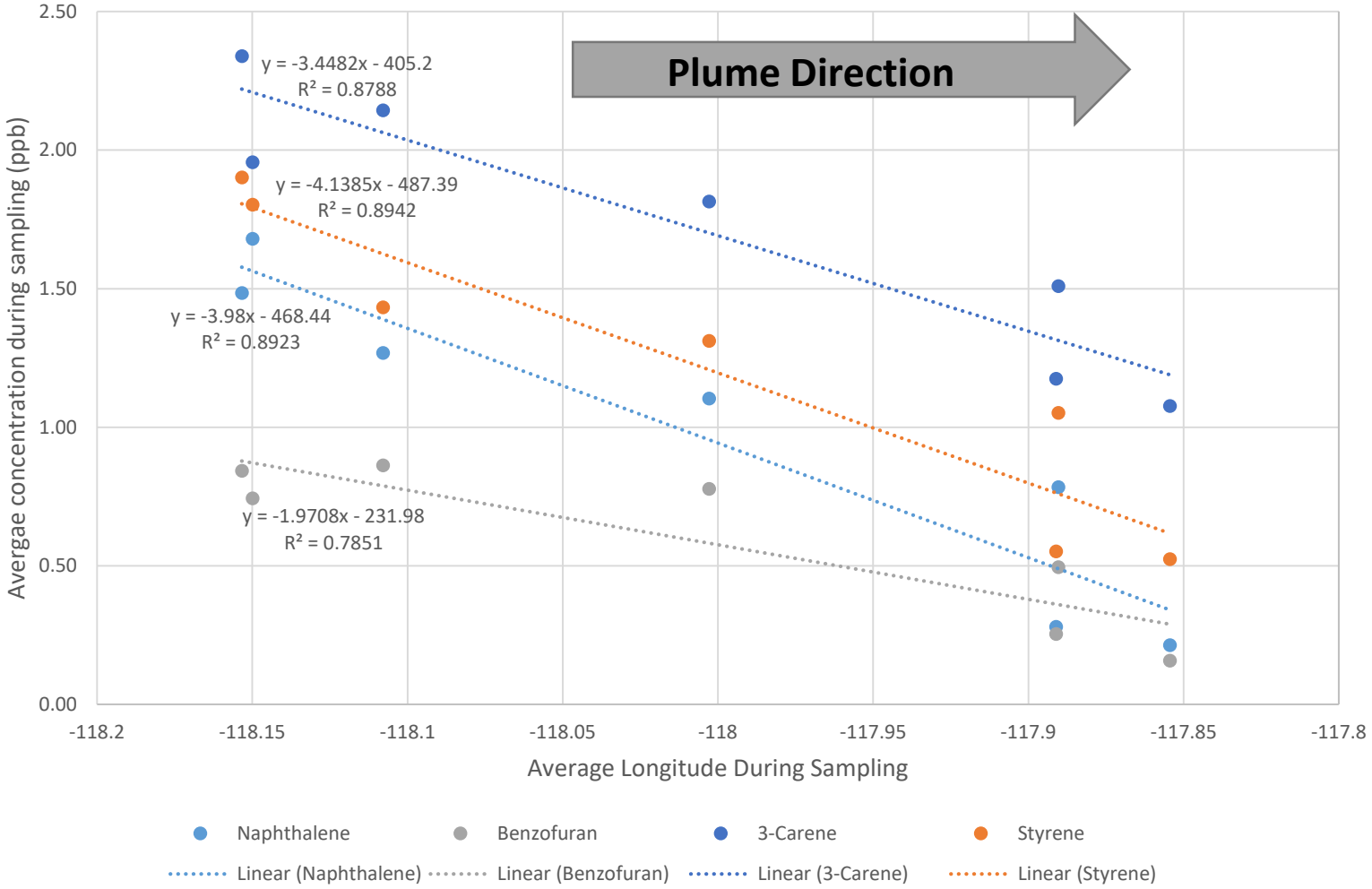


- Contamination makes broad untargeted analysis difficult
- Targeting a list of ~90 compounds to identify and quantify

Targeted Compounds					
à-Pinene	5-Methyl furfural	1-Tetradecene	Anisole	3-Carene	p-Xylene
Methacrolein	Limonene	Sabinene	Phenol, 2,4,6-trimethyl-	Methyl vinyl ketone	o-Xylene
Longifolene	Pentanal	Bornyl acetate	Acenaphthene	Acetonitrile	Benzene, (1-methylethyl)-
Creosol	Styrene	Eugenol	Pyrazine	Phenol, 2,3-dimethyl-	Benzene, propyl-
Pyrrole	Cyclohexanone	Naphthalene, 1-methyl-	Benzaldehyde	Naphthalene, 2-ethyl-	Benzene, 1-methyl-3-(1-methylethyl)-
Indene	m-Cresol	Phenol, 2,5-dimethyl-	Phenol, 2,6-dimethyl-	Phenol, 2,6-dimethoxy-	p-Cymene
Acenaphthylene	Indole	Terpinolene	Acetone	1-Dodecene	o-Cymene
1,13-Tetradecadiene	Cyclohexene	Acetylacetone:2	alpha-Phellandrene	Guaiacol, 4-ethyl	Benzene
ç-Terpinene	Salicylaldehyde	Acetylacetone	à-Methylstyrene	Furan, 2-methyl-	Toluene
Pyridine	á-Myrcene	Isoeugenol, Z-	N-Methylpyrrol	Ocimene	Ethylbenzene
Guaiacol	Furan, 2-acetyl-	Naphthalene, 2-methyl-	Naphthalene, 2,6-dimethyl-	Ocimene:2	Furan, 2,5-dimethyl-
2,3-Dimethylbutadiene	Eucalyptol	Benzofuran	Phthalic anhydride	Phenol, 2,4-dimethyl-	Butanedione
beta-Pinene	Benzonitrile	Acetophenone	Furfural	Naphthalene, 1-ethyl-	o-Cresol
Acrolein	2-Butanone	Benzyl alcohol	Furan	Camphene	Phenol, 3,5-dimethyl-
Camphor	Naphthalene	alpha-Terpinene	Acetic anhydride	á-Phellandrene	Phenylacetylene
p-Cresol					

- We have identified and quantified 10-40 of these compounds for each flight analyzed.

20190828_L3 Concentrations



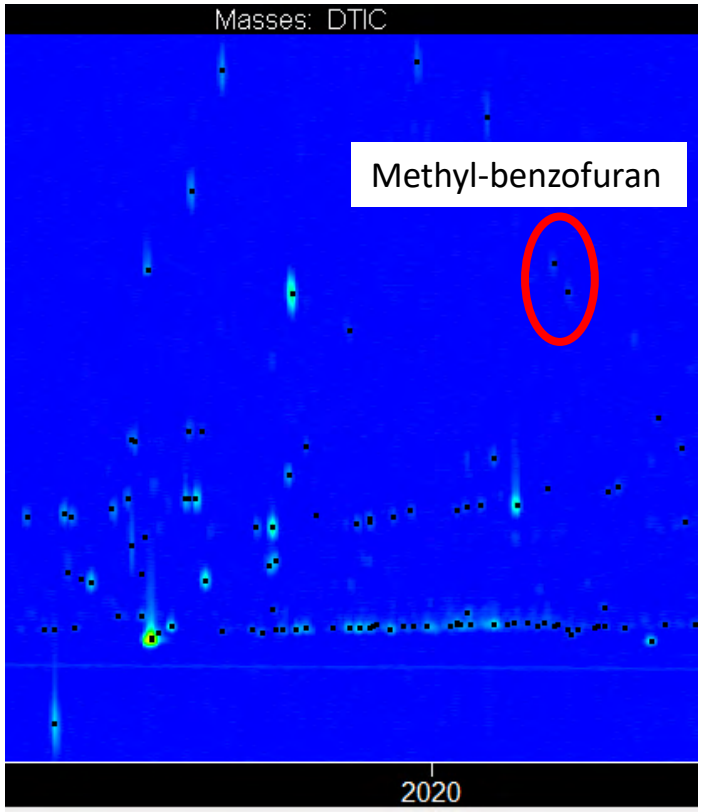
- Despite the contamination, after subtracting blank, we are often seeing nice trends: A good sign!

Data status

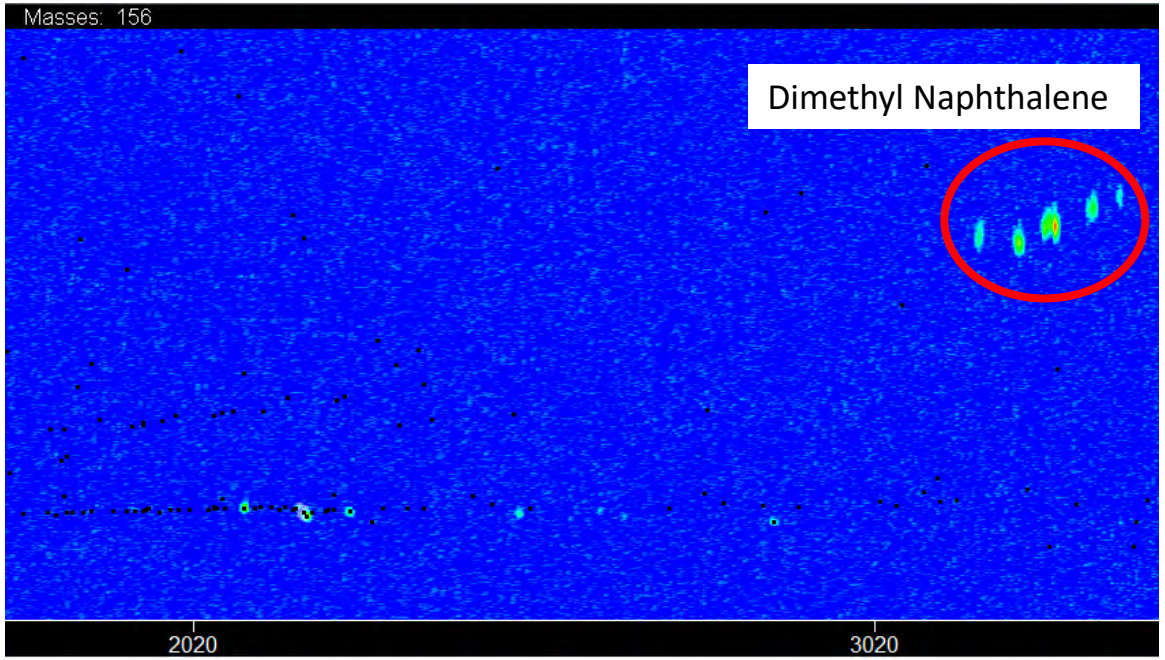
- Twin Otter Samples:
  - Targeted compounds have been identified and quantified
  - Next step: volume correct data and post
- Mobile Lab Samples:
  - Tube cartridges analyzed
  - Next step: run standards, identify/quantify samples

