Monthly Webex Tag-up, 9 July 2015

Agenda

1. Announcements and opportunities

2. Colorado Pipeline Fire

3. Science Presentations

Fall AGU 2015 Abstract Submission (Results)

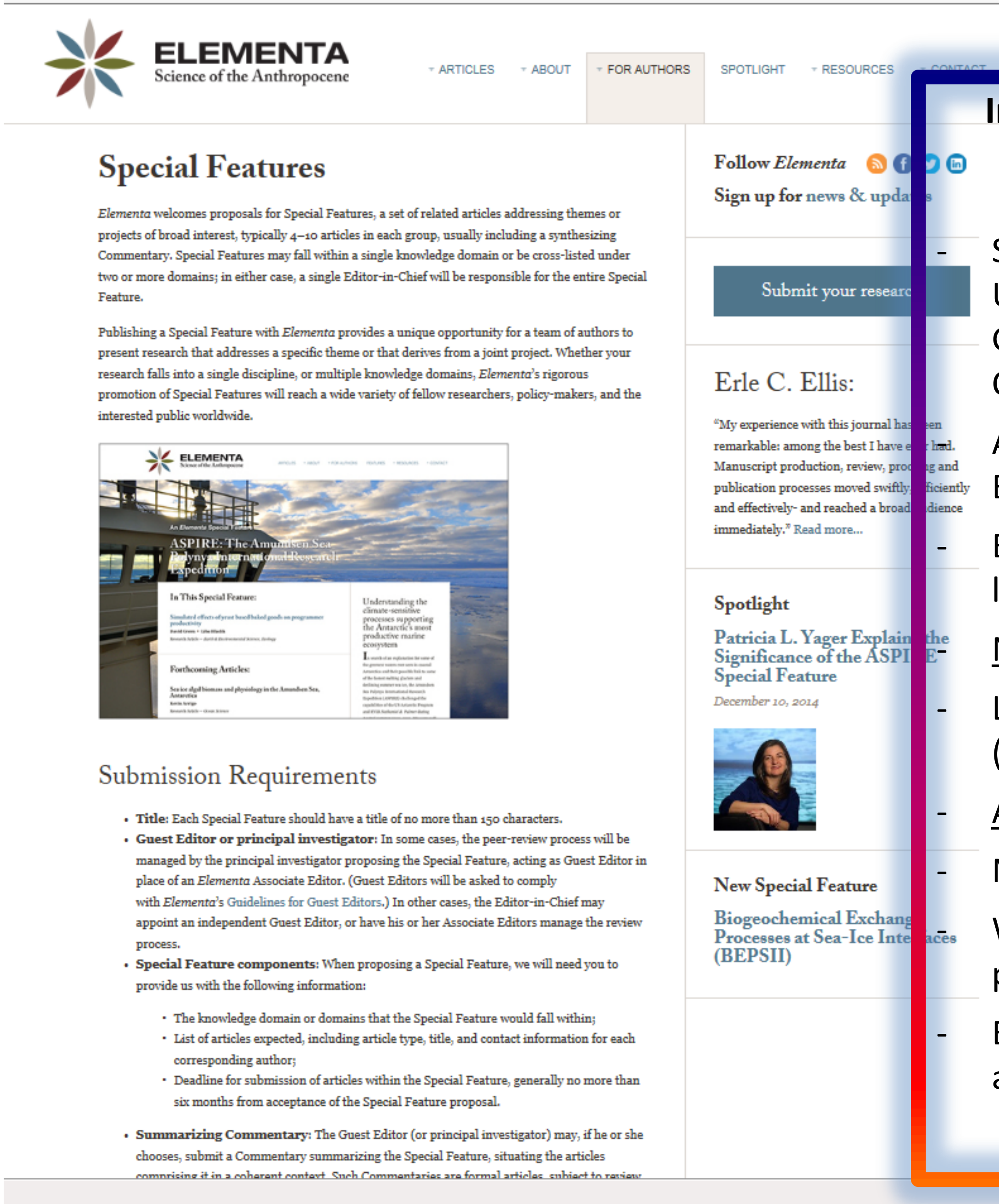
Our two sponsored sessions received an overwhelming response.

A011: Air Quality Research: From Emissions to Impacts
Conveners: Gabi Pfister, Patrick Reddy, Greg Frost, and Annmarie Carlton

150 abstracts submitted

A041: Emergence of a Global Observing System for Air Quality: Integrated Approaches Using Observations and Models of Tropospheric Composition and Pollution to Inform Air Quality Analyses and Applications
Conveners: Jay Al-Saadi, Caroline Nowlan, Gangwoong Lee, and Henk Eskes

75 abstracts submitted



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Science of the Anthropocene

ARTICLES · ABOUT · FOR AUTHORS · SPOTLIGHT · RESOURCES · CONTACT

Special Features

Elementa welcomes proposals for Special Features, a set of related articles addressing themes or projects of broad interest, typically 4–10 articles in each group, usually including a synthesizing Commentary. Special Features may fall within a single knowledge domain or be cross-listed under two or more domains; in either case, a single Editor-in-Chief will be responsible for the entire Special Feature.

Publishing a Special Feature with *Elementa* provides a unique opportunity for a team of authors to present research that addresses a specific theme or that derives from a joint project. Whether your research falls into a single discipline, or multiple knowledge domains, *Elementa*'s rigorous promotion of Special Features will reach a wide variety of fellow researchers, policy-makers, and the interested public worldwide.

ASPIRE: The Amundsen Sea Polynya International Research Expedition

Submission Requirements

- **Title:** Each Special Feature should have a title of no more than 150 characters.
- **Guest Editor or principal investigator:** In some cases, the peer-review process will be managed by the principal investigator proposing the Special Feature, acting as Guest Editor in place of an *Elementa* Associate Editor. (Guest Editors will be asked to comply with *Elementa*'s Guidelines for Guest Editors.) In other cases, the Editor-in-Chief may appoint an independent Guest Editor, or have his or her Associate Editors manage the review process.
- **Special Feature components:** When proposing a Special Feature, we will need you to provide us with the following information:
  - The knowledge domain or domains that the Special Feature would fall within;
  - List of articles expected, including article type, title, and contact information for each corresponding author;
  - Deadline for submission of articles within the Special Feature, generally no more than six months from acceptance of the Special Feature proposal.
- **Summarizing Commentary:** The Guest Editor (or principal investigator) may, if he or she chooses, submit a Commentary summarizing the Special Feature, situating the articles comprising it in a coherent context. Such Commentaries are formal articles, subject to review

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Erle C. Ellis:

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Spotlight

Patricia L. Yager Explains the Significance of the ASPIRE Special Feature

December 10, 2014

New Special Feature

Biogeochemical Exchange Processes at Sea-Ice Interfaces (BEPSII)

Invitation for a FRAPPE/DISCOVER-AQ Special Feature in Elementa

- Six Knowledge Domains, all hosted by major US universities (Dartmouth, Univ. Michigan, Georgia Tech., Univ. Washington, Univ. of Colorado)
- Atmospheric Science Domain hosted by CU Boulder (Detlev Helmig Editor-in-Chief)
- Elementa will set up dedicated website with listing of papers and ancillary information
- Non-profit peer-reviewed journal
- Low, discounted flat rate publication fee (~$1,200 for special feature articles)
- All open access
- No page limit
- Well recognized by public, media, and policy makers
- Experienced Associate Editor Board; can appoint Special Feature Guest Editor

NGL Pipeline Fire during Discover AQ/Frappe Campaigns

Aug 13, 2015

Tara Yacovitch, Aerodyne Research Inc.

tyacovitch@aerodyne.com

Overland Pass Pipeline (OPLL)

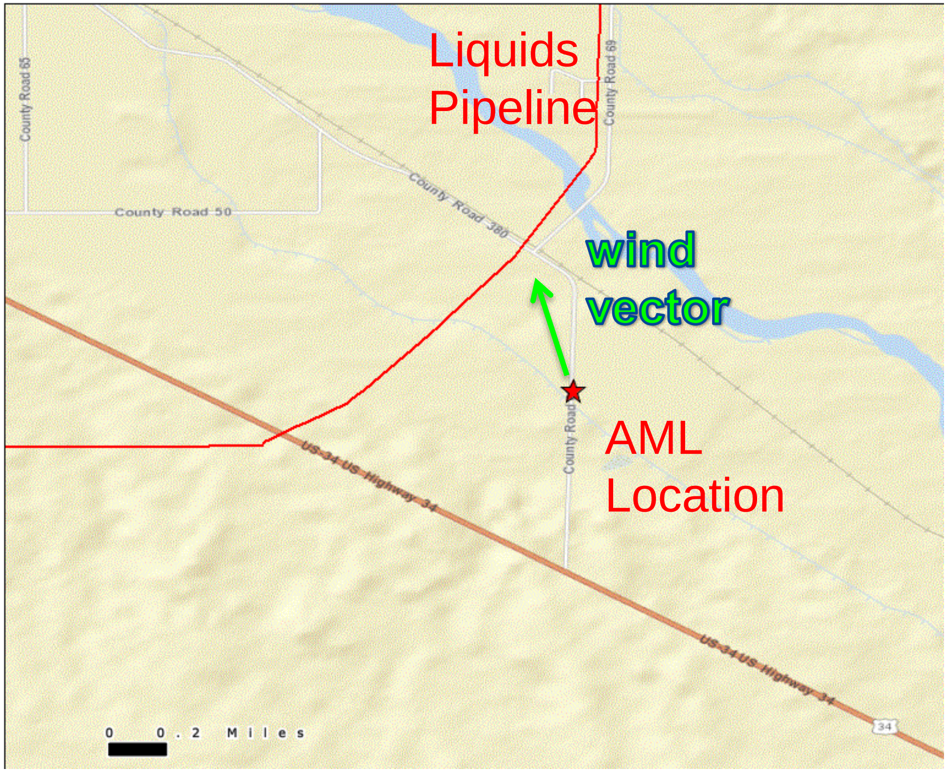


Image from the National Pipeline Mapping System, https://www.npms.phmsa.dot.gov/PublicViewer/composite.jsf

- Estimated Lat/Lon of pipeline fire:

  40.34641 -104.41852

- Duration of Fire:

