Leveraging monitoring activities to improve modeling in the LISTOS region

2020 MARAMA Air Quality Monitoring Training Committee Virtual Workshop

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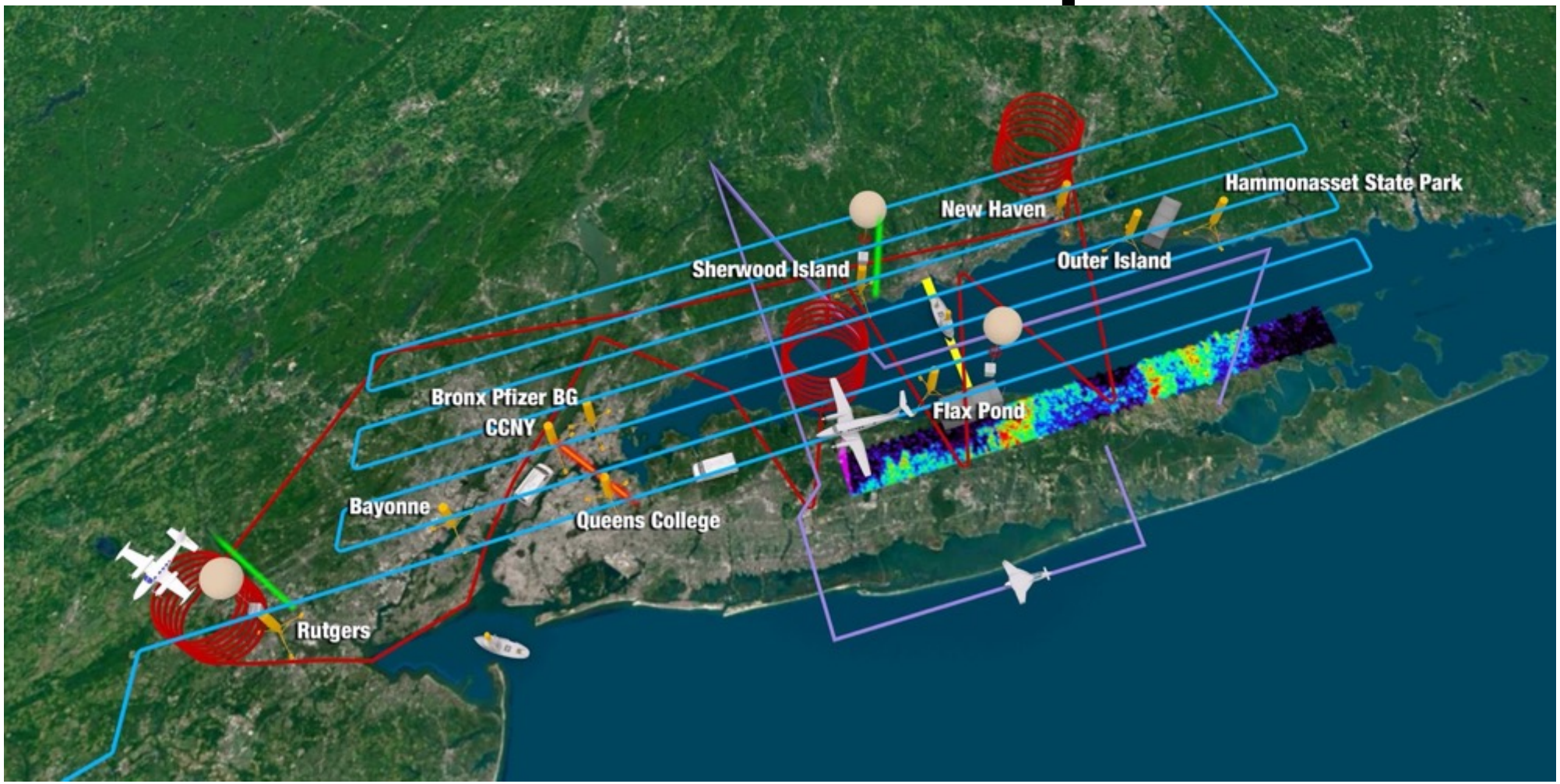
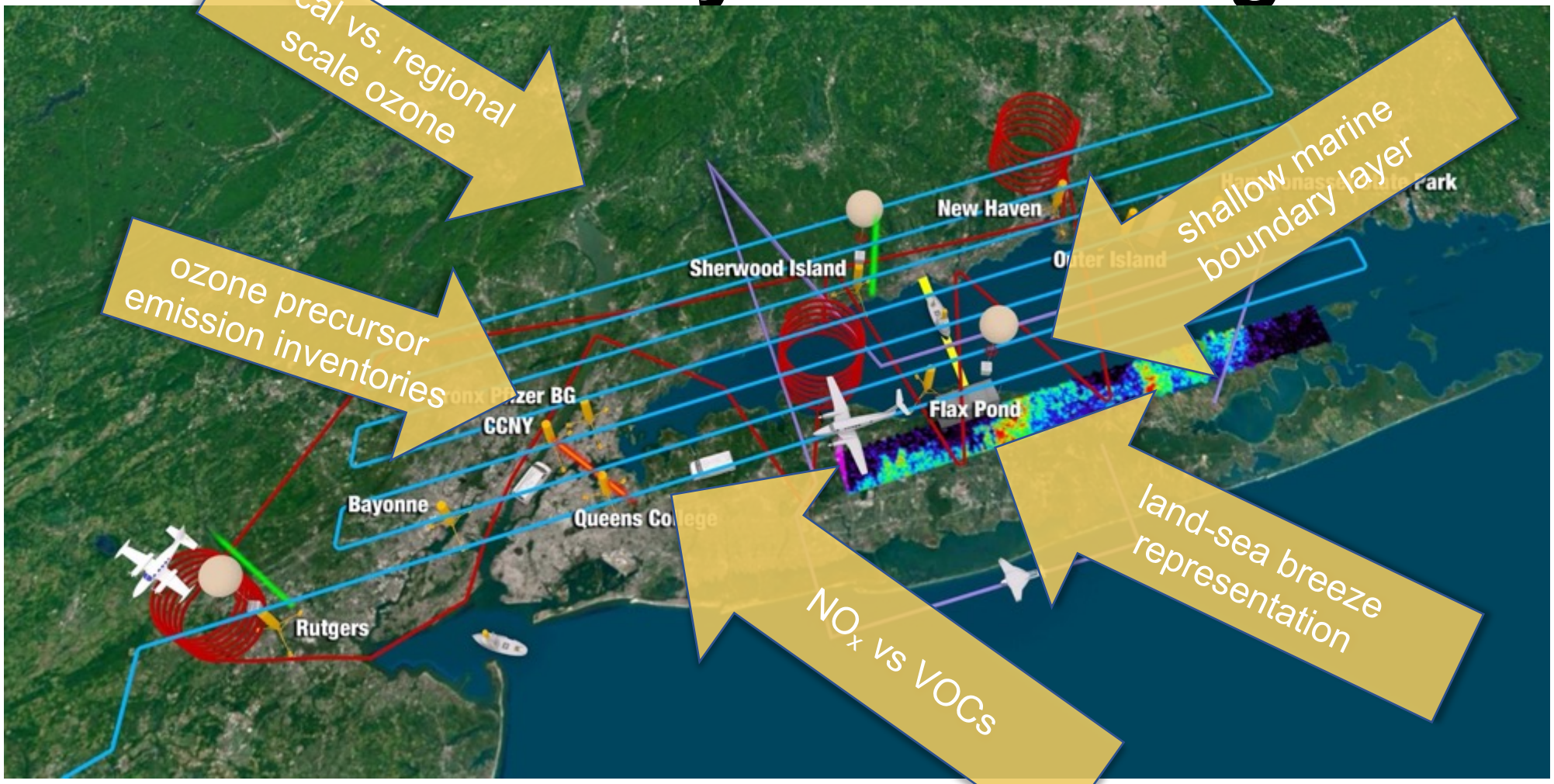
10 December 2020