GCxGC data to be posted (Twin Otter)	
20190816	L2, L3
20190817	L1, L2
20190820	L1, L2, L3
20190821	L1, L2
20190824	L2, L3
20190825	L1, L2, L3
20190827	L1, L2
20190828	L1, L2, L3
20190903	L1, L2, L3
20190904	L1, L2, L3
20190905	L1, L2

Untargeted Approach



Search for specific mass (here, we are looking at 156)



- Willing to work with other groups upon request to look for more compounds. If you have a specific compound/flight you are interested in, please feel free to send me an email (pvanr001@ucr.edu)

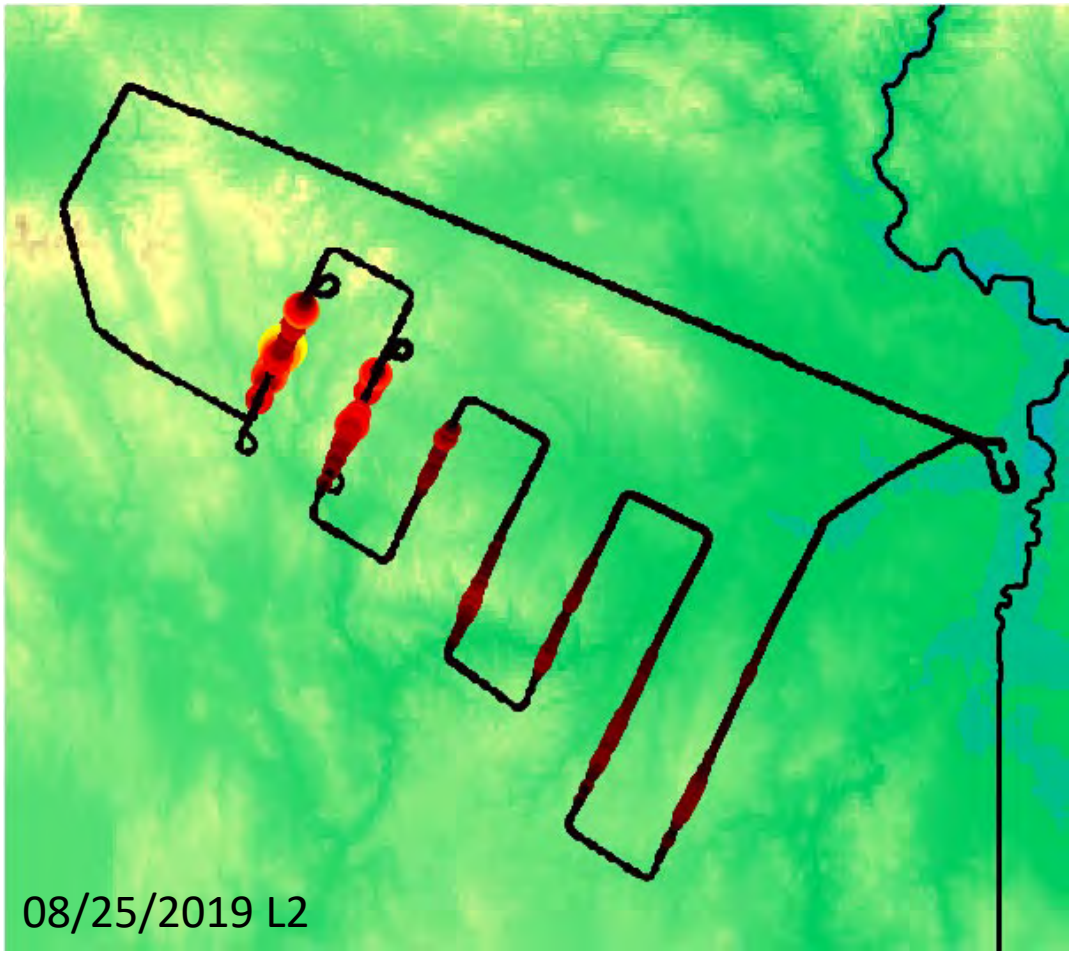
UW CIMS

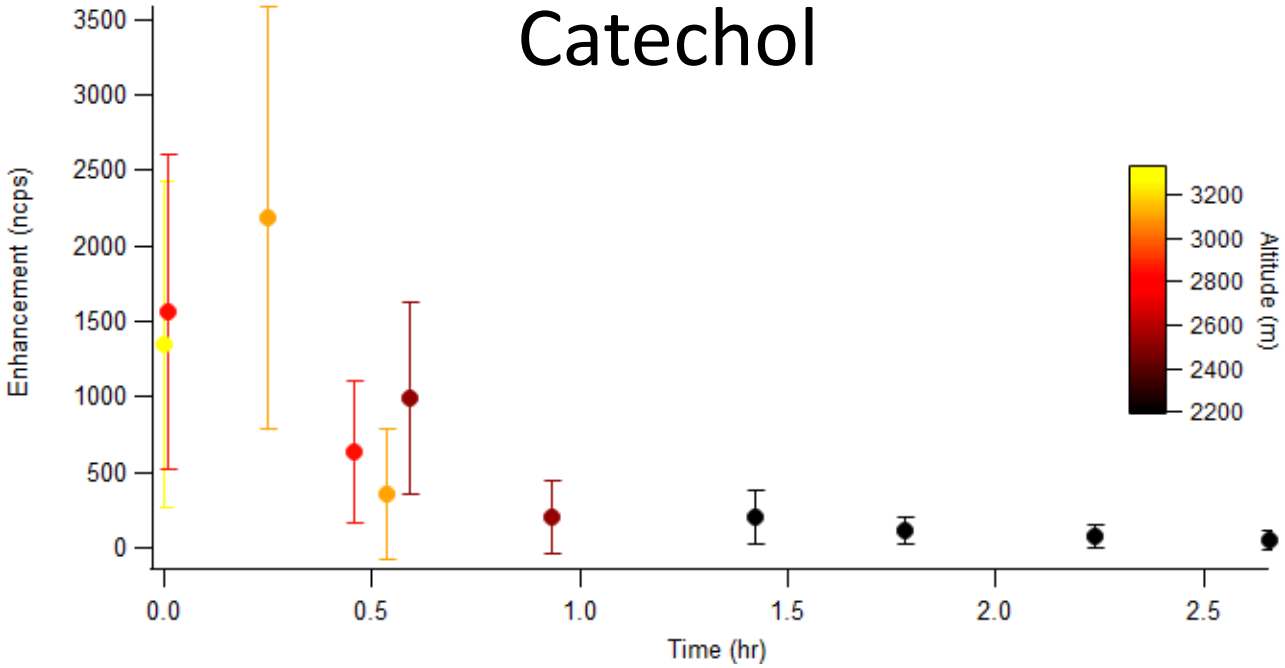
FIREX-AQ Chem Otter Data Meeting
01/31/2020

R0 Will be Available Before the (new) Deadline

- R0 will include
  - HCN
  - HNCO
  - HNO_3
  - HNO_2
  - CH_2O_2
  - $C_2H_4O_2$
  - SO_2
  - HCl (tbd)
  - N_2O_5
  - $ClNO_2$
  - C_6H_6O (includes phenol)
  - $C_6H_6O_2$ (includes catechol)
  - C_7H_8O (includes cresol)
  - $C_5H_{10}O_3$
  - $C_5H_9O_4N$
  - $C_9H_{14}O_4$
  - $C_{10}H_{16}O_3$
  - $C_6H_{10}O_5$

BBVOC Oxidation (Oxy. Aromatics)