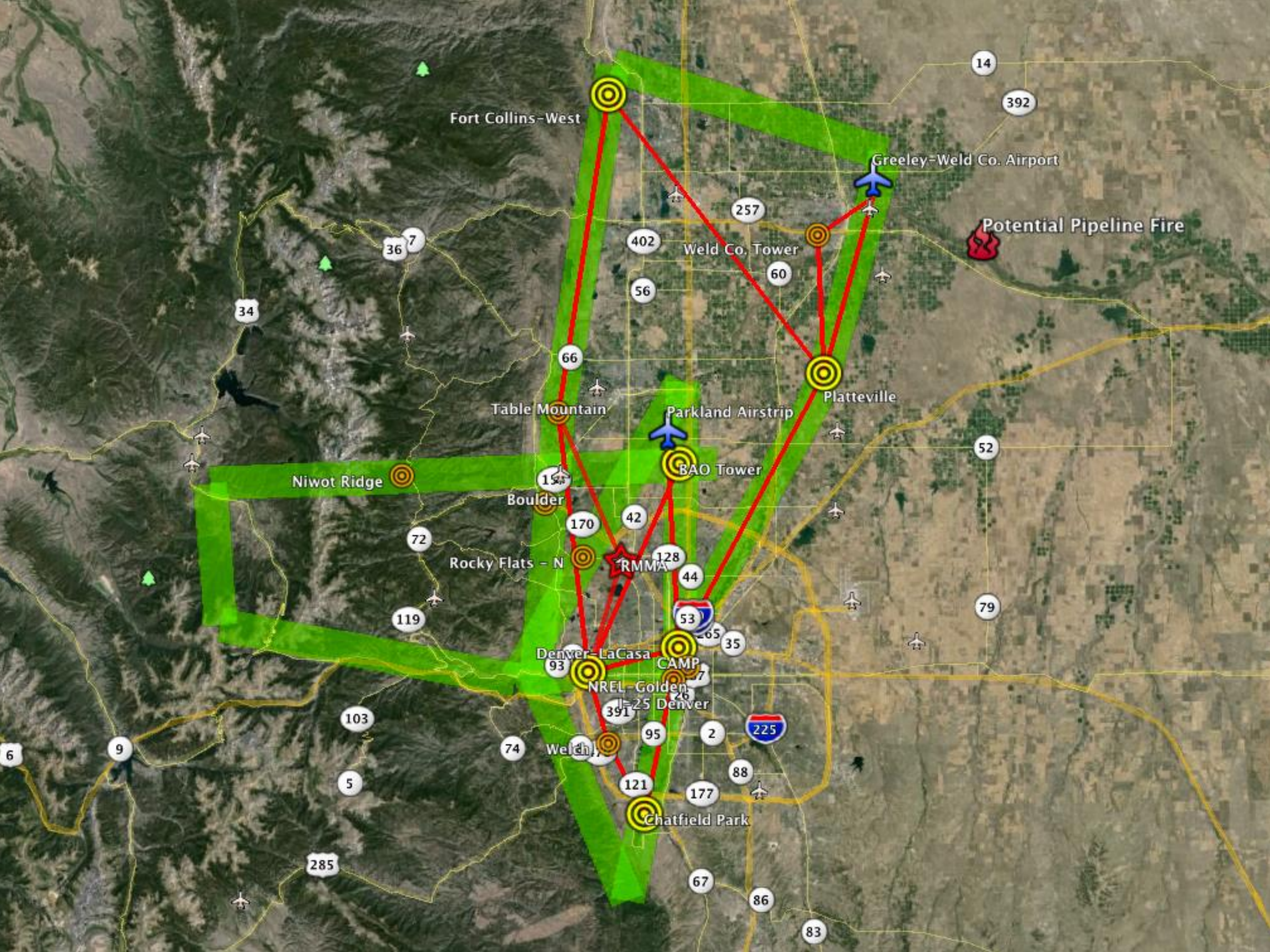
  July 21 – July 27

A helpful comment from Brad Pierce in response to discussion about the location of the fire…

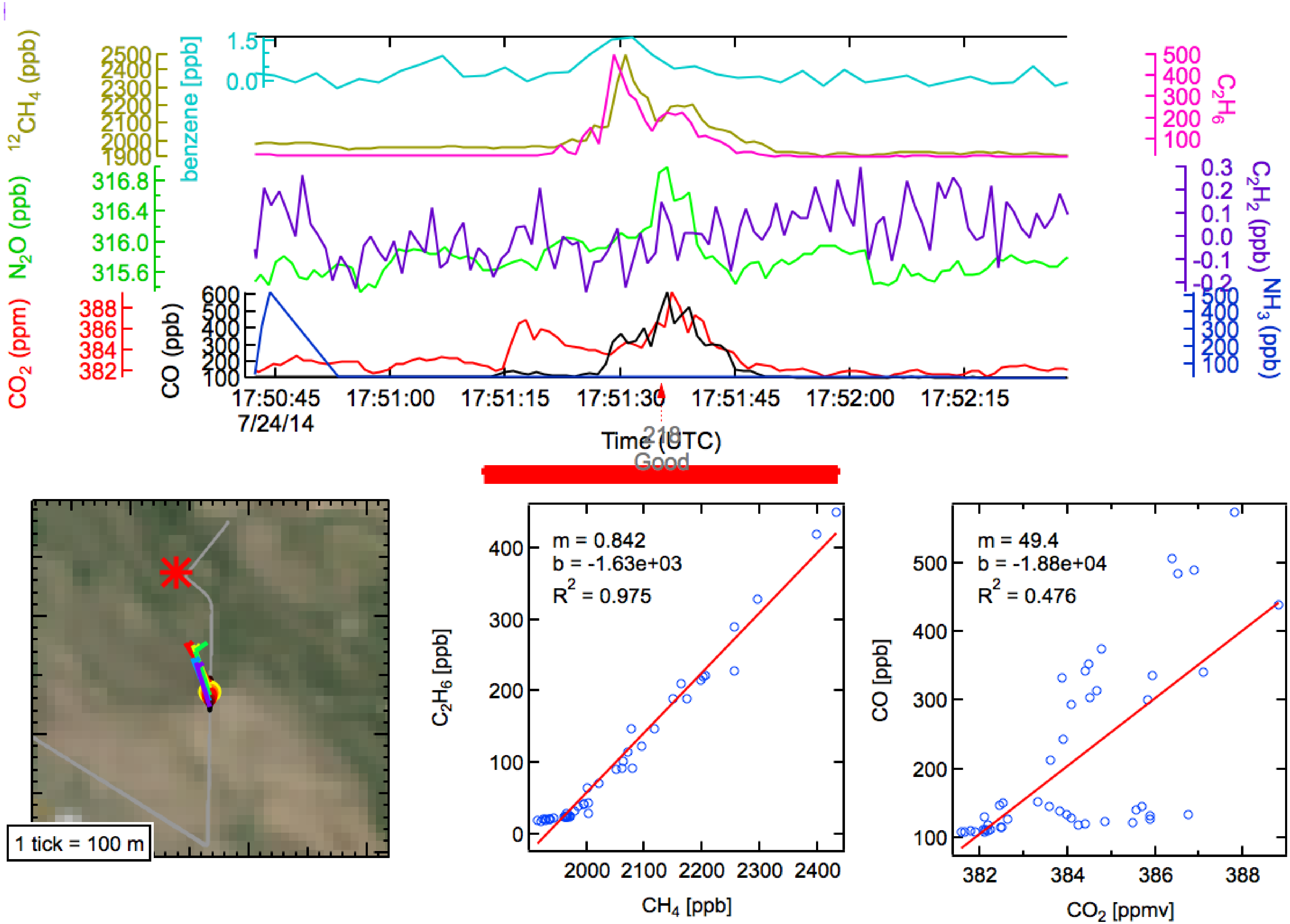
The NOAA National Geophysical Data Center (NGDC) Earth Observation Group (EOG, http://www.ngdc.noaa.gov/eog/index.html) uses VIIRS Day Night Band (DNB) data along with other VIIRS channels, to detect nighttime fires and distinguish fires (relatively cold planck temperatures) from flares (high planck temperatures). Could use these measurements to further characterize the flaring associated with the liquid pipeline fire. There are kml files with flare detections and temperatures at:

http://www.ngdc.noaa.gov/eog/viirs/download_viirs_fire.html

The main POC for this effort is Chris Elvidge at NGDC (chris.elvidge@noaa.gov).



Fort Collins-West
Greeley-Weld Co. Airport
Potential Pipeline Fire
Weld Co. Tower
Platteville
Table Mountain
Parkland Airstrip
BAO Tower
Niwot Ridge
Boulder
Rocky Flats - N
RMMA
Denver-LaCasa
CAMP
NREL-Golden
I-25 Denver
Welch
Chatfield Park



$^{12}CH_4$ (ppb)
2500
2400
2300
2200
2100
2000
1900
benzene [ppb]
1.5
0.0
500
400
300
200
100
C_2H_6
N_2O (ppb)
316.8
316.4
316.0
315.6
0.3
0.2
0.1
0.0
-0.1
-0.2
C_2H_2 (ppb)
CO_2 (ppm)
388
386
384
382
CO (ppb)
600
500
400
300
200
100
NH_3 (ppb)
17:50:45
7/24/14
17:51:00
17:51:15
17:51:30
17:51:45
17:52:00
17:52:15
Time (UTC)
218
Good
1 tick = 100 m
m = 0.842
b = -1.63e+03
R^2 = 0.975
C_2H_6 [ppb]
CH_4 [ppb]
m = 49.4
b = -1.88e+04
R^2 = 0.476
CO [ppb]
CO_2 [ppmv]

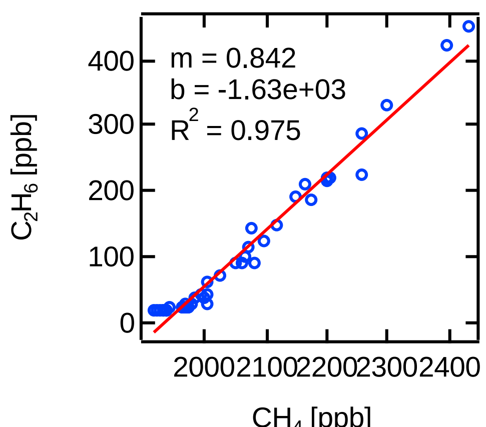
NGL Composition

Raw Product:

- 0.012% CH_4, 10% C_2H_6
- $C_2H_6/CH_4 = 844$

Uncombusted:

- $C_2H_6/CH_4 = 0.842$



What are natural gas liquids and how are they used?

NGL Attribute Summary				eia
Natural Gas Liquid	**Chemical Formula**	**Applications**	**End Use Products**	**Primary Sectors**
Ethane	C_2H_6	Ethylene for plastics production; petrochemical feedstock	Plastic bags; plastics; anti-freeze; detergent	Industrial
Propane	C_3H_8	Residential and commercial heating; cooking fuel; petrochemical feedstock	Home heating; small stoves and barbeques; LPG	Industrial, Residential, Commercial
Butane	C_4H_{10}	Petrochemical feedstock; blending with propane or gasoline	Synthetic rubber for tires; LPG; lighter fuel	Industrial, Transportation
Isobutane	C_4H_{10}	Refinery feedstock; petrochemical feedstock	Alkylate for gasoline; aerosols; refrigerant	Industrial
Pentane	C_5H_{12}	Natural gasoline; blowing agent for polystyrene foam	Gasoline; polystyrene; solvent	Transportation
Pentanes Plus*	Mix of C_5H_{12} and heavier	Blending with vehicle fuel; exported for bitumen production in oil sands	Gasoline; ethanol blends; oil sands production	Transportation

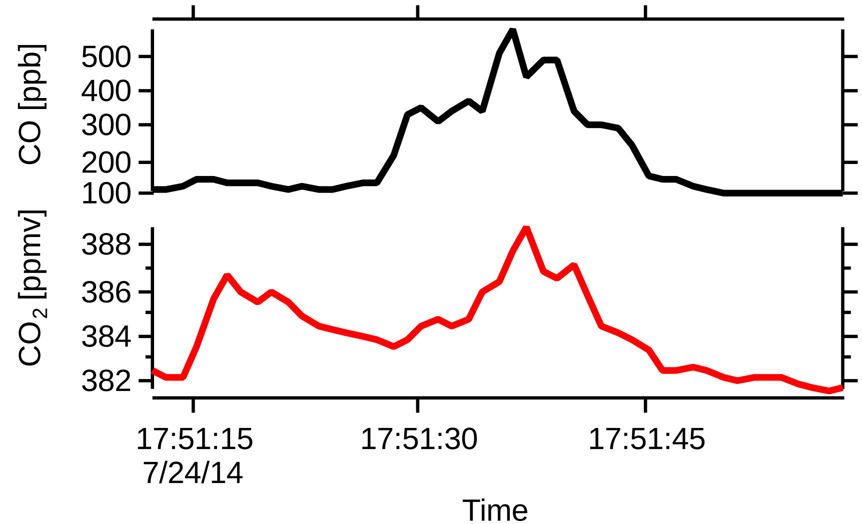
C indicates carbon, H indicates hydrogen; Ethane contains two carbon atoms and six hydrogen atoms