2018 LISTOS in one picture



LISTOS Analysis Challenges



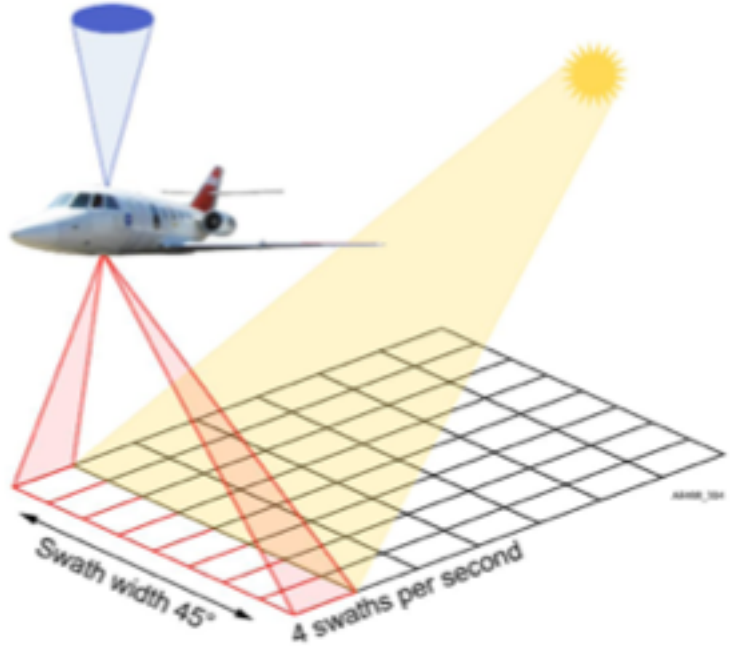
* Not an all-encompassing list of challenges

2018 LISTOS Participants & Activities

1. State AQI forecasters predicting ozone episodes to launch activities
2. NOAA-ESRL oxygenated/consumer product VOC mobile van measurements in NYC during March and July
3. Univ. Maryland 8-12 flights (depends on episodes, flight durations)
4. Maine DEP and NYS DEC labs VOC canister analysis
5. NASA GeoTASO/GCAS 20-30 high altitude flights; ozonesondes at Rutgers, NJ
6. EPA Pandoras Long Island Sound (LIS) coastline, Rutgers PAMS, NYC; ozonesondes & continuous HCHO at Westport, CT
7. CCNY boat-based air pollution measurements in LIS
8. CCNY aerosol LIDAR in northern Manhattan
9. Stony Brook Univ. oxygenated VOC measurements at Flax Pond PAMS site (Long Island north shore) during summer
10. Stony Brook Univ. aircraft fine resolution wind field measurements over LIS
11. Univ. at Albany O_3, NOx, VOC mobile measurements across Long Island south to north shore transects
12. Univ. at Albany ozonesondes at Flax Pond, Long Island, NY
13. NASA ozone LIDARs upwind at Rutgers Univ., NJ, and downwind on CT's LIS shoreline
14. CT DEEP ozone monitor on LIS ferry between Bridgeport, CT and Port Jefferson, NY
15. PAMS VOC measurements at Rutgers, NJ & the Bronx, with new NYS DEC PAMS site at Flax Pond, Long Island
16. Yale Univ. Coastal Field Station – VOCs on CT coast