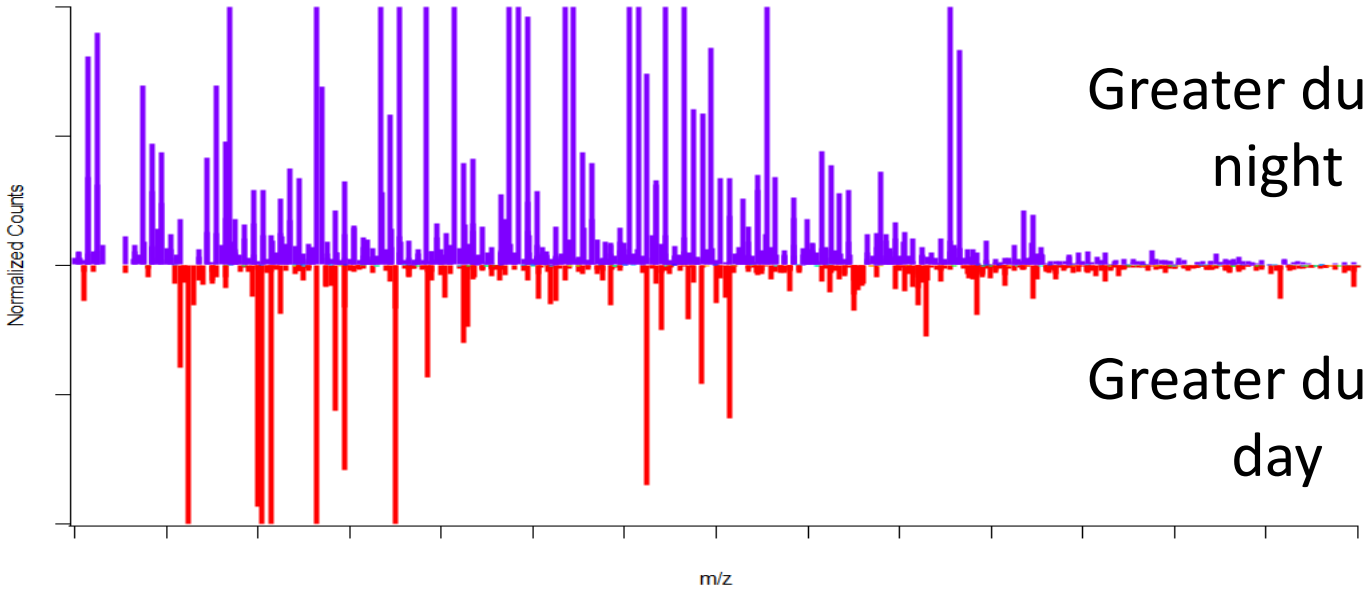




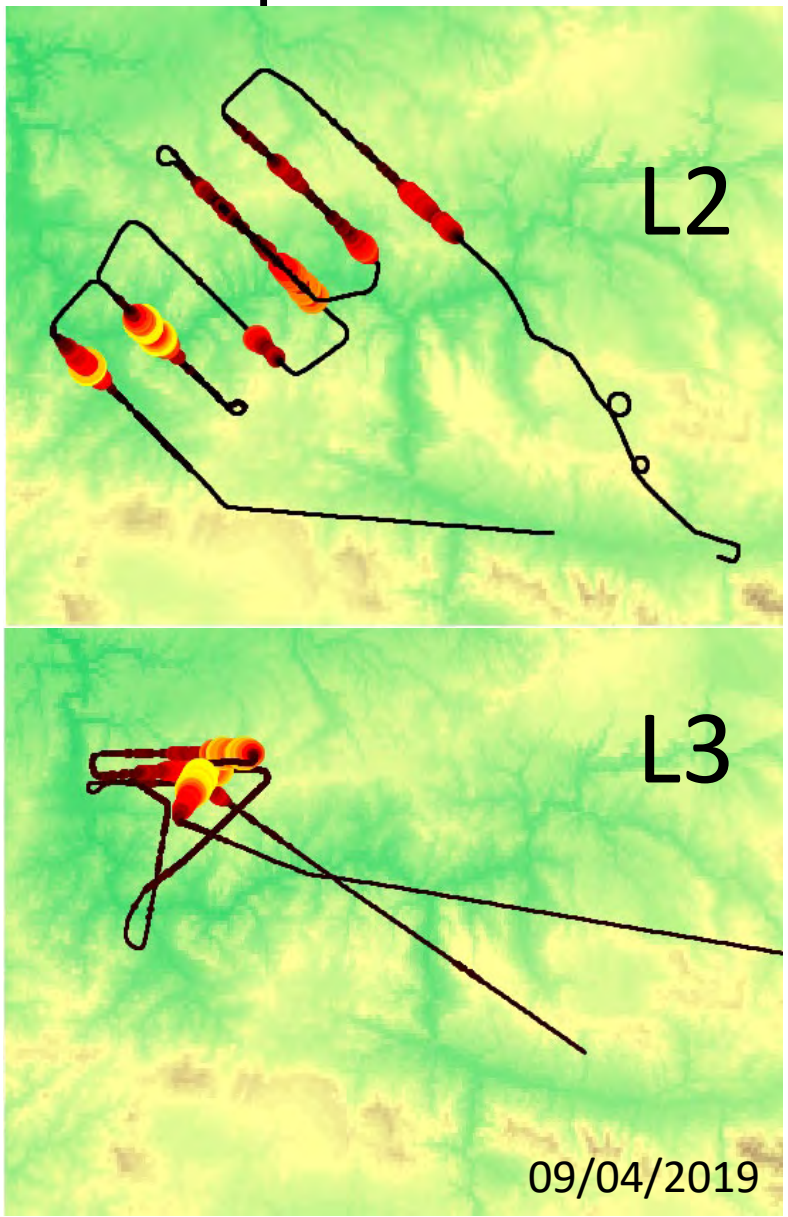
- No conclusions here
- Not dilution corrected

Zach Decker

Day vs Night Emissions and Plume Composition

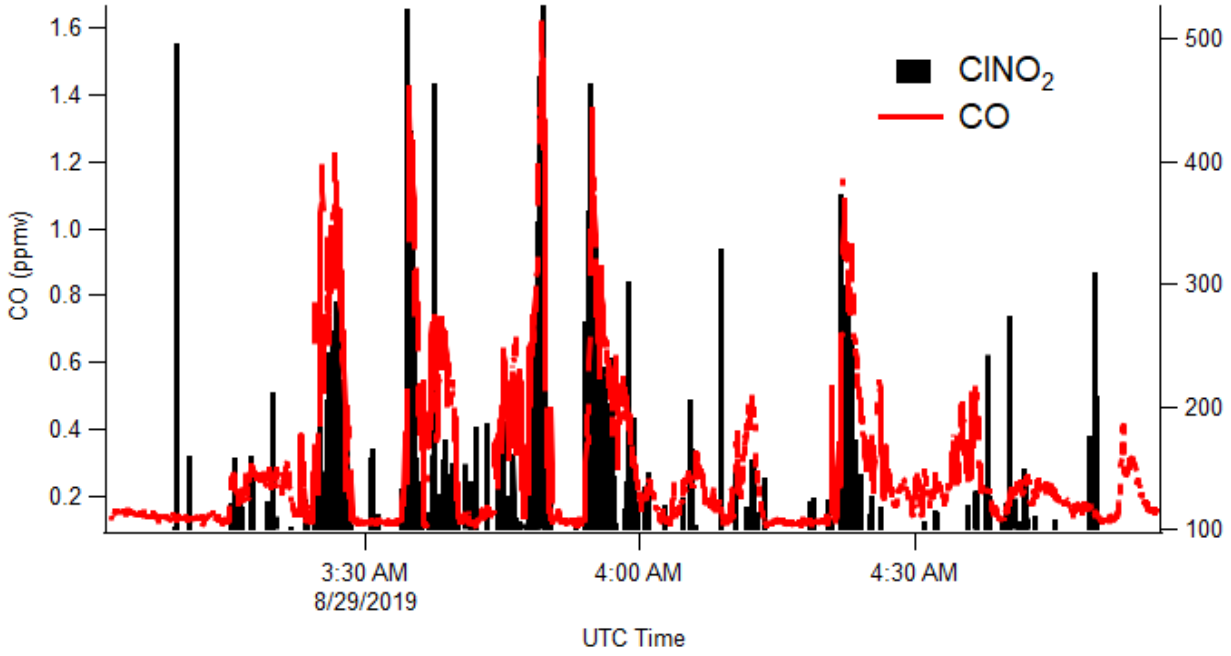


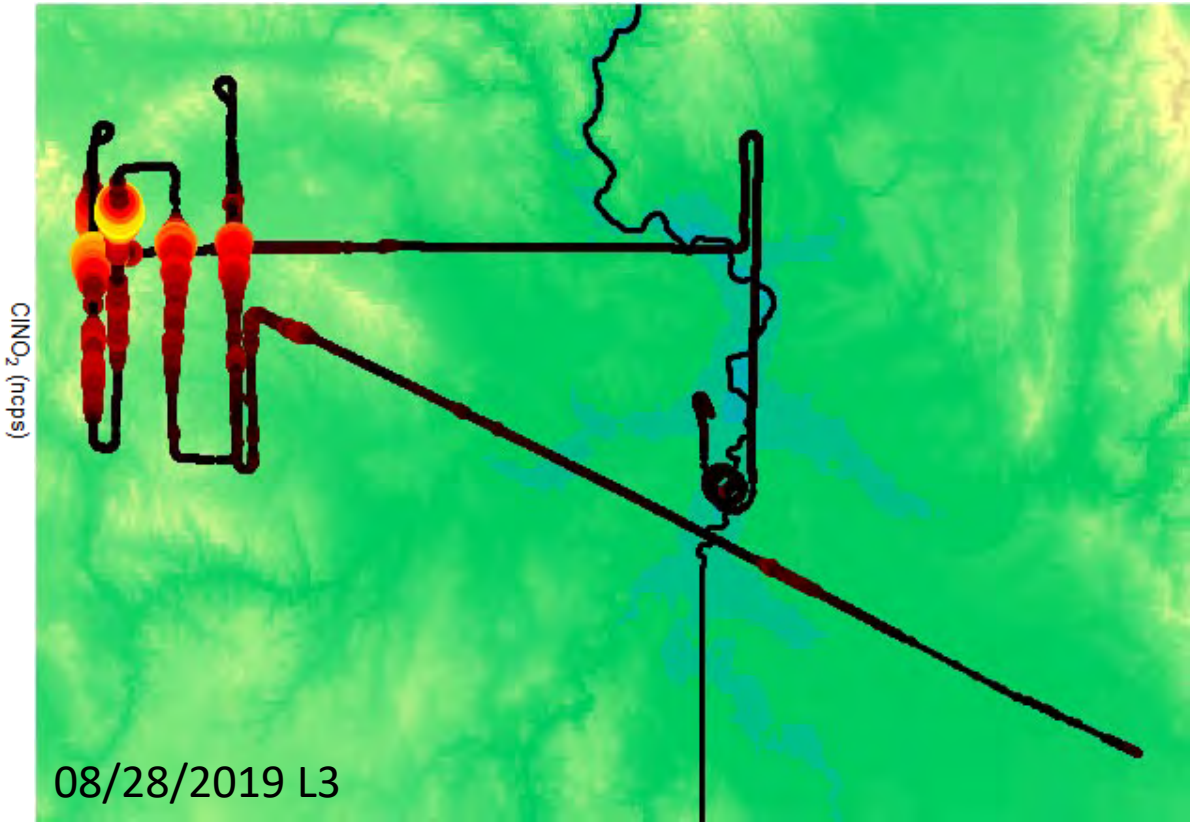
- No conclusions here
- There are a lot of unanswered questions on how to compare day and night plumes.
- We plan to focus on some of these questions