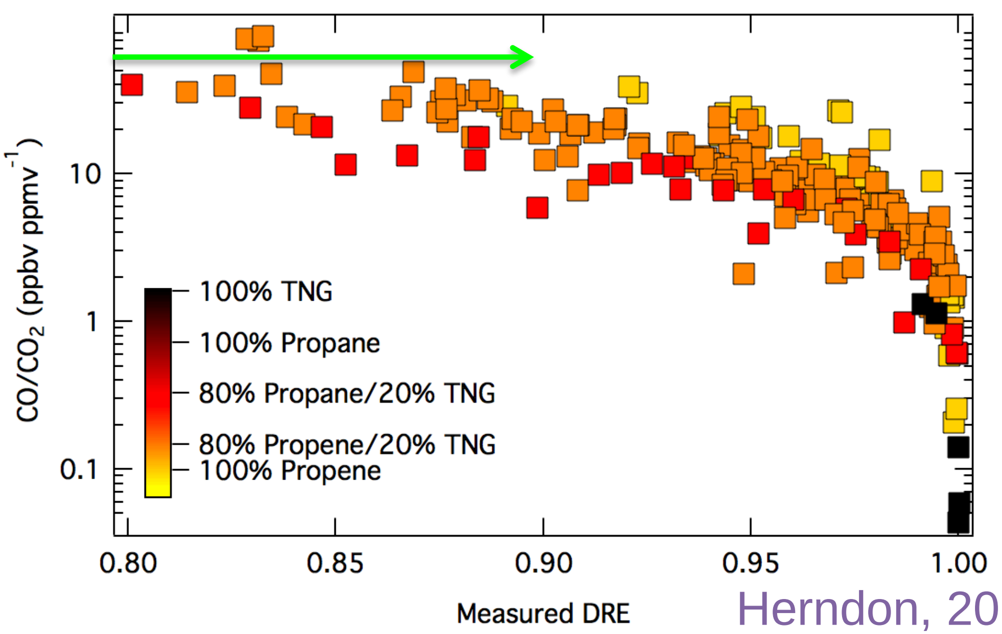
*Pentanes plus is also known as "natural gasoline." Contains pentane and heavier hydrocarbons.

Source: U.S. Energy Information Administration, Bentek Energy LLC.

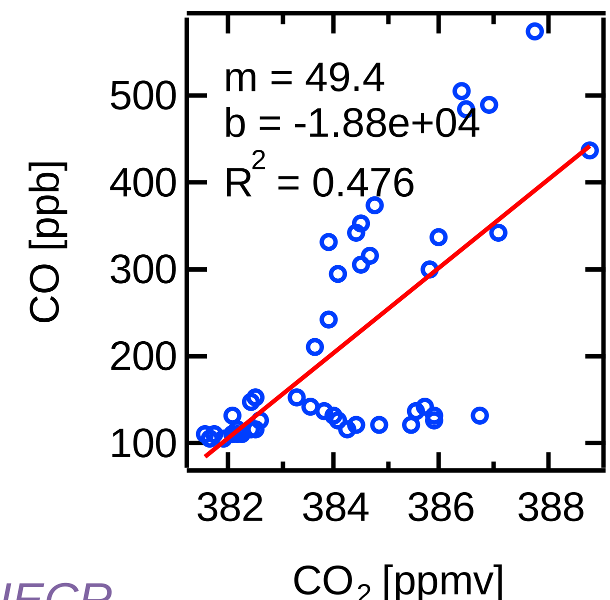
Flare/Fire Destruction

- $CO/CO_2 = 0.049$ (0.49%)
- $CO/CO_2 < 0.01$:
  - – functioning process flare



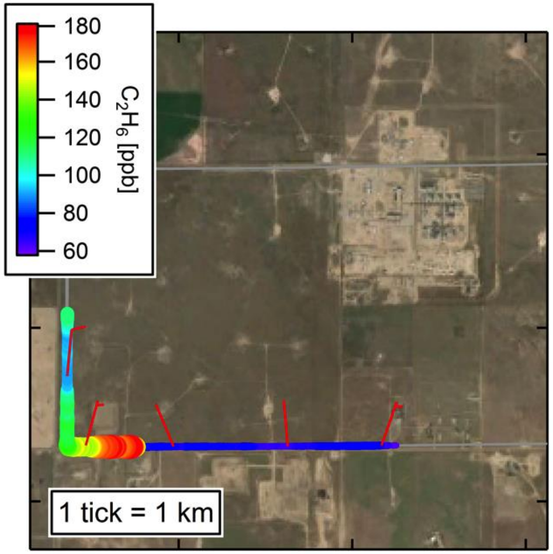


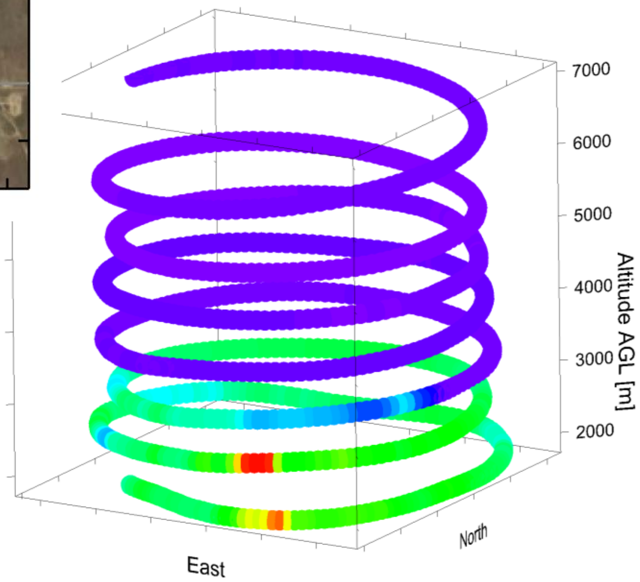
Herndon, 2012, *IECR*



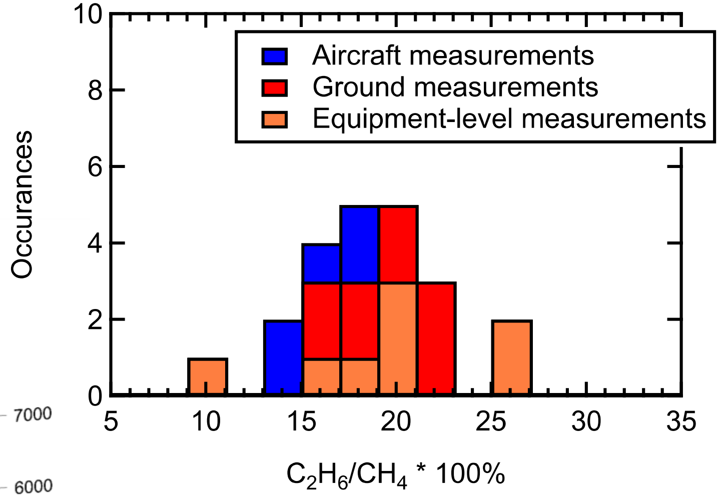
Impact on Other Sites

- Ethane at Ft-Lupton (Platteville)





- C_2H_6/CH_4 : 15-22%



Disruption at Wattenberg Plant as well.

Info From Operator, courtesy Daniel Bon:

"The Overland Pass Pipeline did have a fire event (reported to CDPHE) at a block valve south of the South Platte River crossing in July, 2014. This fire was an upset condition that occurred to the block valve mechanical equipment. The incident is contained in the PHMSA Database hl2010toPresent.xlsx. The event started on July 21st and was extinguished when the pipeline was empty on July 27, 2014. The Overland Pass Pipeline (OPPL) system contains natural gas liquids (NGL). NGL is considered a highly volatile liquid (HVL). NGL are created from gas processing and would have been liquid coming from nearby gas plants. The shutdown of the NGL line did cause gas processing facilities to temporarily shut down because there was no outlet for the NGL. NGL carry only a small amount of methane. The material released from the fire only had 0.012% of methane based on samples taken nearby. The ethane content of the liquid was about 10%. Ethane can be as much as 50% in an NGL pipeline, but due to the very low ethane prices, gas processing plants in Colorado are currently not separating out ethane specifically as they are considered in "ethane rejection". This practice has been in place throughout all of 2014 and is presently continued. It was estimated that about 2,255.2 bbls of NGL's were released during the event. The VOC content is just about 100%, although the regulated VOC's in this liquid were about 89-90% due to the presence of ethane (which is not a regulated VOC). The NGL's were either released through the fire, which efficiently burned through the event (no smoking was observed which indicated complete burn), or in portable flares that were brought to the site to remove liquid from the pipeline. Therefore, an overall estimated control of 95% was used to estimate emissions released to the atmosphere. The total estimated release to the atmosphere was 40 lbs of methane and 1.26 tons of ethane.

Do we have any questions we would like to ask Williams about the incident?

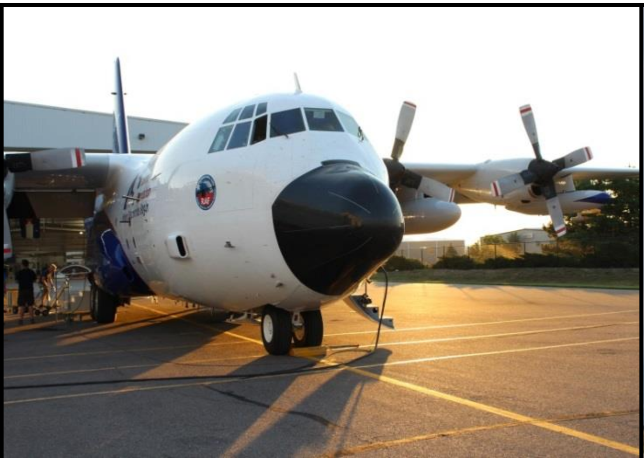
Daniel Bon has agreed to collate any requests for information and communicate with them on our behalf.