Instruments used in LISTOS

Credit: Xinrong Ren, NOAA; Russ Dickerson, UMD



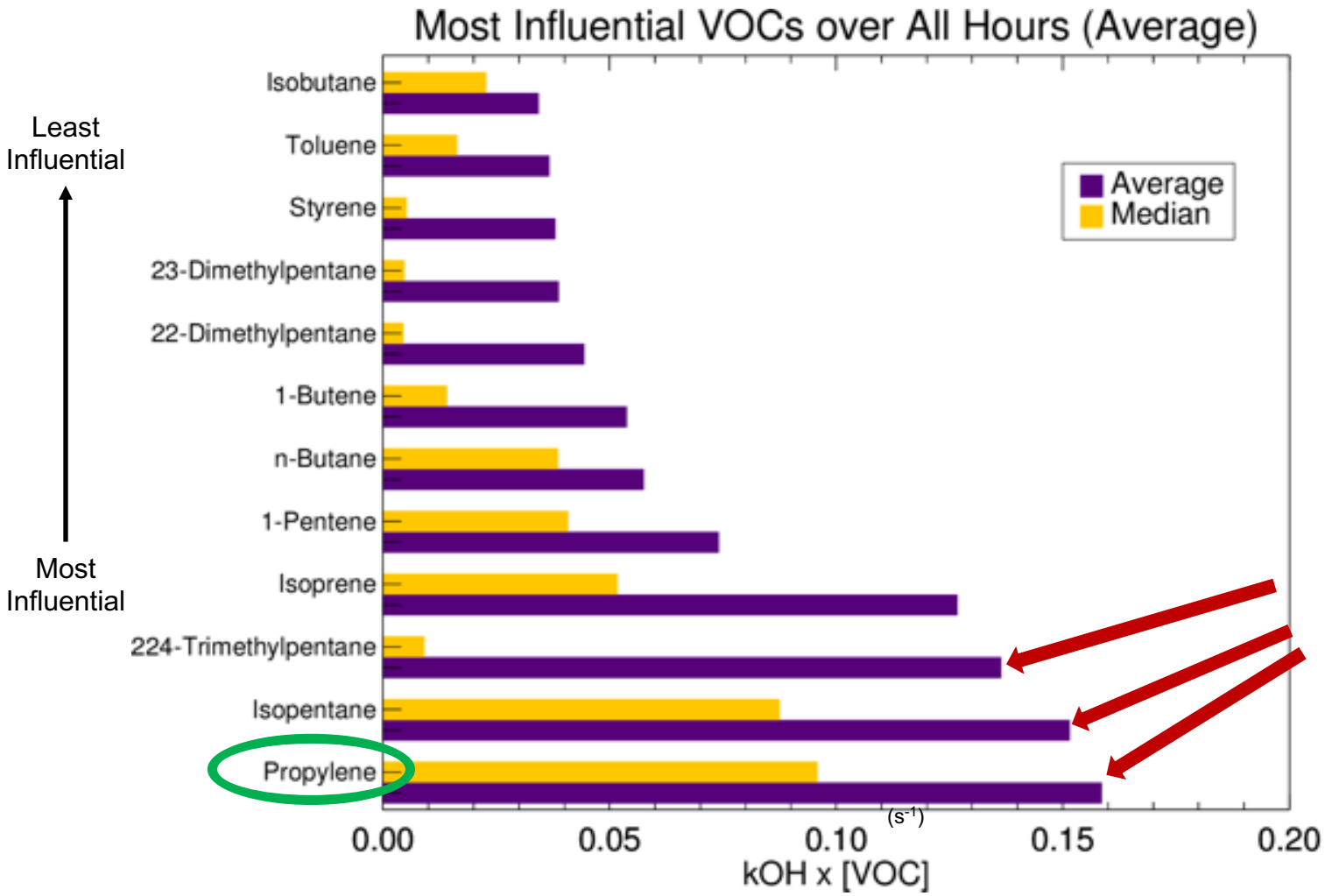
LISTOS Follow-up Studies Post-2018

1. Staten Island special monitoring site
2. Continuous formaldehyde monitoring
3. New ozone LIDAR based in NYC
4. Winter-time high-res speciated VOC and VCP monitoring
5. Long Island south shore monitoring site
6. CMAQ: Using LISTOS data to inform modeling

1. Staten Island Special Monitoring Site

- Temporary monitoring site to measure VOCs from shipping and petrochemical facilities
- Follow-up of 2017 VOC aircraft measurements seeing relatively high propylene levels over NYC

VOCs Measured May 17 and 18, 2017



- Pre-LISTOS measurements
- Ranked by Reactivity with OH (UMD Flight Canister Data), *Average* of All VOC Canister Data (Purple)
- Information important to addressing ozone precursors in region
- Where is propylene coming from?

Isoprene is not dominant – Why?