Zach Decker

Nighttime Chemical Pathways → Heterogeneous





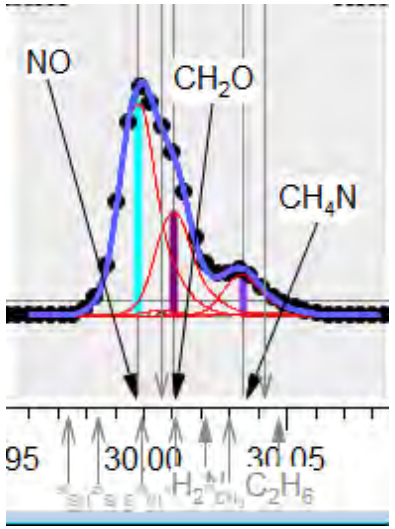
Zach Decker

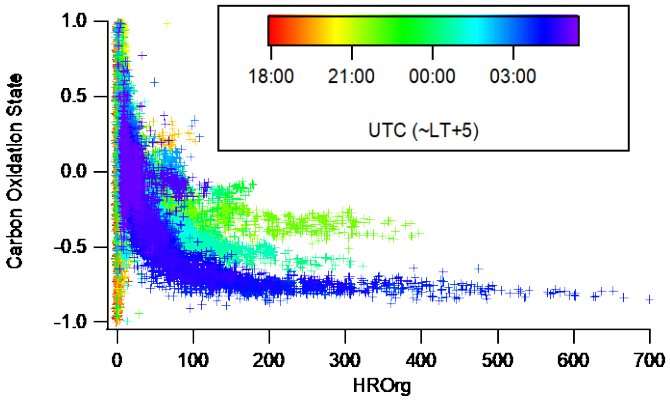
Twin Otter Aerosol Instruments

Instrument	Species Measured	Investigators	Institution
High-Resolution AMS	Aerosol composition	Ann Middlebrook, Ale Franchin, Kathy Hayden, Shao-Meng Li	NOAA CSD Environment Canada
Aethelometer	Aerosol absorption at three wavelengths	Ale Franchin	NOAA CSD
Optical Particle Counter	Aerosol size distribution	Ale Franchin, Ann Middlebrook	NOAA CSD
Brown Carbon PILS	Water-soluble aerosol absorption Water-soluble organic carbon concentration	Rebecca Washenfelder, Lisa Azzarello	NOAA CSD
Water and Filter Samples	Aerosol composition, size-resolved absorption	Cora Young, Lisa Azzarello	York University
Aerosol Impactor	Particle morphology, composition, and mixing state	Alex Laskin, Jay Tomlin, Felipe Rivera, Kevin Jankowski	Purdue University

Aerosol Rack Data Status: AMS, UHSAS, and CLAP

- Fit HR-AMS spectra to over 1000 ions
  - Good separation of inorganic/organic ions
- Main AMS species will be reported in final data
  - Folks need to request for particular ions
  - Possibly add carbon oxidation state
- Still working on R0 data for all three instruments
  - Want reasonable closure between them
  - Expect to be done by the Feb 14 deadline





Ale Franchin and Ann Middlebrook

Relationship between optical properties and chemical composition

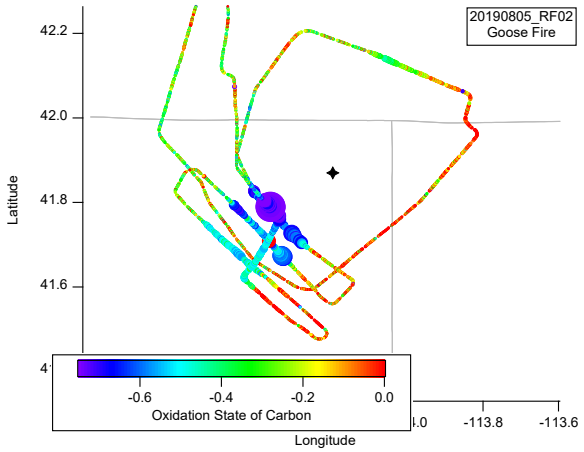
- Is there a chemical signature for absorbing aerosols?
- Is there a difference between day and night, plume age and/or time of day emitted?
- Is there a difference between the plume edges and the plume center?
- Do we see similarities/differences in the altitude profiles?
- By using the CLAP absorption measurement at 653 nm we would like to generate a black carbon proxy, using a MAC from the literature
- Investigate fast oxidation within the first tens of minutes

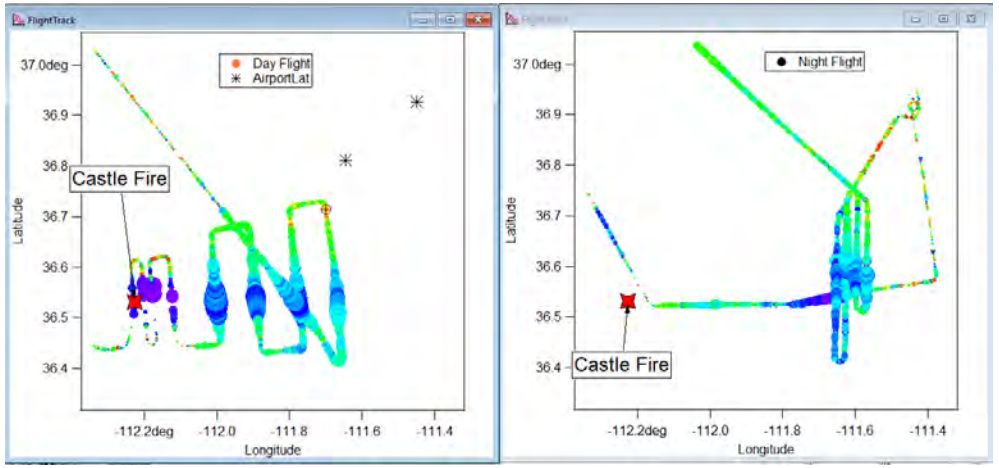
Ale Franchin and Ann Middlebrook

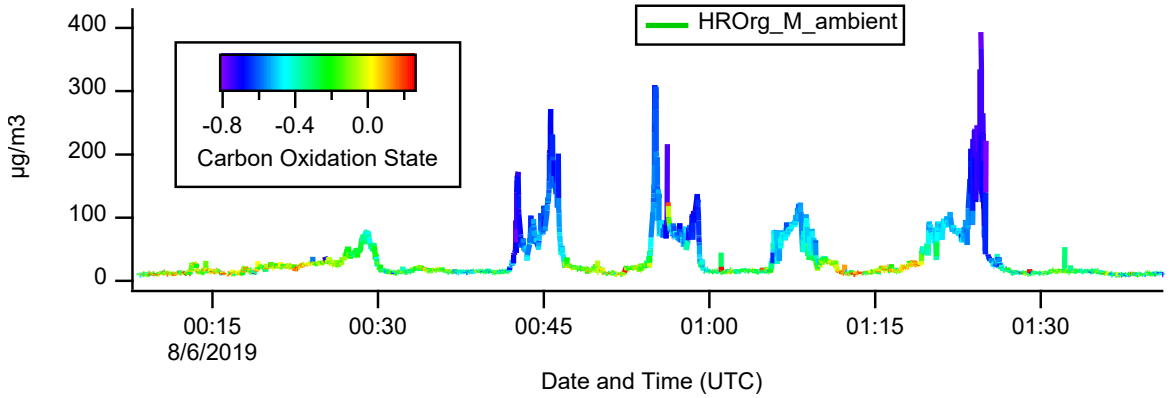
Fast (10s of minutes) Daytime Oxidation? What Controls Oxidation State at Night?

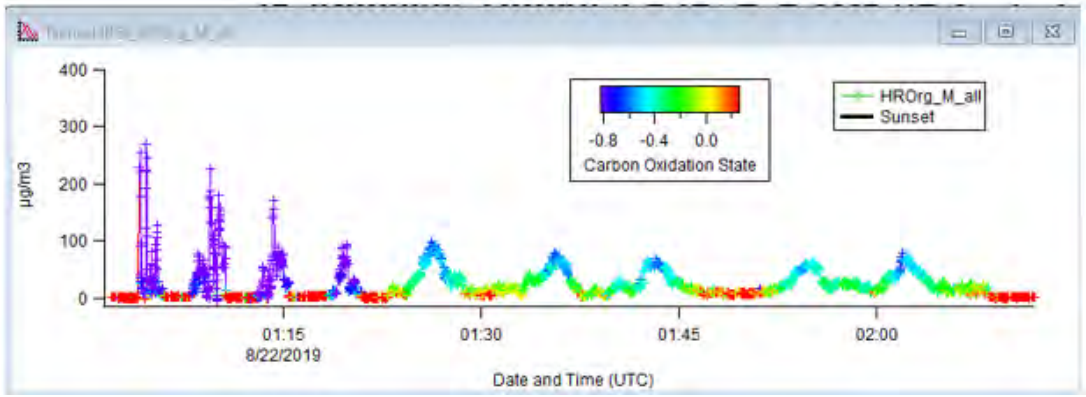
Need to examine

- fire intensity,
- time since emission
- time in sunlight.