SCIENCE PRESENTATIONS

Observations of VOCs in the Colorado Front Range during FRAPPÉ

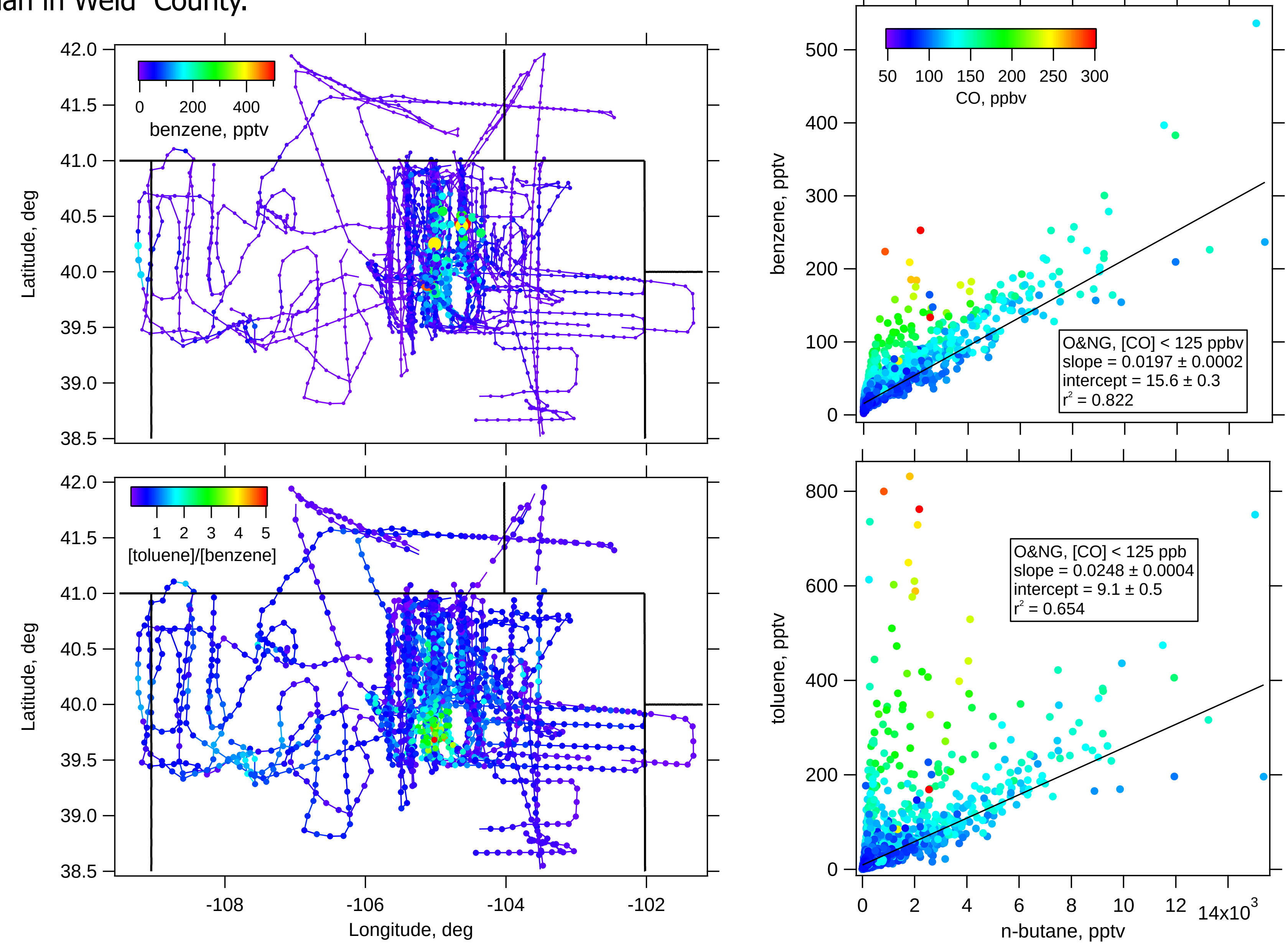
Rebecca Hornbrook[1,*], Eric Apel[1], Alan Hills[1], Don Blake[2], Nicola Blake[2], Jason Schroeder[2], Alan Fried[3], Petter Weibring[3], Dirk Richter[3], Jim Walega[3], Andy Weinheimer[1], Deedee Montzka[1], Meghan Stell[1], John Orlando[1], Geoff Tyndall[1], Teresa Campos[1], Brian Heikes[4], Victoria Treadaway[4], Dan O'Sullivan[5], Greg Huey[6], David Tanner[6], Ron Cohen[7], Frank Flocke[1], Gabi Pfister[1], and the FRAPPÉ science team

[1]NCAR, Boulder, CO, *rsh@ucar.edu; [2]University of California, Irvine, CA; [3]University of Colorado, Boulder, CO; [4]University of Rhode Island, Kingston, RI; [5]United States Naval Academy, Anapolis, MD; [6]Georgia Institute of Technology, Atlanta, GA; [7]Univeristy of California , Berkeley, CA.



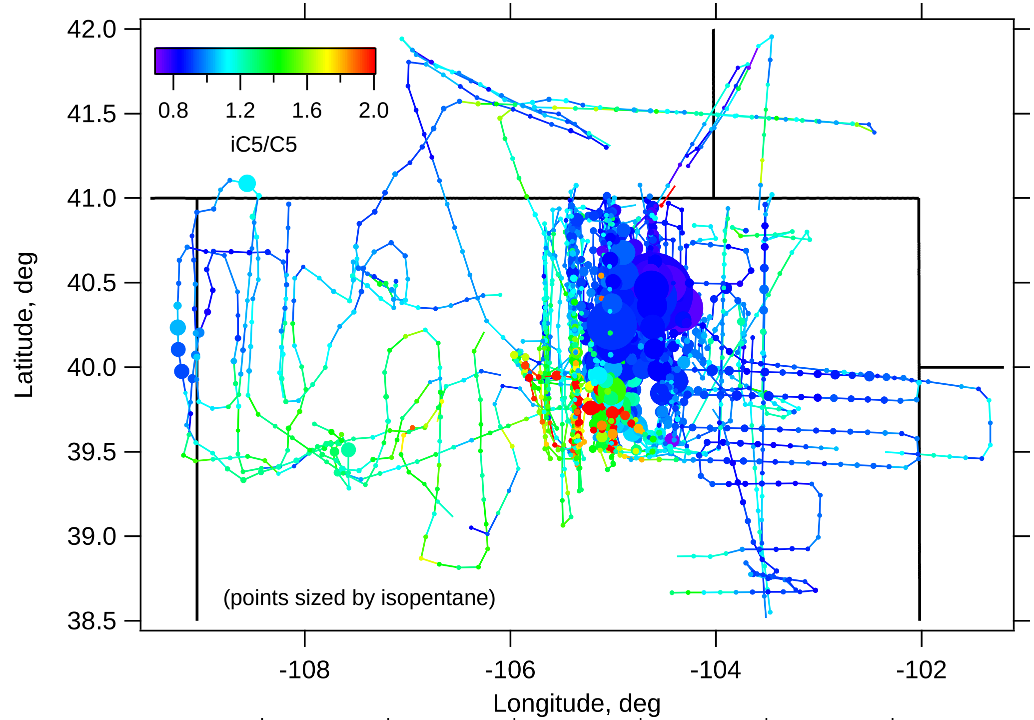
Benzene and Toluene

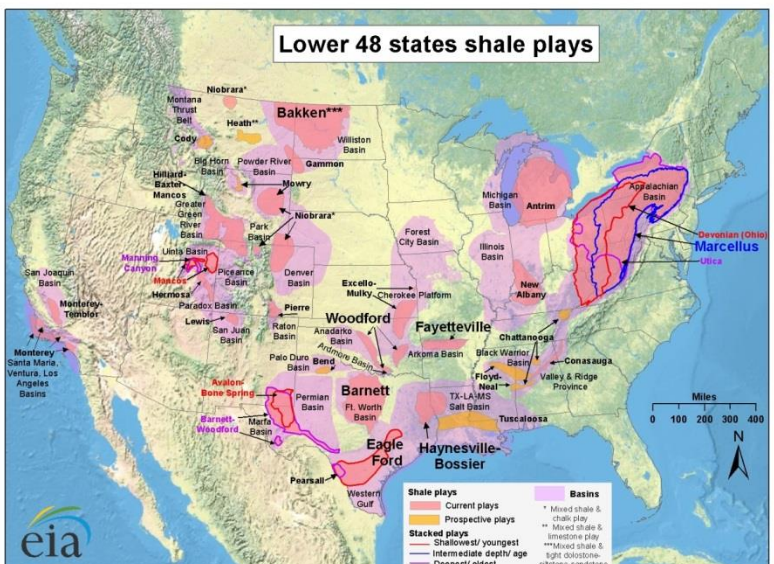
Emission ratios [VOC]/[CO] of benzene and toluene vary significantly between Denver and Weld County. Both are correlated with *n*-butane emissions where CO is low, but in the Denver area, [toluene]/[benzene] ratios are much higher than in Weld County.



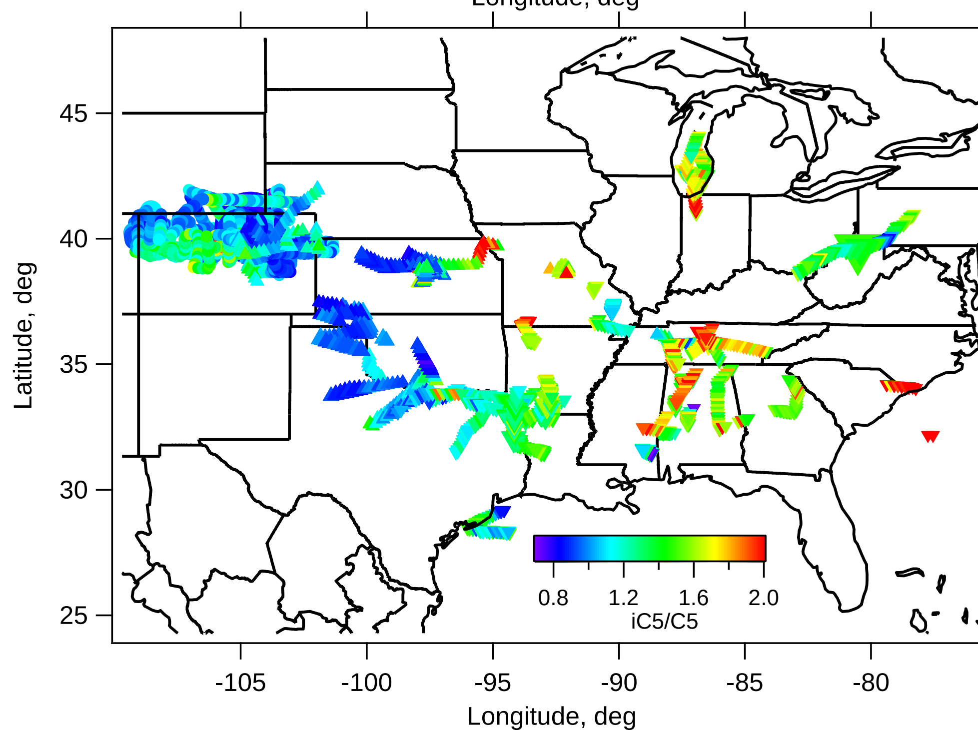
Pentane Ratios

Ratios of isopentane/n-pentane (iC5/C5) are useful for contrasting Oil & Natural Gas (O&NG) (0.8-1.0) vs. urban emissions (1.5-2.5).