Based on the 50 VOCs measured

Does not include oxygenates, consumer products

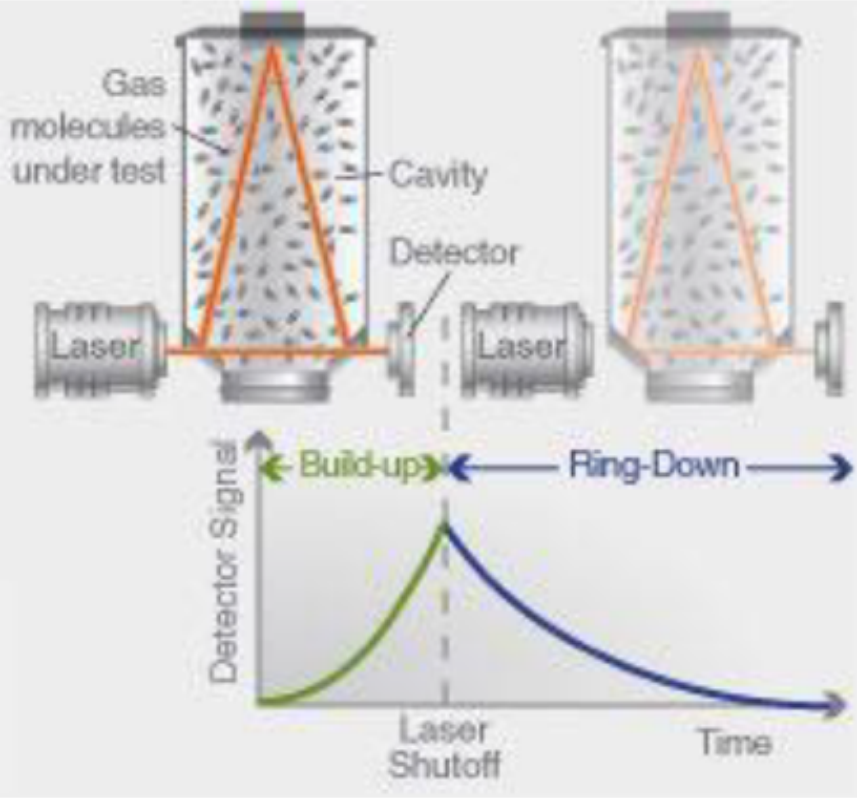
From A. Ring, UMD, et al., in prep.; VOC can analysis by ME DEP

2. Continuous Formaldehyde Monitoring

- NYS DEC now has 3 Picarro “cavity ring-down ” formaldehyde analyzers
- 2 are for continuous HCHO measurements at PAMS sites:
  1. NY Botanical Garden, The Bronx
  2. Flax Pond, Stony Brook (north shore Long Island)
- 1 for special monitoring site on Staten Island

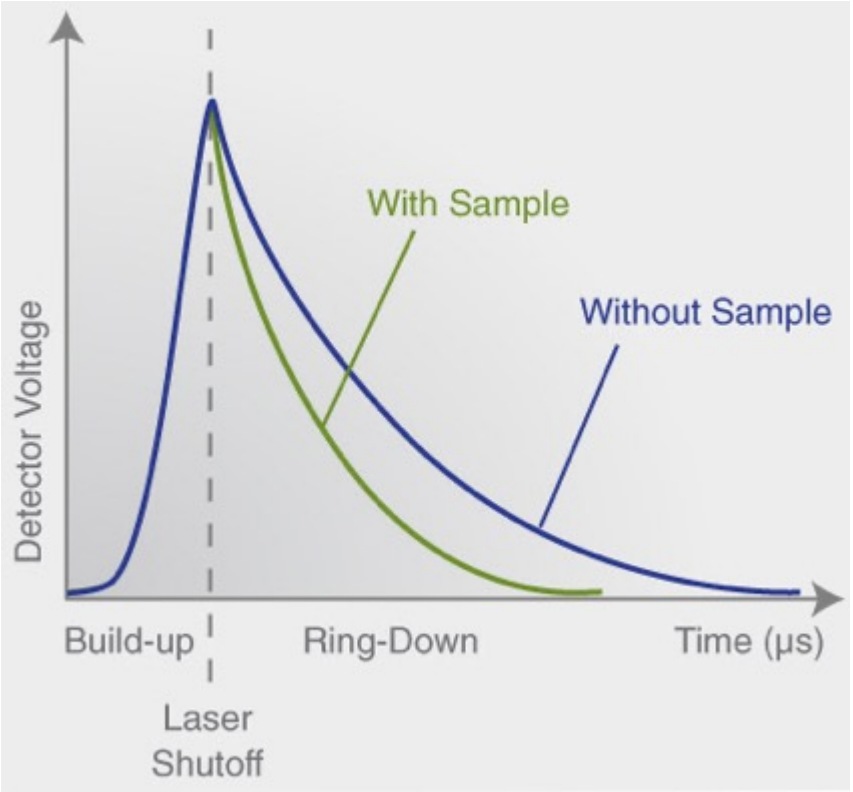
Formaldehyde Picarro: locations and findings