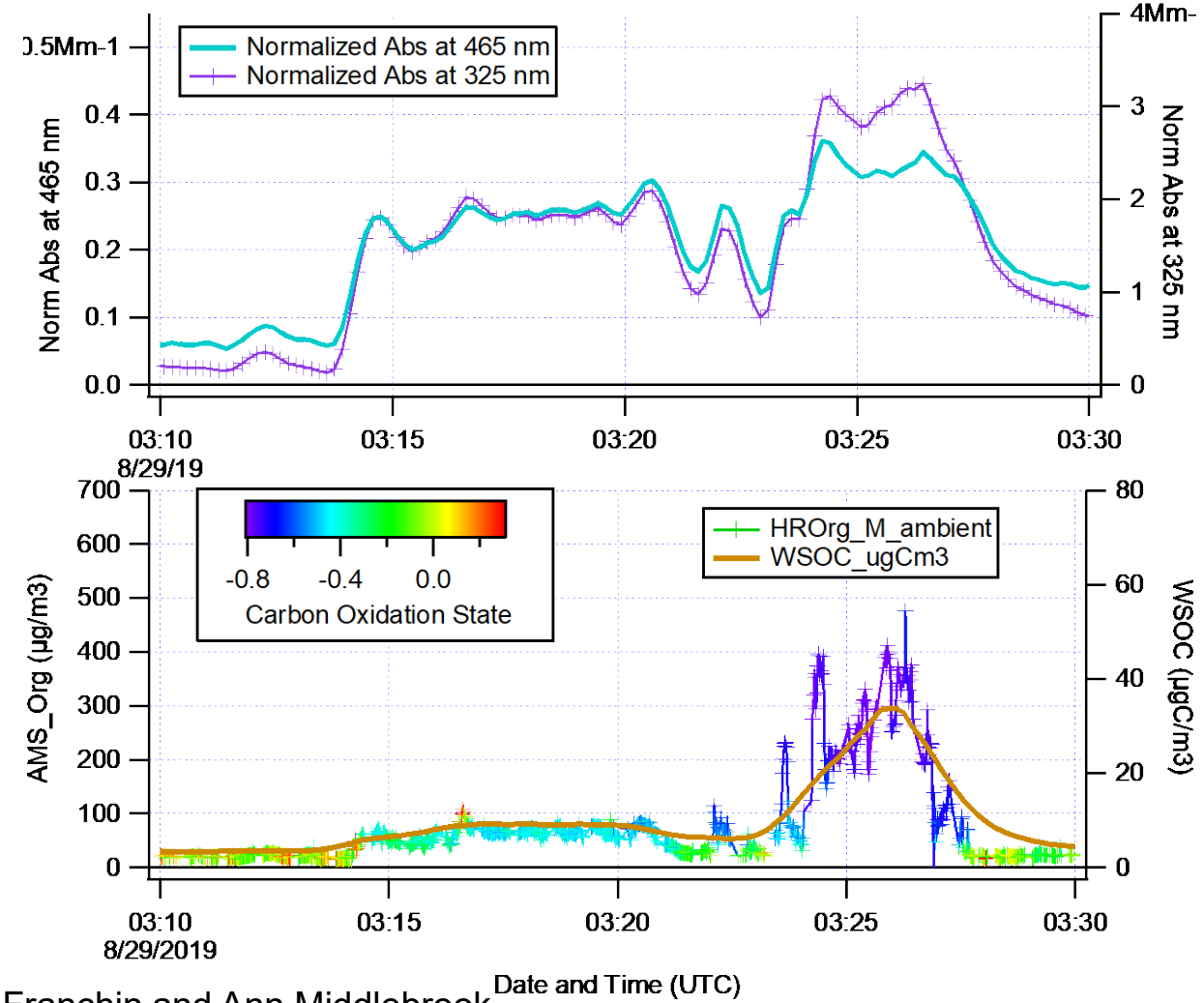






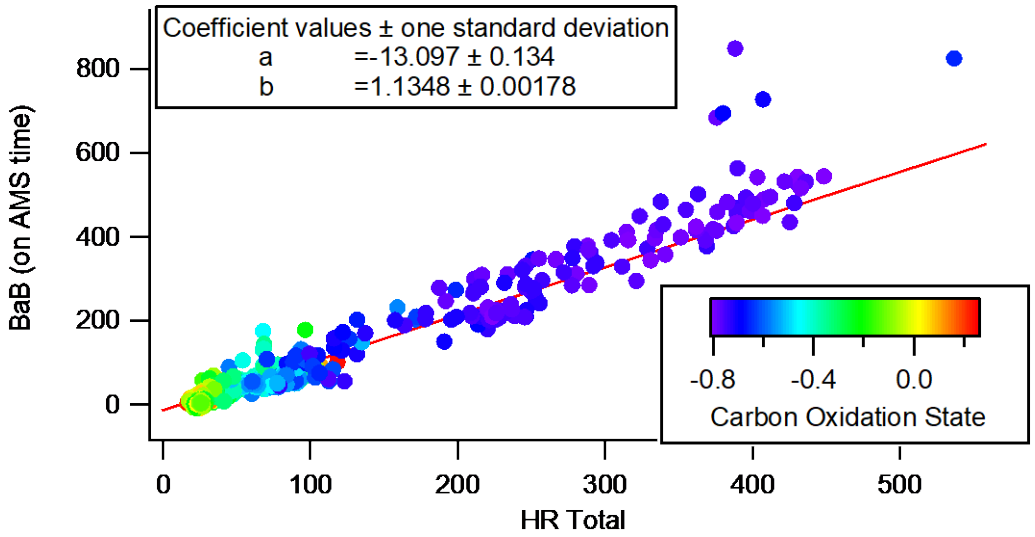
Ale Franchin and Ann Middlebrook

Water Soluble and CLAP Optical Properties and Carbon Oxidation State



Normalized WSOC absorption is enhanced at 325 nm when aerosol is less oxidized, whereas at 465 nm it is fairly constant.

CLAP transmission data at 467 nm also appears relatively constant despite lower oxidation state.



Ale Franchin and Ann Middlebrook

Brown Carbon - PILS

Date	Fire	Availability
7/29	Colorado Test Flight	L1
8/3	McCall Test Flight	L1
8/5	Goose	L1/L2/L3
8/9	Granite/HK/Nethker	L1/L2/L3
8/10	Nethker	L1
8/11	Nethker	L1
8/16	Granite	L1/L2/L3
8/17	Granite	L1/L2
8/20	Little Bear	L1/L2/L3
8/21	Little Bear / Castle	L1/L2/L3
8/24	Cow	L1/L2/L3
8/27	Cow	L1/L2
8/28	Cow	L1/L2/L3
9/3	Cow	L1/L2/L3
9/4	Canyon 66	L1/L2/L3
9/5	Smith Knob	L1/L2

RA Posted

Partial data or problems

No data

RA data posted and roughly time-aligned:

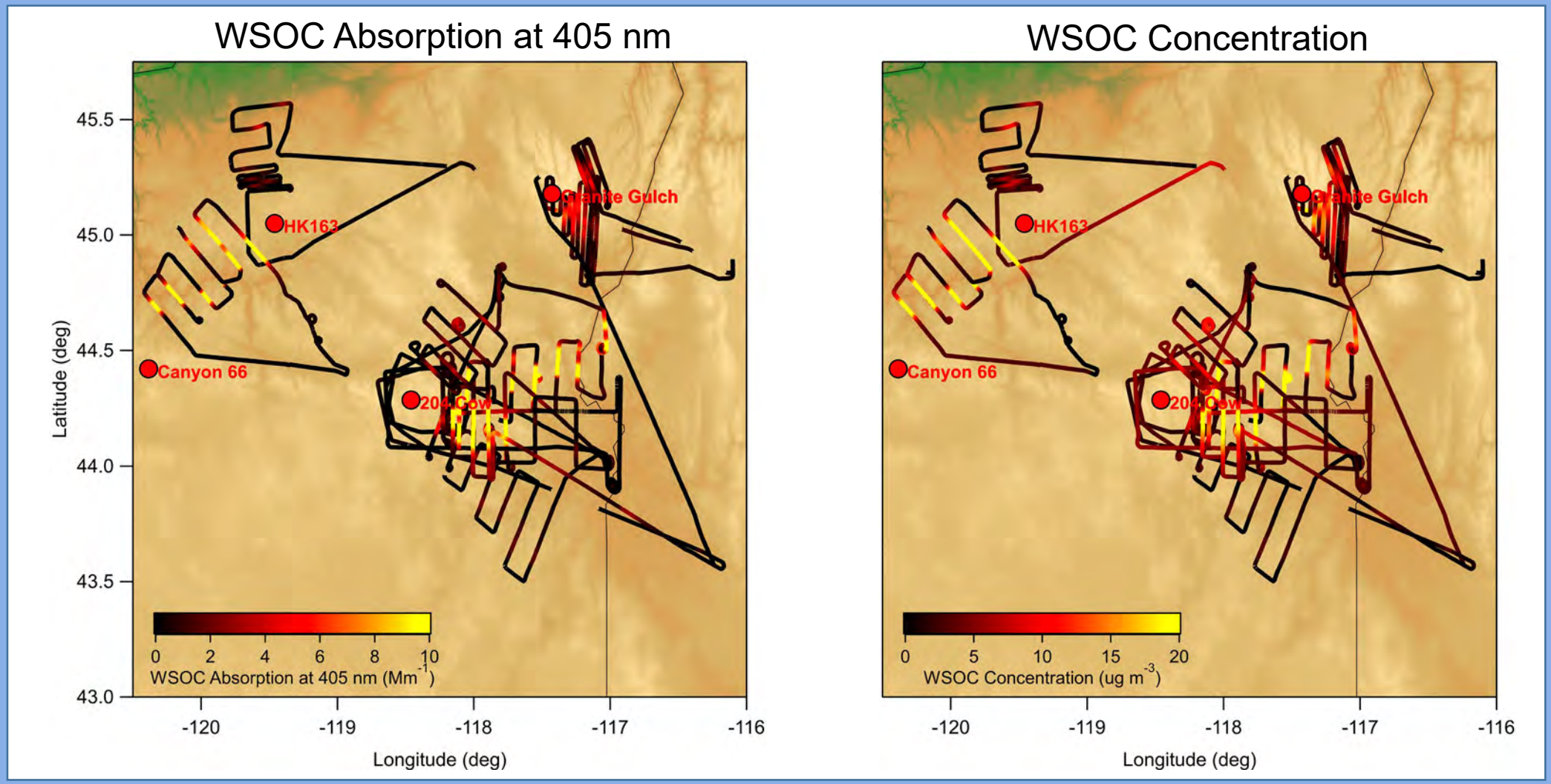
- Water-soluble organic carbon
- Water-soluble absorption from 310 – 500 nm

Next: Final data!

Rebecca Washenfelder

Example flights with consistent wind direction

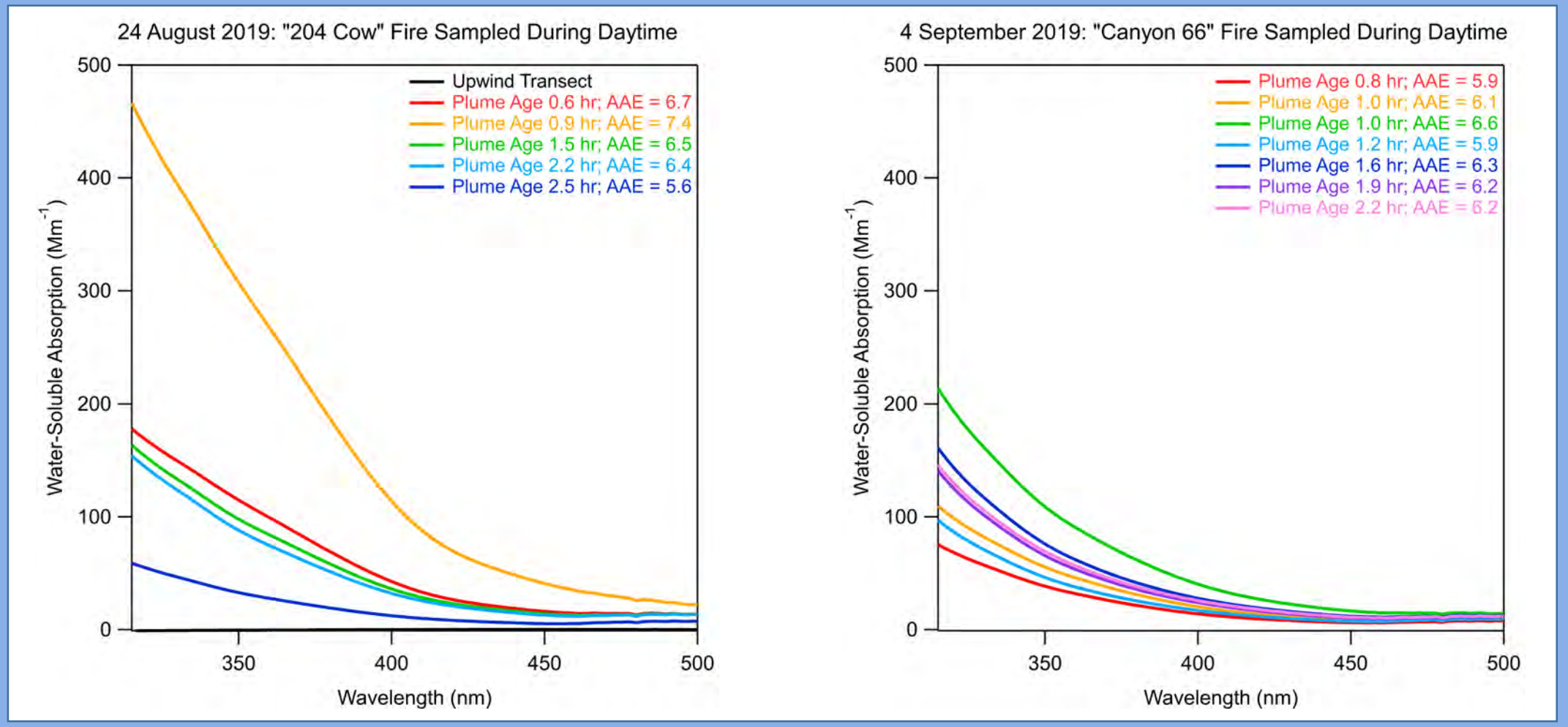
A subset of the 40 flights had consistent wind directions and well-organized plumes.
Ten examples are shown here: August 9, 16, 17, 24, 25, and 28; September 4 and 5.