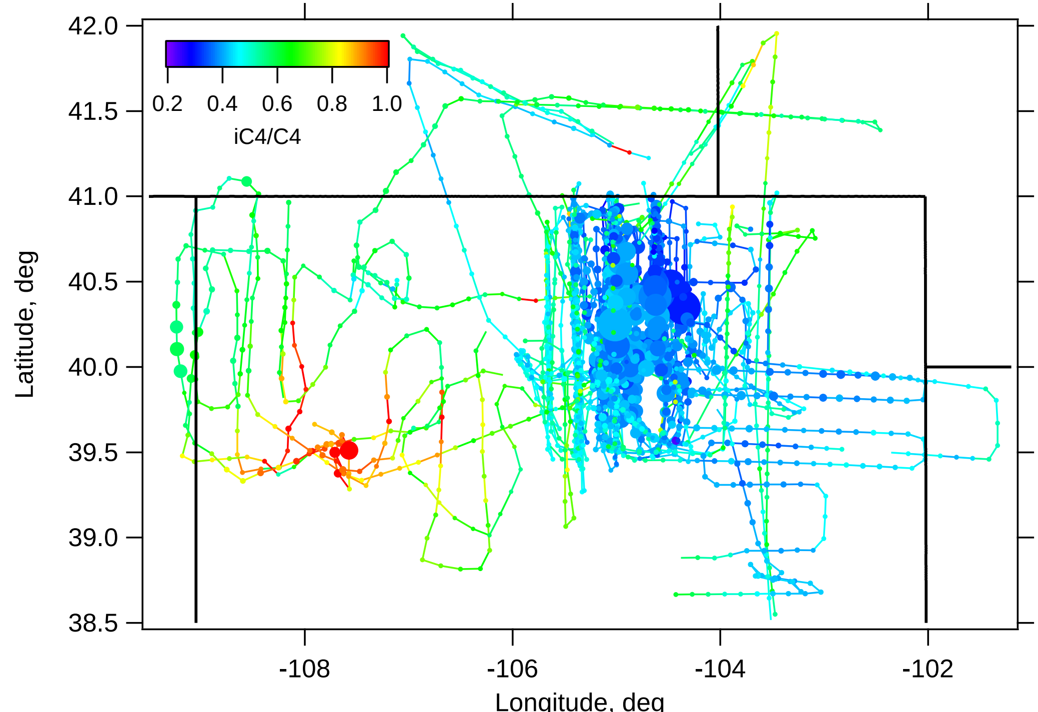


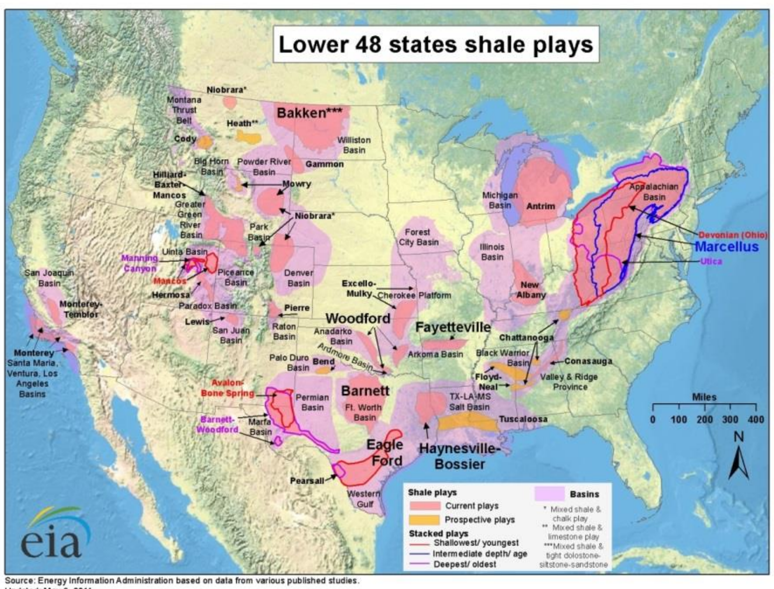
Source: Energy Information Administration based on data from various published studies.
Updated: May 9, 2011

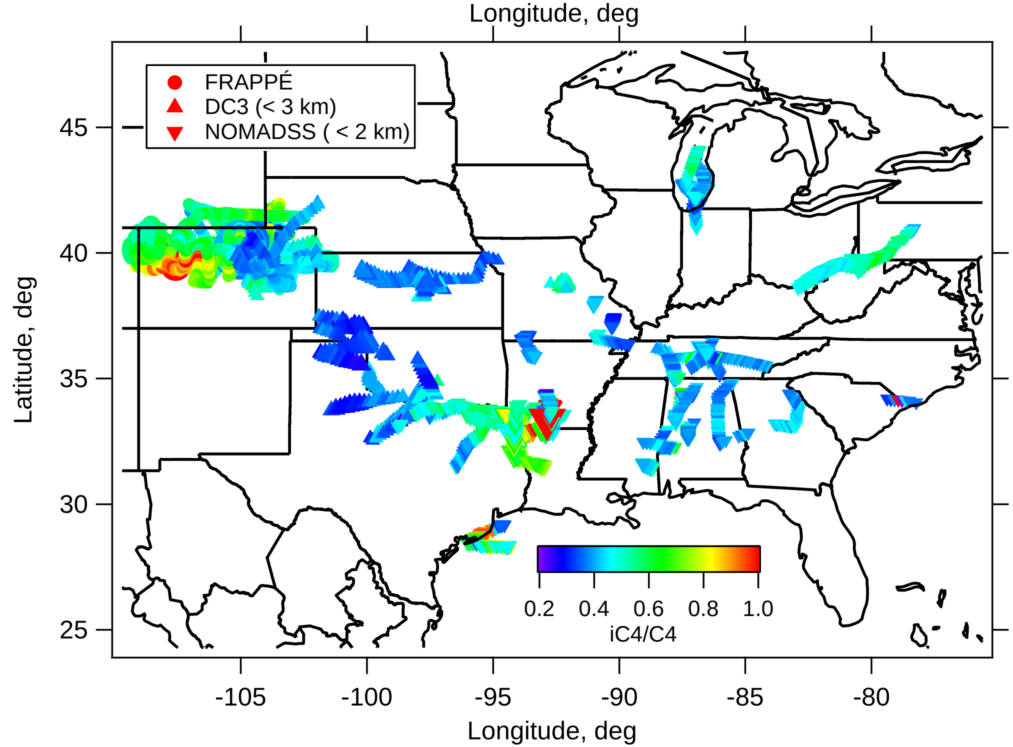


Butane Ratios

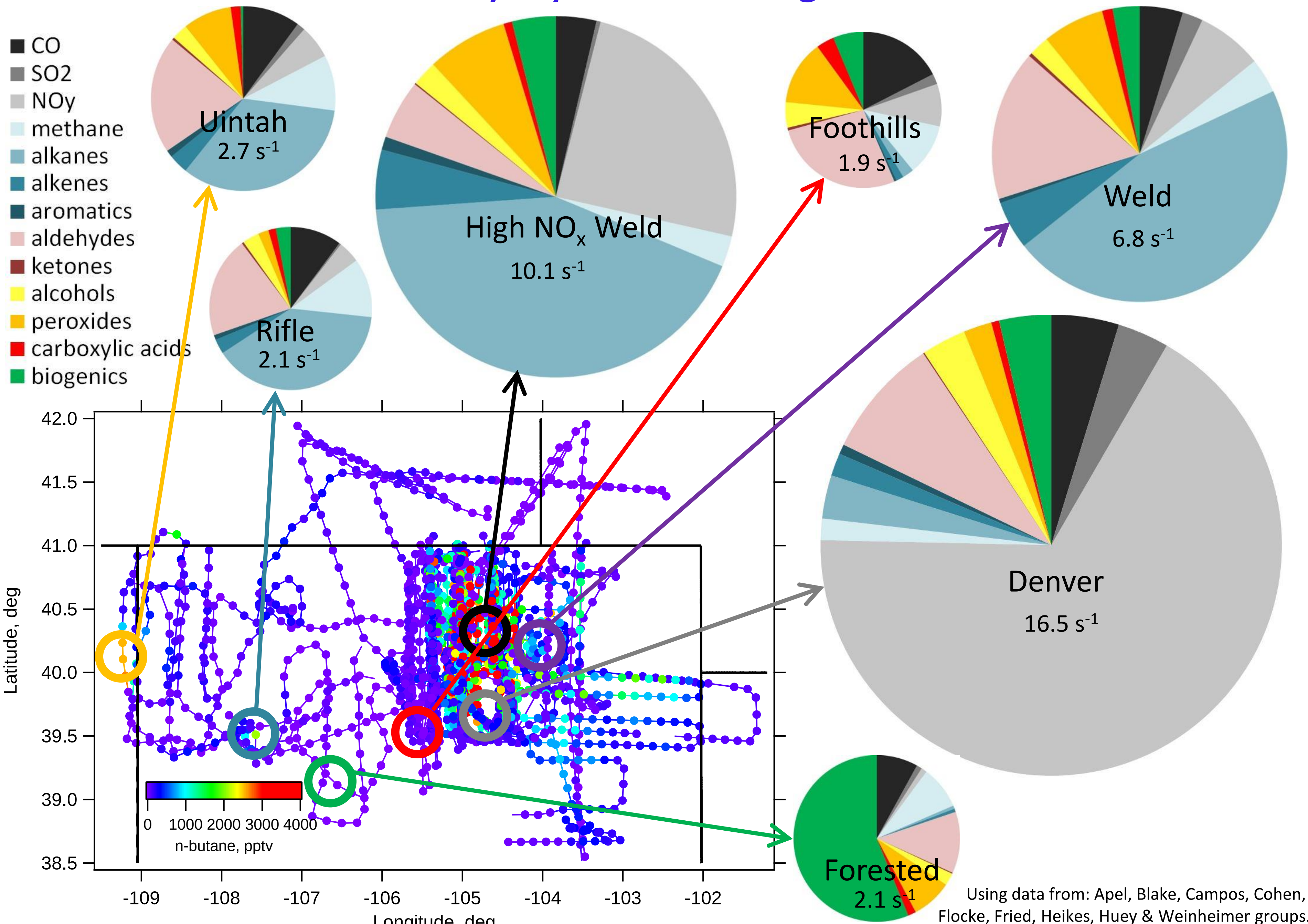
Similarly, ratios of isobutane/ n-butane (iC4/C4) can be used to differentiate between different O&NG extraction activities and different shale plays.







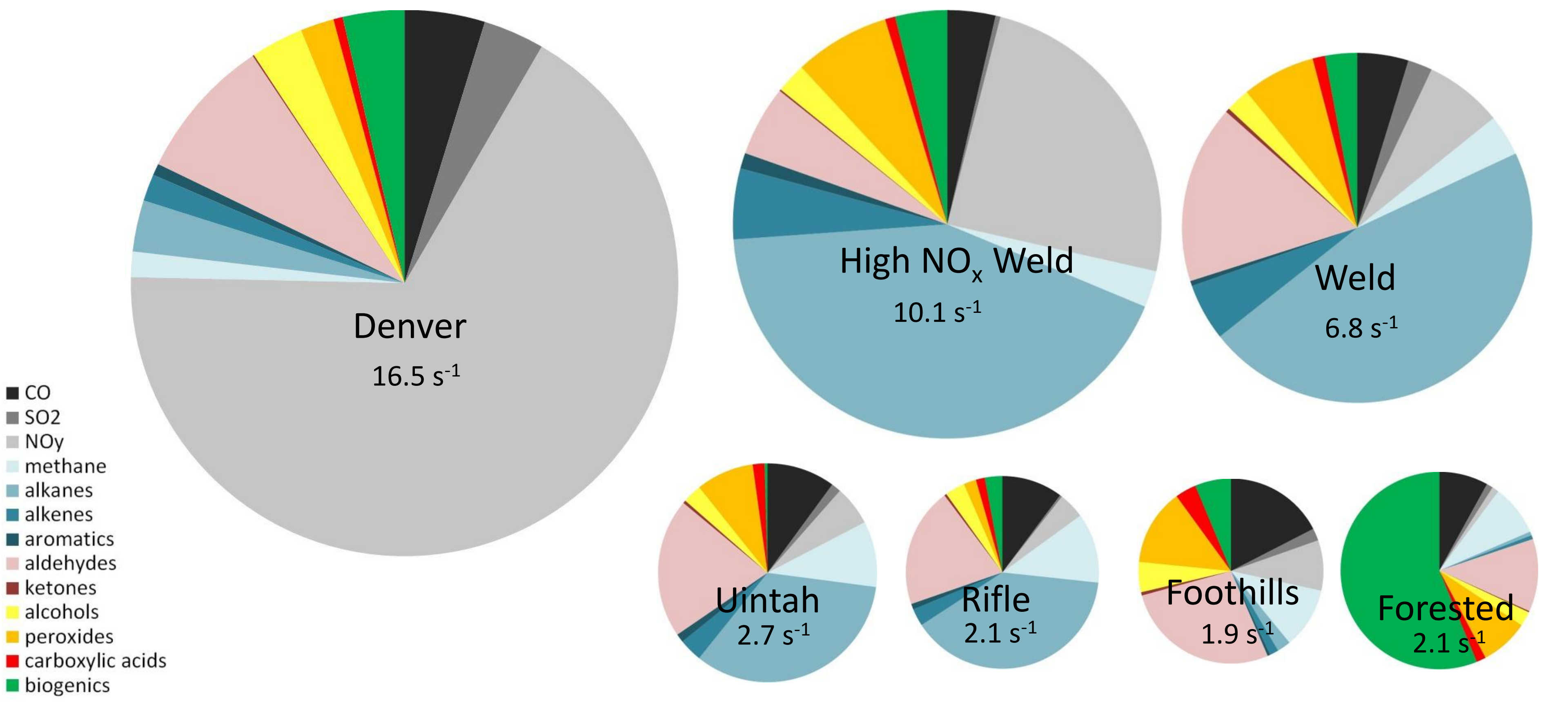
Calculated OH Reactivity by FRAPPÉ region



Using data from: Apel, Blake, Campos, Cohen, Flocke, Fried, Heikes, Huey & Weinheimer groups.