Cavity Ring-Down Spectroscopy (CRDS)



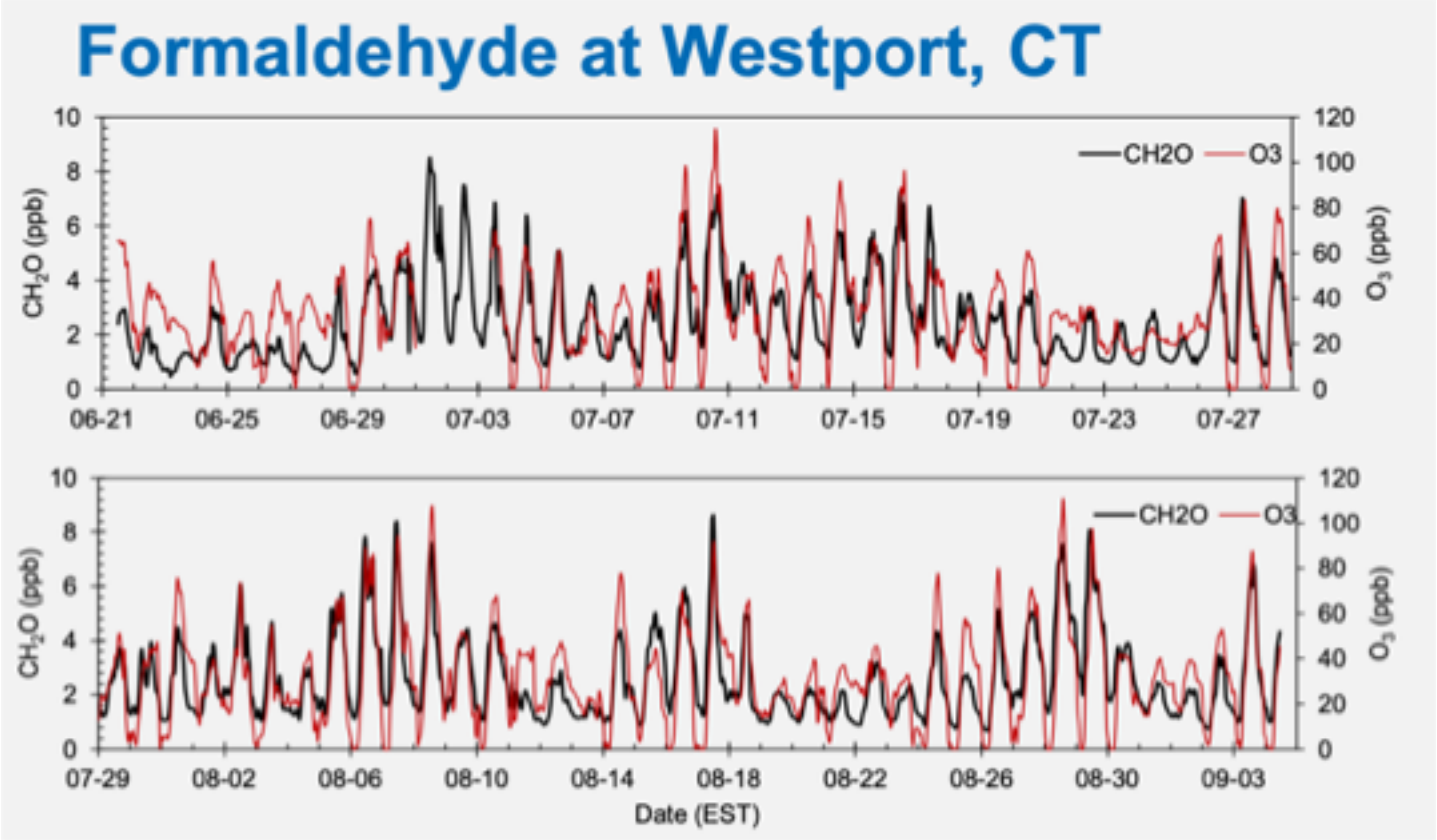
Light from a single frequency laser enters a cavity where three mirrors reflect the laser light