Rebecca Washenfelder

Absorption Angstrom Exponent

Absorption Angstrom Exponent (AAE) describes the wavelength-dependence of absorption: $\alpha_{absorption} = K\lambda^{-AAE}$



Literature AAE values for brown carbon are 2 – 6.

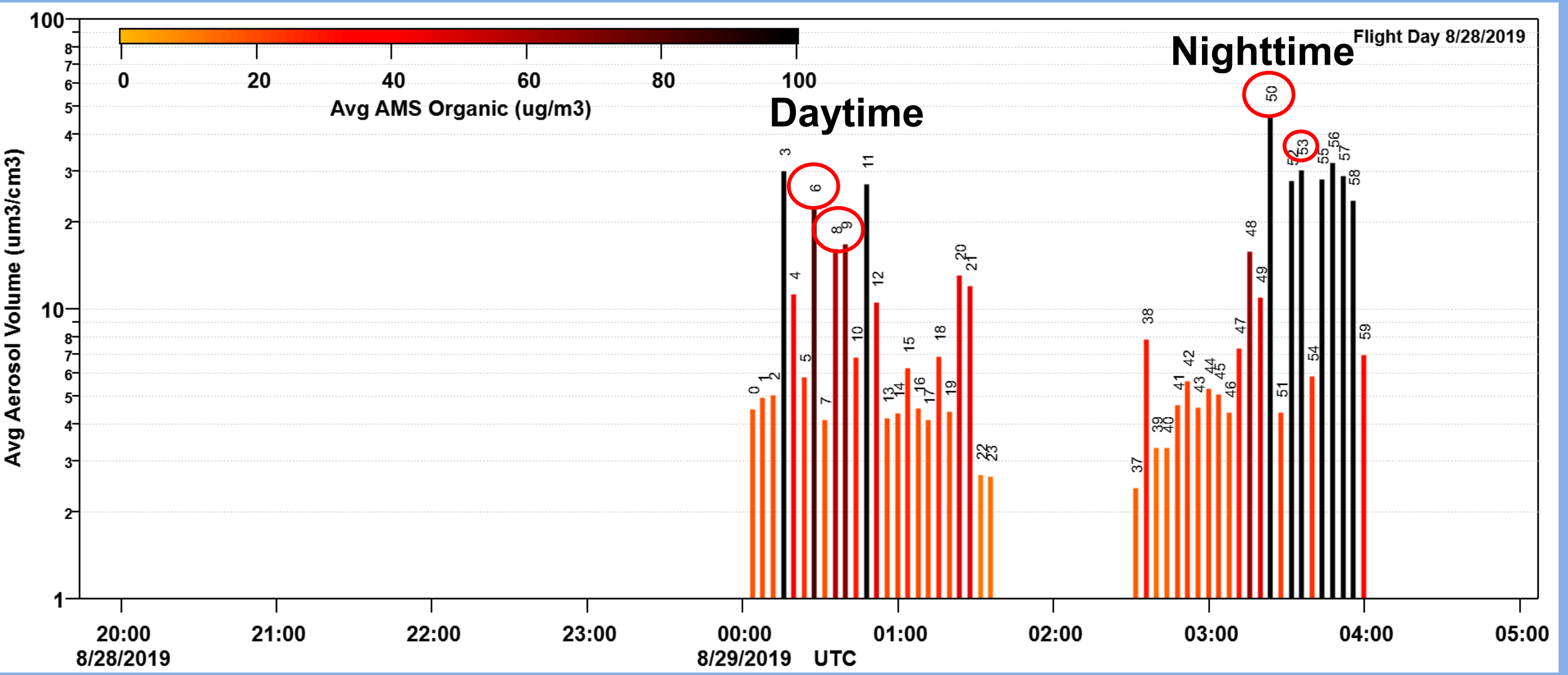
For smoke sampled 0 – 3 hours downwind, the water-soluble AAE values were 5 – 7.

Rebecca Washenfelder

August 28th, 2019 (204 Cow Fire) FIREX-AQ Particles CCSEM Data Summary

Jay Tomlin and Felipe Rivera

Sample selection



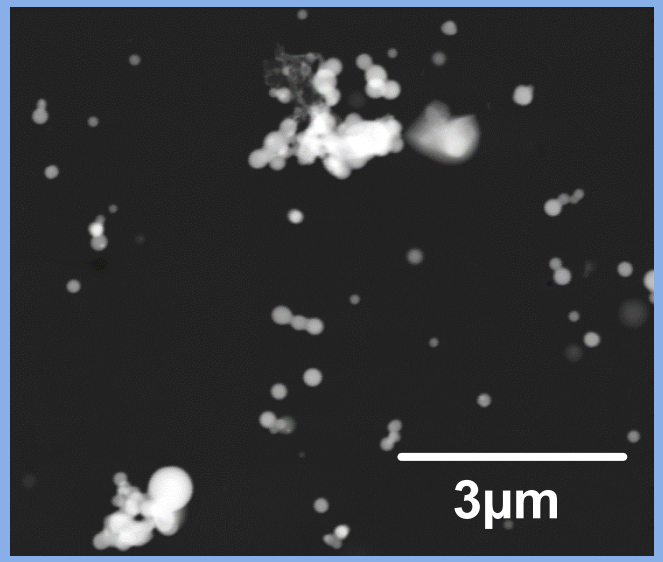
Jay Tomlin and Felipe Rivera

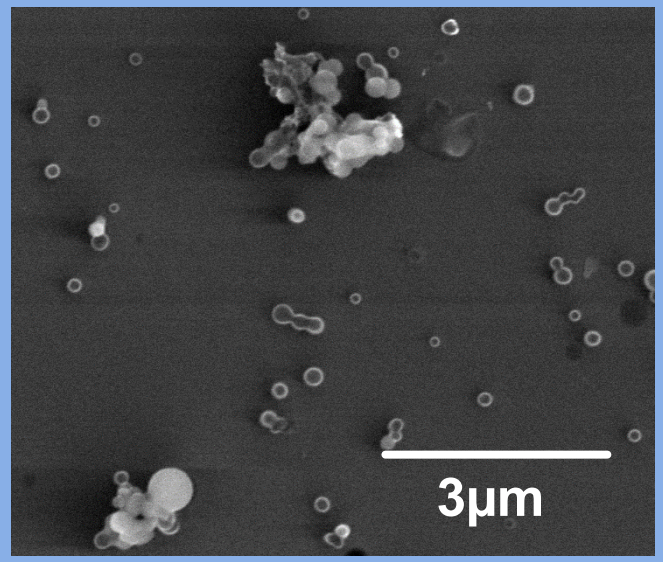
Representative SEM image for 20190828 sample