Ten largest contributors to OH reactivities by region

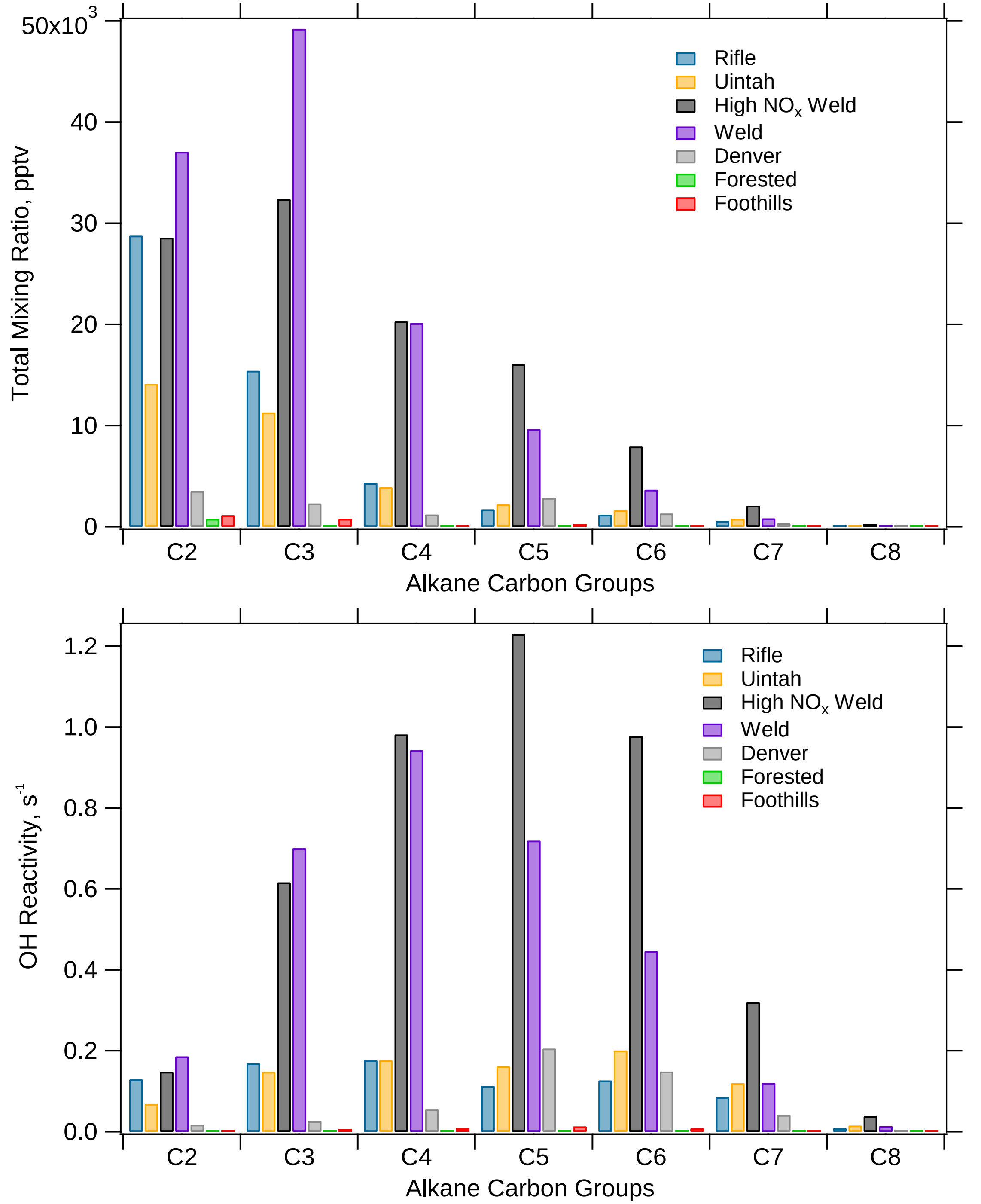
Denver		High NO_x Weld		Weld County		Uintah		Rifle		Foothills		Forested	
NO	9.75	NO_2	2.15	butane	0.74	CO	0.27	CH_4	0.24	HNO_3	0.39	isoprene	0.94
NO_2	7.40	NO	1.13	propane	0.70	HCHO	0.26	HCHO	0.23	HCHO	0.39	HCHO	0.20
CO	0.78	butane	0.75	CH_3CHO	0.57	CH_4	0.26	CO	0.21	CO	0.33	CH_4	0.18
HCHO	0.73	pentane	0.67	HNO_3	0.44	CH_3CHO	0.24	propane	0.17	CH_4	0.20	CO	0.17
SO_2	0.60	CH_3OOH	0.65	NO_2	0.43	HNO_3	0.22	CH_3CHO	0.15	CH_3OOH	0.18	HNO_3	0.16
CH_3CHO	0.55	propane	0.62	CH_3OOH	0.42	CH_3OOH	0.19	ethane	0.13	CH_3CHO	0.11	MVK	0.16
HNO_3	0.51	isopentane	0.51	HCHO	0.41	propane	0.15	HNO_3	0.11	NO_2	0.09	CH_3OOH	0.12
isoprene	0.44	CO	0.37	pentane	0.40	butane	0.12	butane	0.09	NO	0.08	MBO	0.06
ethanol	0.30	butenes	0.32	CO	0.32	NO_2	0.10	isobutane	0.09	methanol	0.07	CH_3CHO	0.05
CH_3OOH	0.29	2-methylpentane	0.29	butenes	0.28	methylcyclohexane	0.08	NO	0.06	H_2O_2	0.07	H_2O_2	0.05



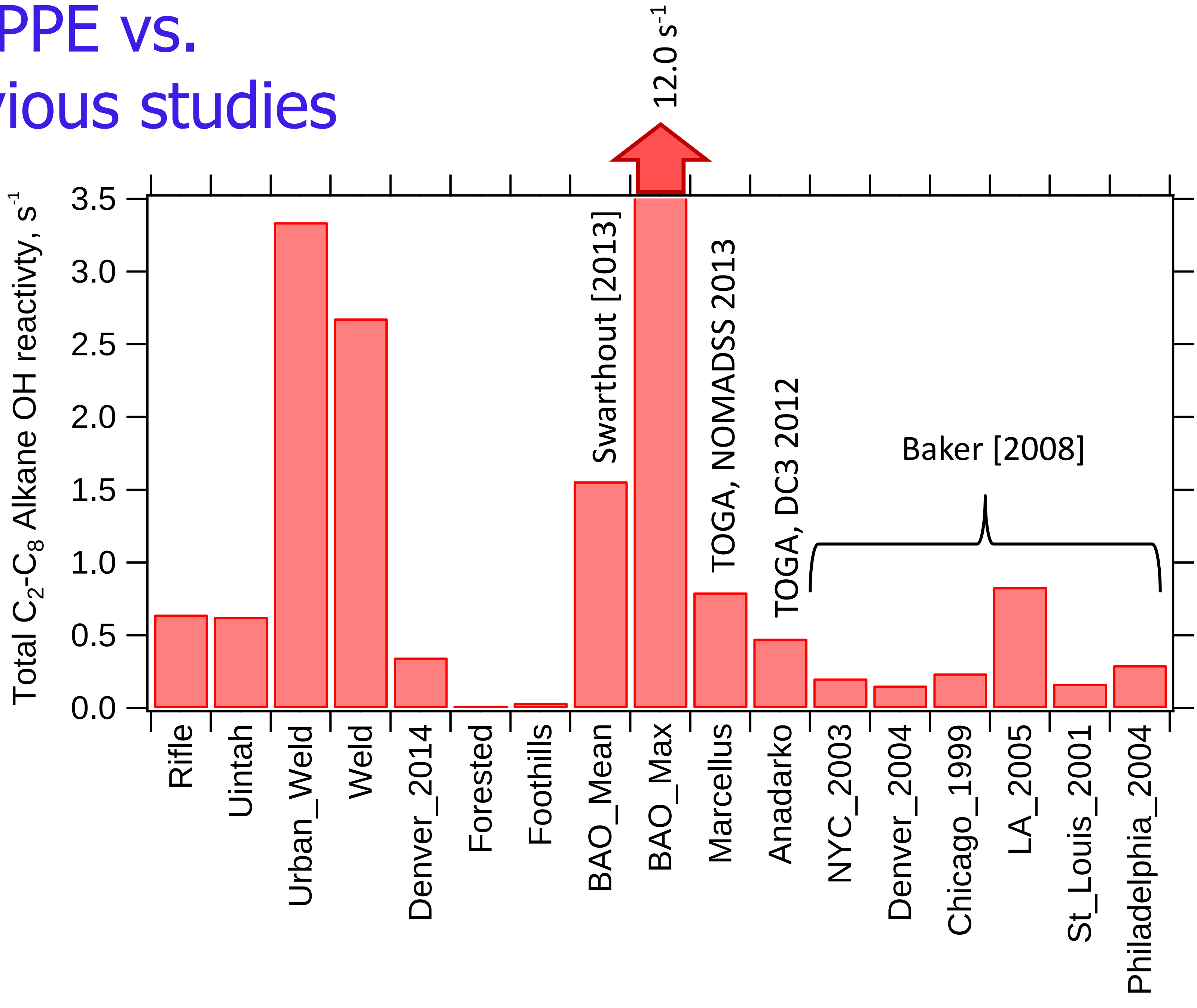
Alkane OH Reactivity Contributions

Total alkane mixing ratio by carbon number (top), and total alkane OH reactivity by carbon number (bottom). Alkane OH reactivities in Denver and high-NO_x Weld regions are greatest at C_5, while the lower-NO_x Weld

region is centered around C_4.



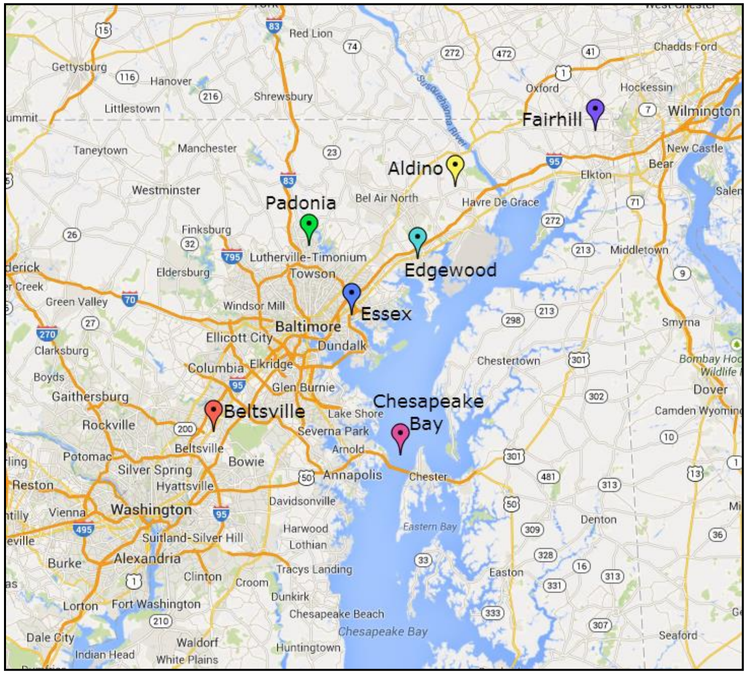
FRAPPÉ vs. previous studies



Large Vertical Gradient of Reactive Nitrogen Oxides in the Boundary Layer: Modeling Analysis of DISCOVER-AQ 2011 Observations

Yuzhong Zhang, Yuhang Wang, Gao Chen, Charles Smeltzer, James Crawford, Jennifer Olson, James Szykman, Andy Weinheimer, Armin Wisthaler, Alan Fried, Glenn Diskin

DISCOVER-AQ July, 2011 Baltimore



200+ vertical profiles measured over 6 sites

Questions

1. How do pollutants distribute in the boundary layer?
2. How well is the boundary layer mixed?
3. What factors affect the mixing state of pollutants?

Classification of vertical profiles

Height Stability	Deep >1km	Medium 0.5-1km	Shallow <0.5km
Turbulent (<0.1K/km)	40	-	-
Neutral (0.1-1K/km)	123	24	-
Stable (>1K/km)	-	7	12

Stability: potential temperature gradient

Distributions of profile category

	Deep &Turbulent	Deep &Neutral	Medium &Neutral	Stable	Total
Distribution of profile categories at varied local time					
6:00 -10:00	2	10	8	9	29
10:00 - 14:00	29	75	12	7	123
14:00 - 18:00	9	38	4	3	54
Distribution of profile categories at varied sites					
Padonia	5	24	2	3	34
Fairhill	9	25	5	1	40
Aldino	8	21	5	2	36
Edgewood	7	27	5	2	41
Essex	6	22	3	3	34
Beltsville	5	3	3	4	15
Chesapeake Bay	0	1	1	4	6

Analysis using a 1D model

200+ vertical profiles from Discover-AQ

$$\frac{dC_i}{dt} = K_i \frac{\partial^2 C_i}{\partial z^2}$$

1D-REAM

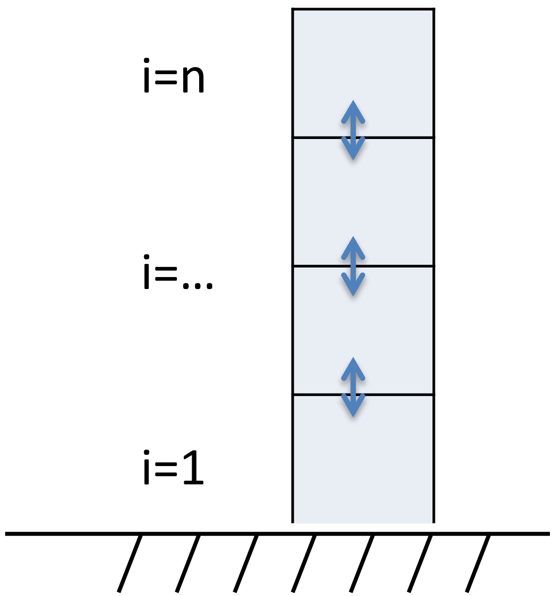
Radiation

O3-NOx-VOC Photochemistry
(Bey et al., 2001; Carter, 2009)

Dry/wet deposition

1D vertical transport

Weather Research and Forecast Model (WRF) meteorology field



Discover-AQ measurements as constraints

Ozone, CO, CH_2O

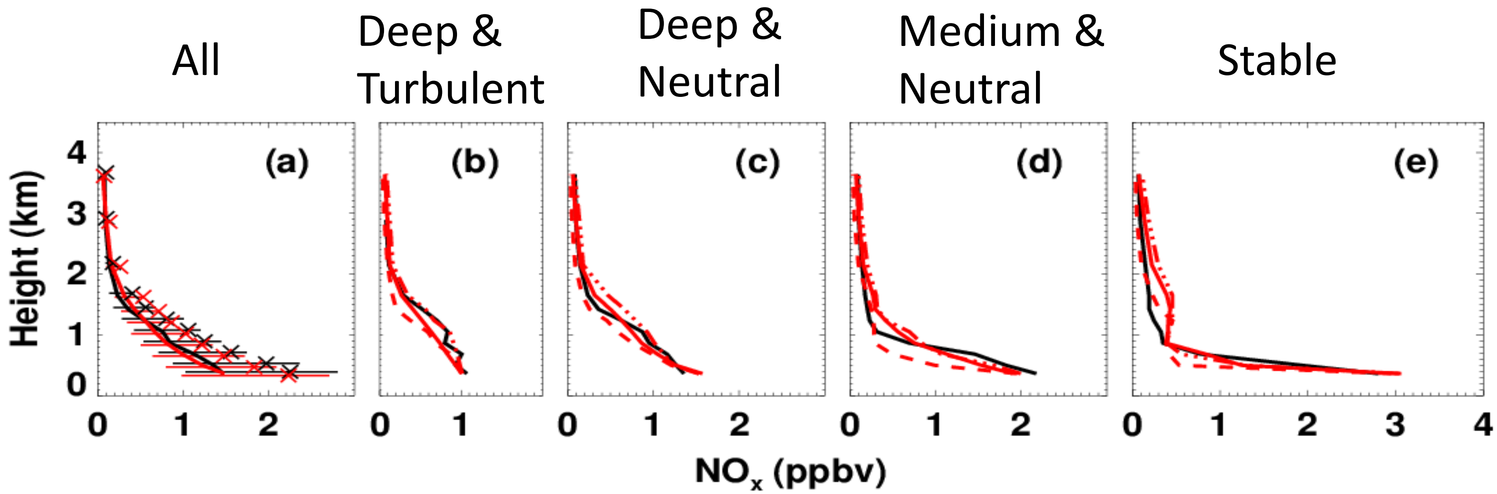
NO_x, toluene, xylene, isoprene

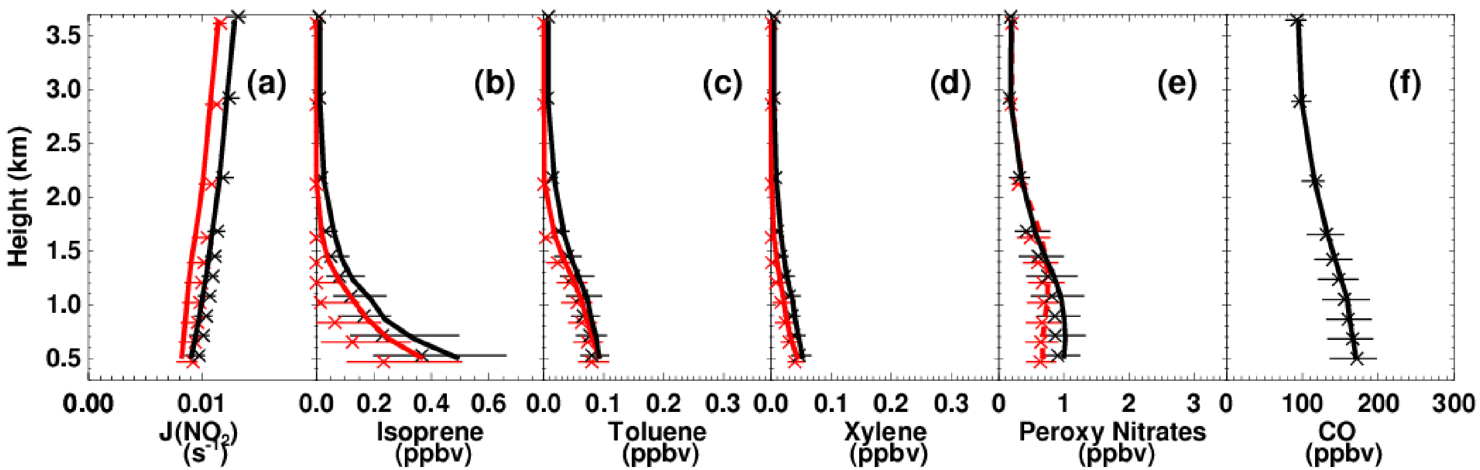
3D model

Alkane C>4, alkene C>=3, ethane, and propane

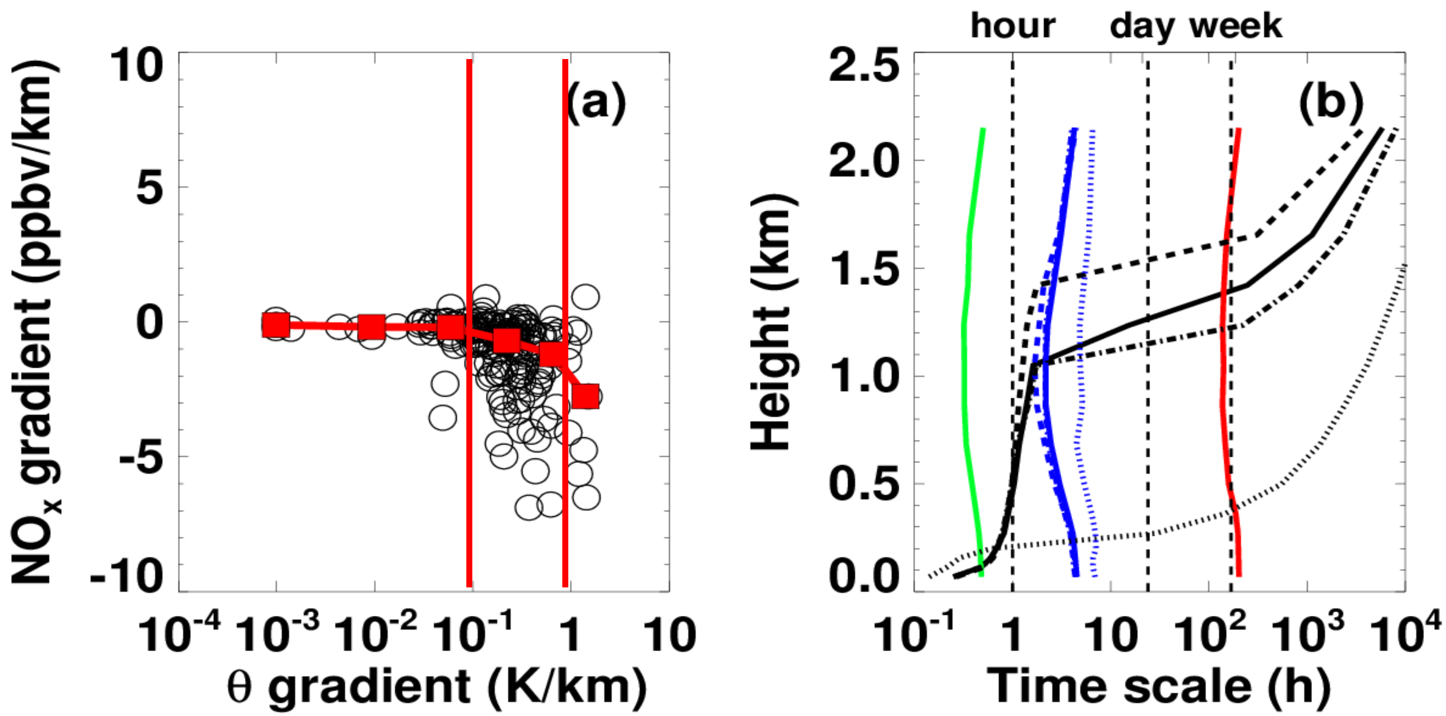
Simulated and observed median profiles

Black: observations
Solid red: ACM2
Dash-dotted red: YSU
Dashed red: MYJ





NOx gradient affected by BL stability



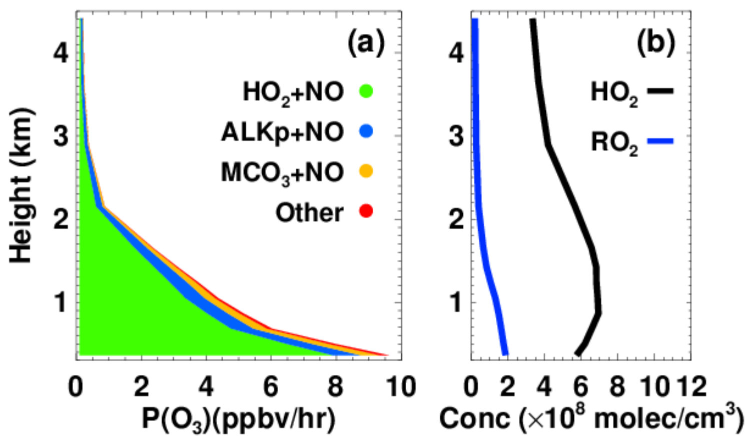
Dot: stable
Dash-dot: deep & neutral
Dash: deep & turbulent
Solid: all profiles