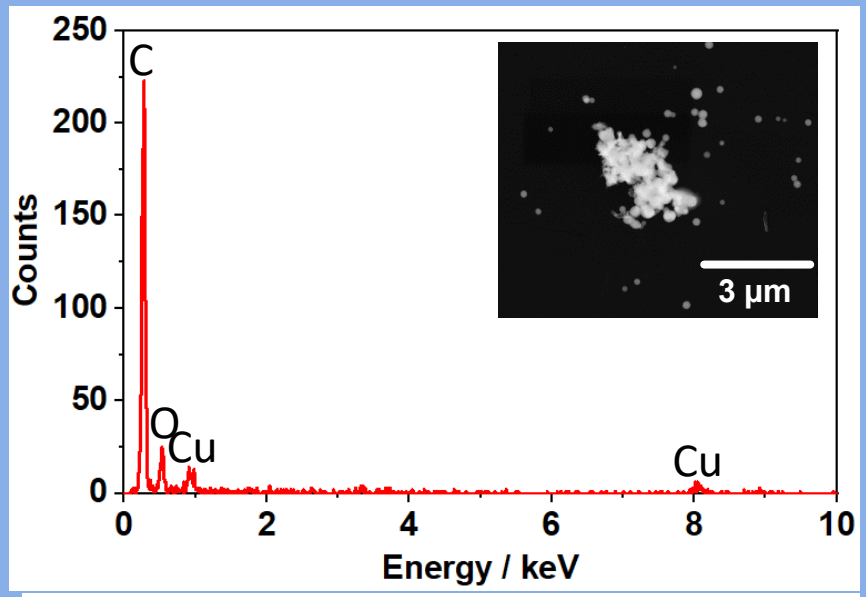
Secondary electron

Backscattered

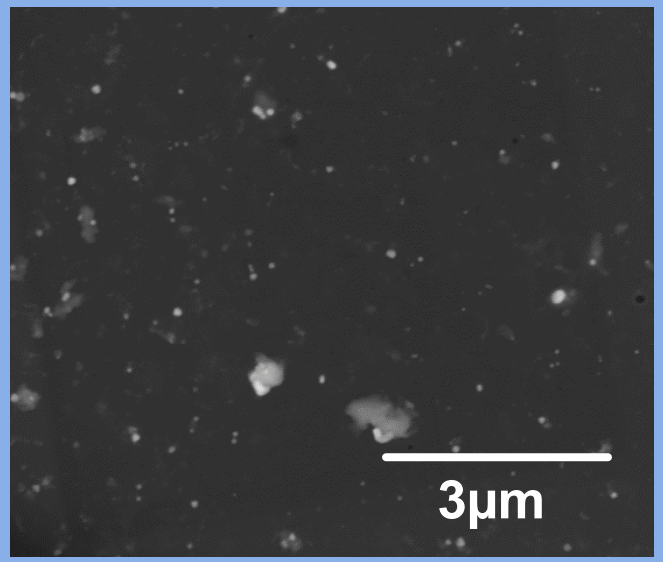
Daytime

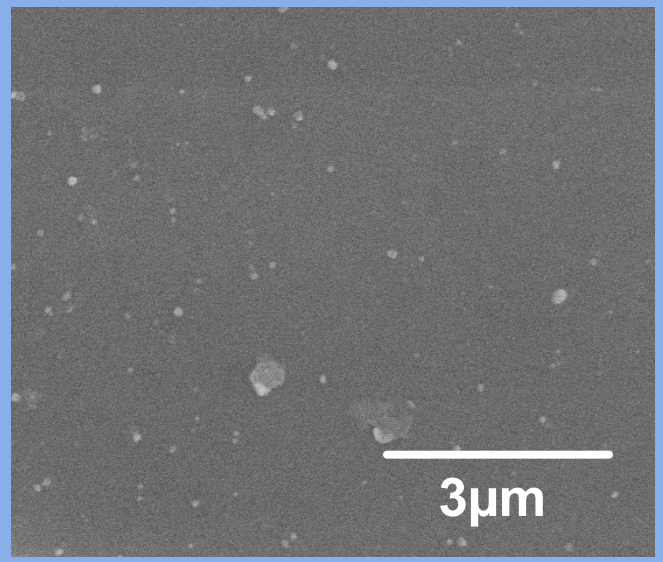


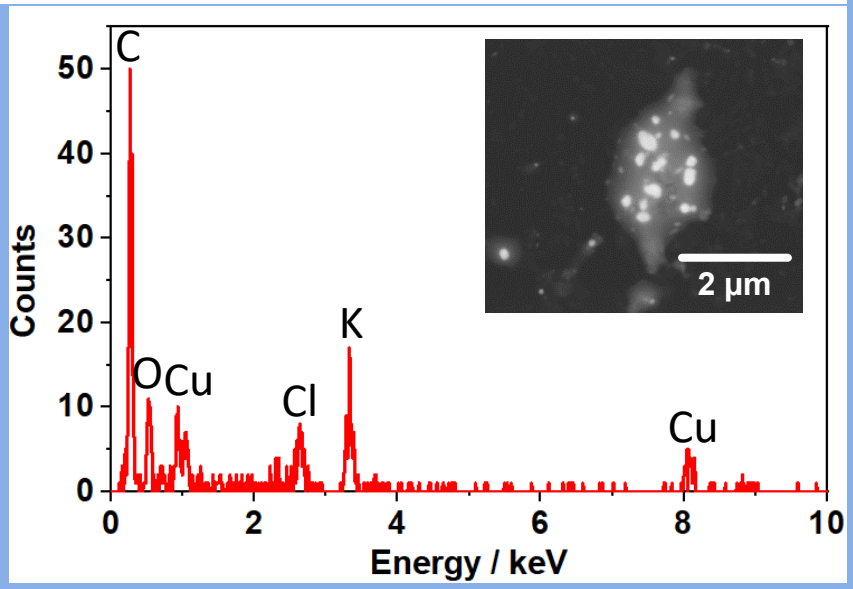




Nighttime

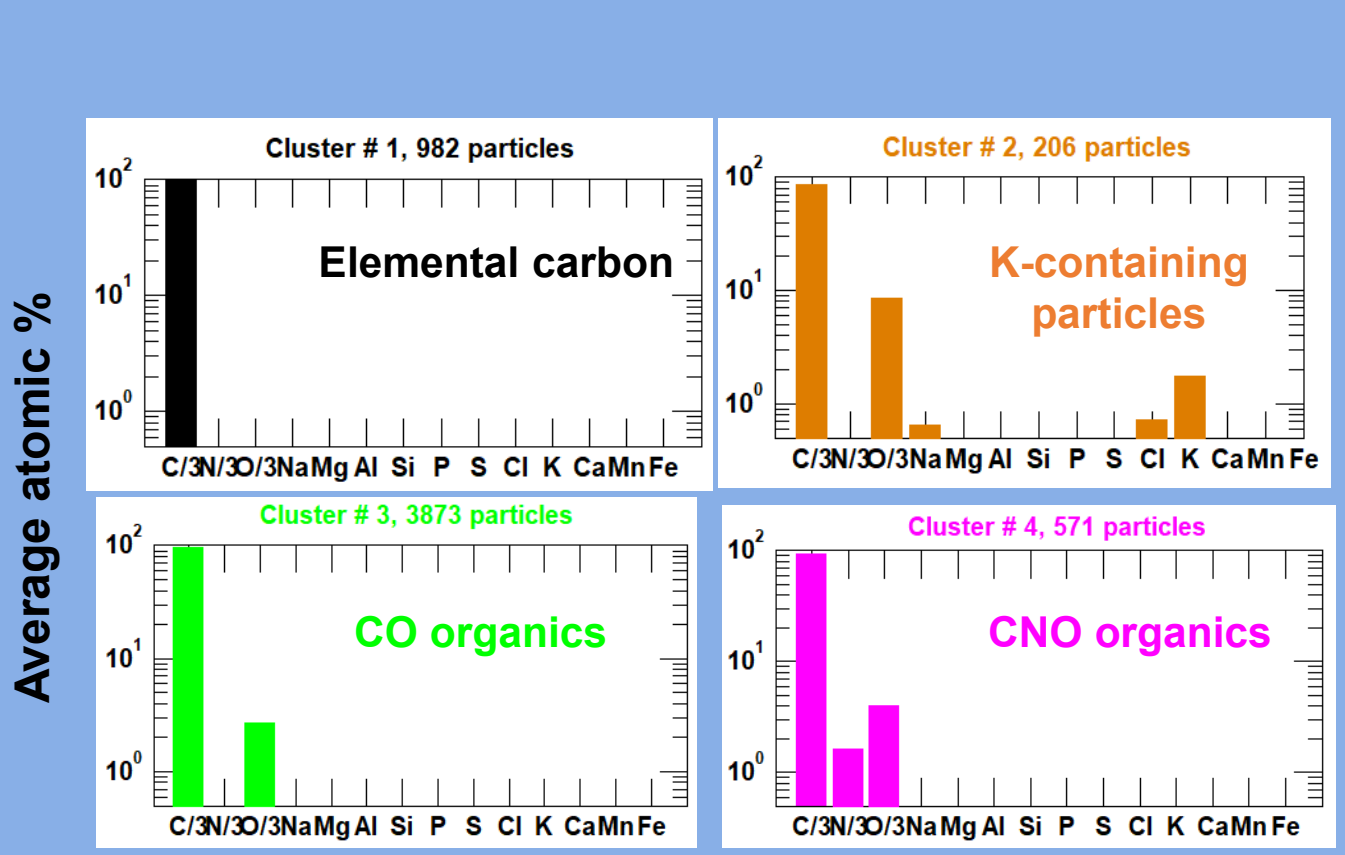


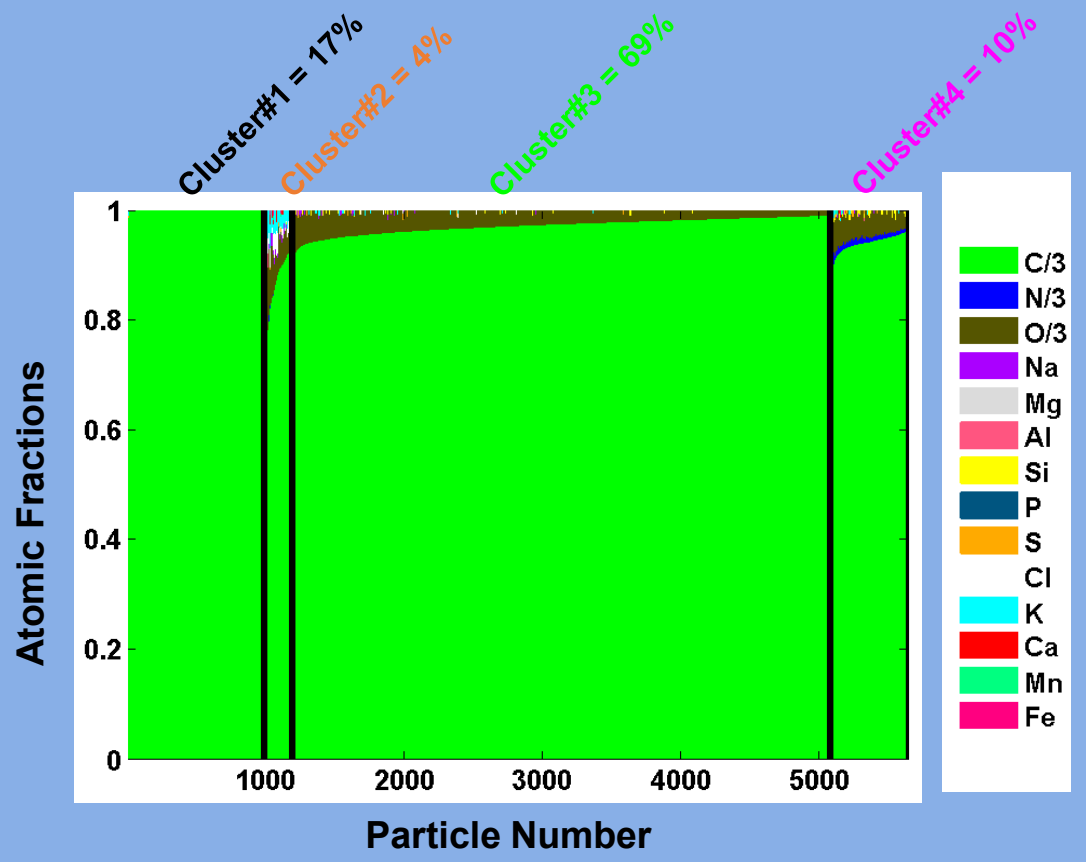




Jay Tomlin and Felipe Rivera

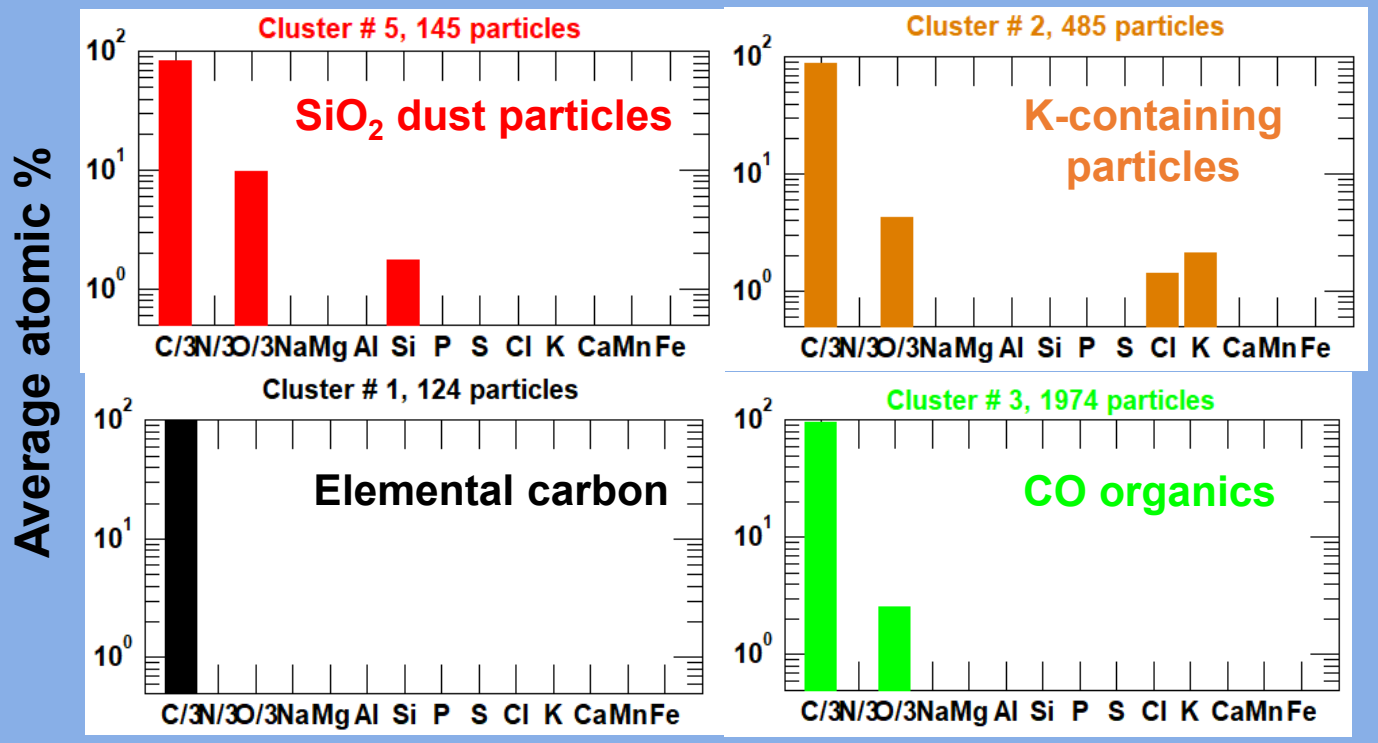
K-means cluster analysis for 20190828 Daytime

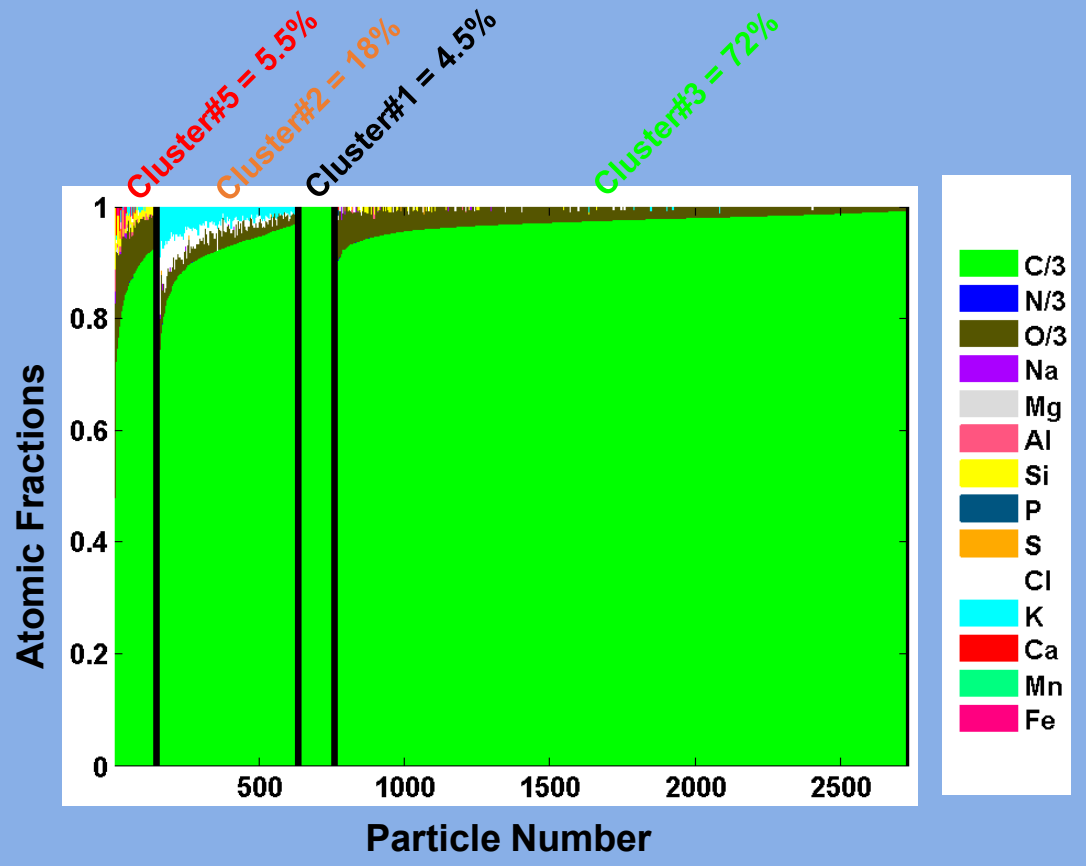




Jay Tomlin and Felipe Rivera

K-means cluster analysis for 20190828 Nighttime





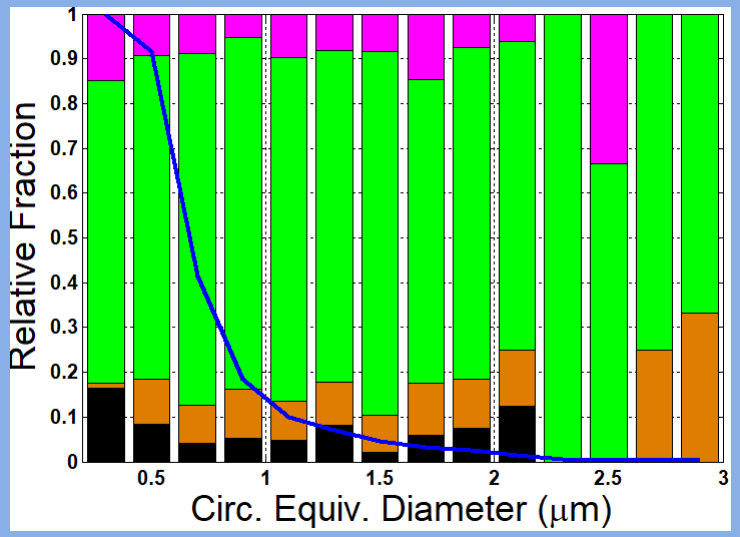
Note the absence of N containing particles for the nighttime sample

Jay Tomlin and Felipe Rivera

Cluster size distribution for 20190828 sample

Daytime

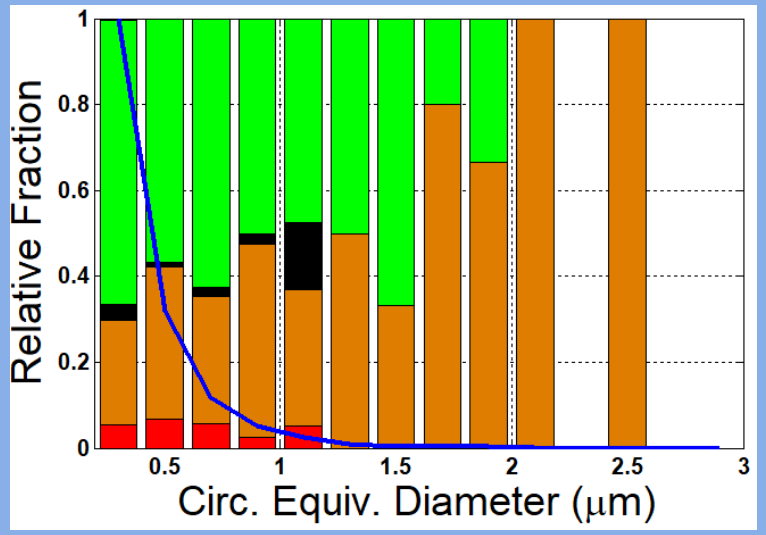
5632 particles analyzed



Cluster#1: Elemental carbon
Cluster#2: K-containing particles
Cluster#3: CO organics
Cluster#4: CNO organics
Cluster#5: SiO_2 dust particle
Particle size distribution

Nighttime

2728 particles analyzed



Daytime sample contained more Oxygenated organic particles while nighttime had a noticeable increase in K-containing particles contribution

Jay Tomlin and Felipe Rivera

Twin Otter Other Instruments

Instrument	Species Measured	Investigators	Institution
GoPro	Photons	Zach Decker	NOAA CSD
Meteorology	Temperature, pressure, altitude, wind speed, wind direction	Mike Robinson	NOAA CSD

Flight Footage

Zach Decker

FIREX-AQ Data Meeting 01/31/2020

https://drive.google.com/drive/folders/1TQ0zZKLWZikVT6U1ftV9AVQbn7pBbJrk?usp=sharing

Photos taken for almost all flights

- Camera was mounted on an interior bubble window with view of inlets.
- Photo taken every 2 seconds
- Drive includes all photos as well as flights in video form.
- Unfortunately photo time stamps are not accurate.

Files are here:

https://drive.google.com/drive/folders/1TQ0zZKLWZikVT6U1ftV9AVQbn7pBbJrk?usp=sharing

Met data update

Mike Robinson

Questions?