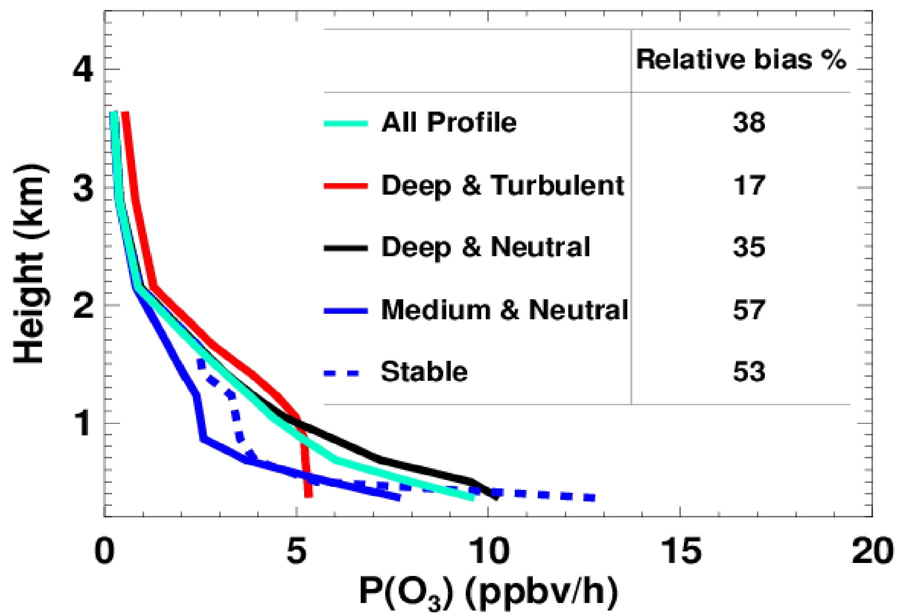
Black: mixing time
Green: isoprene
Blue: NOx
Red: CO

Impact on ozone production calculation

O3 production $$P(O_3)_i = k_{0,i}[NO]_i[HO_2]_i + \sum_{j=1}^{n} k_{j,i}[NO]_i[RO_2]_{j,i}$$

BL-averaged O3 production $$P(O_3)_{BL} = \frac{\sum_{i=k_{BLB}}^{k_{BLT}} P(O_3)_i \cdot h_i}{h_{BL}}$$

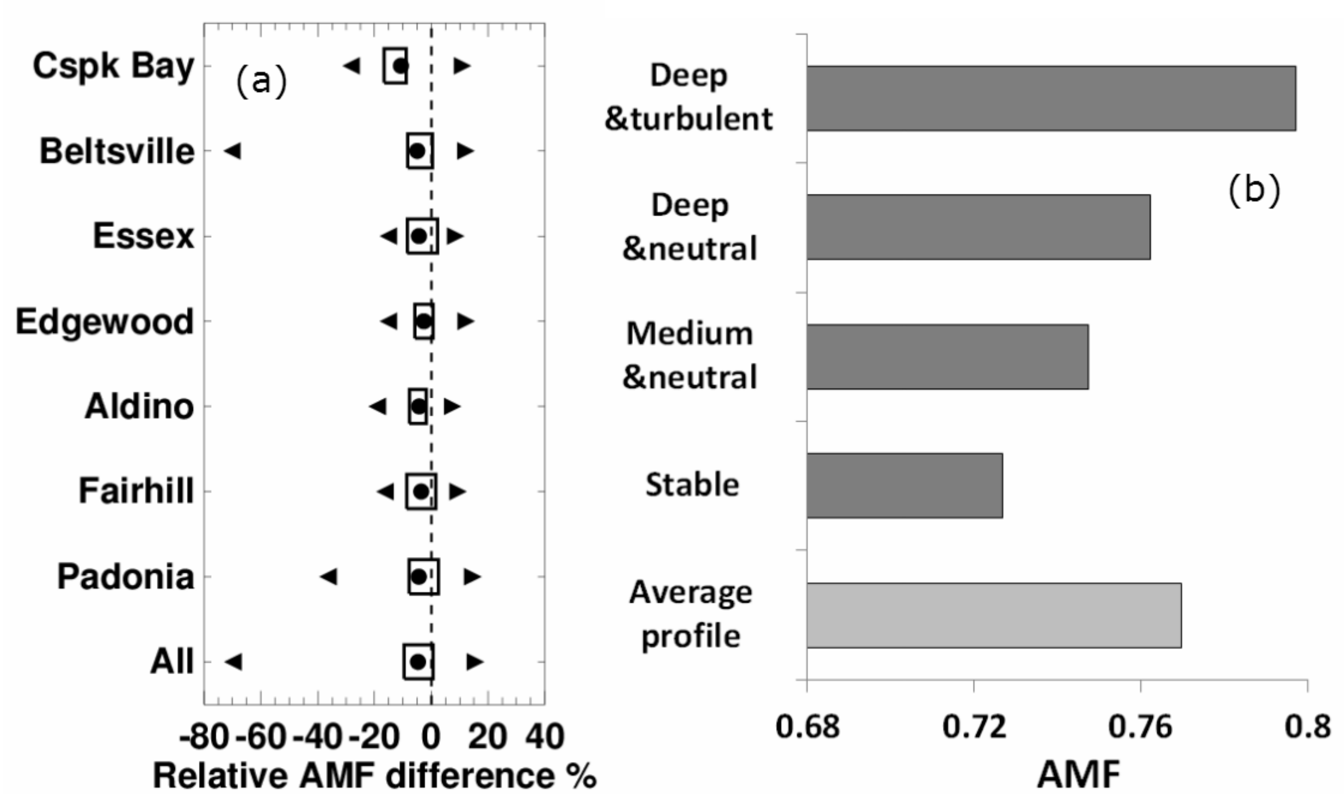




Impact on satellite NOx retrieval calculation

$$Vertical\_Column = \frac{Slant\_Column}{AMF}$$

$$\mathrm{AMF} = \frac{\int \mathrm{amf_h} \cdot \mathrm{c_h} \cdot d\mathrm{h}}{\int \mathrm{c_h} \cdot d\mathrm{h}}$$

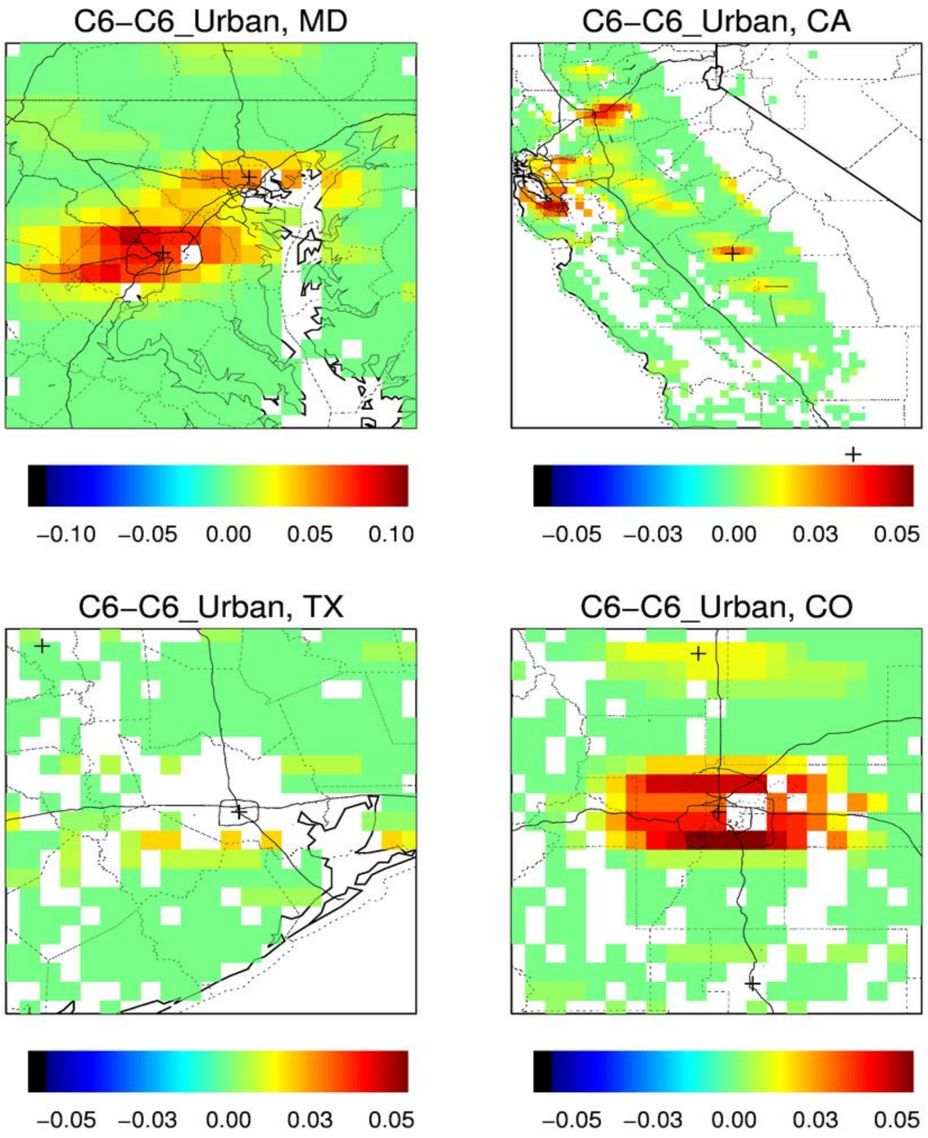


Conclusions

- NOx gradient is sensitive to the strength of vertical mixing
- A 1D model could generally capture the gradient. Using different WRF schemes lead to varied performance for different categories.
- Using surface measurement to calculate ozone production leads to ~30% high bias
- The ability of model to reproduce the shape of vertical profile impact NO2 retrieval process

MODIS DTA C6_Urban AOD Retrieval over DISCOVER-AQ Field Campaigns

- C6U retrieved AOD Data can be made available to DISCOVER-AQ Team.
- Region/Period covering all four deployments
- Data format?
  - MOD04 format (will have all the parameters except DeepBlue parameters (each file size is about 50mb)
  - Just AOD SDS as binary file corresponding to each granule
  - AOD maps only



- ✓ . C6U Provide more accurate AOD values over cities
- ✓ . C6U retrieval provides better continuity between city and surroundings

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