Then the laser is turned off and the intensity of the light reaching the detector decreases. The decay, or "ring-down," is measured in real time by the photodetector, and is proportional to HCHO concentration.



Why is formaldehyde important for understanding ozone?

- Volatile organic compound (VOC) and O_3 precursor
- Byproduct of isoprene oxidation
- Proxy for other VOCs in satellite and other remote sensing measurements
- Tracks well with O_3 under some conditions (e.g., local O_3)
- Tracks poorly with O_3 on others (e.g., transported O_3)

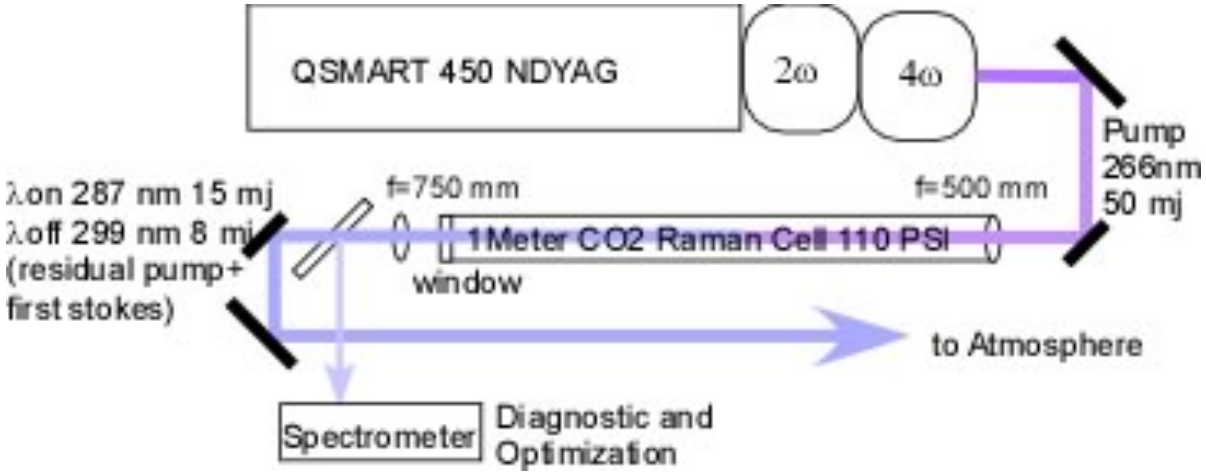


Formaldehyde
Ozone

Adapted from A.R. Whitehill LISTOS presentation

3. Ozone Light Detection and Ranging (LIDAR) System

- Use LIDAR to observe O_3 in the vertical column
- Two sites: upwind and downwind of NYC
  - Provides insights into long-range O_3 transport
- New ”mobile” LIDAR being built by Prof. Fred Moshary, CCNY, and will be part of TOLNET



NYC “inflow”

NASA Goddard Tropospheric Ozone Lidar (TROPOZ)

Rutgers site, ~ 50 km SW of NYC
PI: John Sullivan, NASA GSFC
john.t.sullivan@nasa.gov 301-614-5549

NYC “outflow”

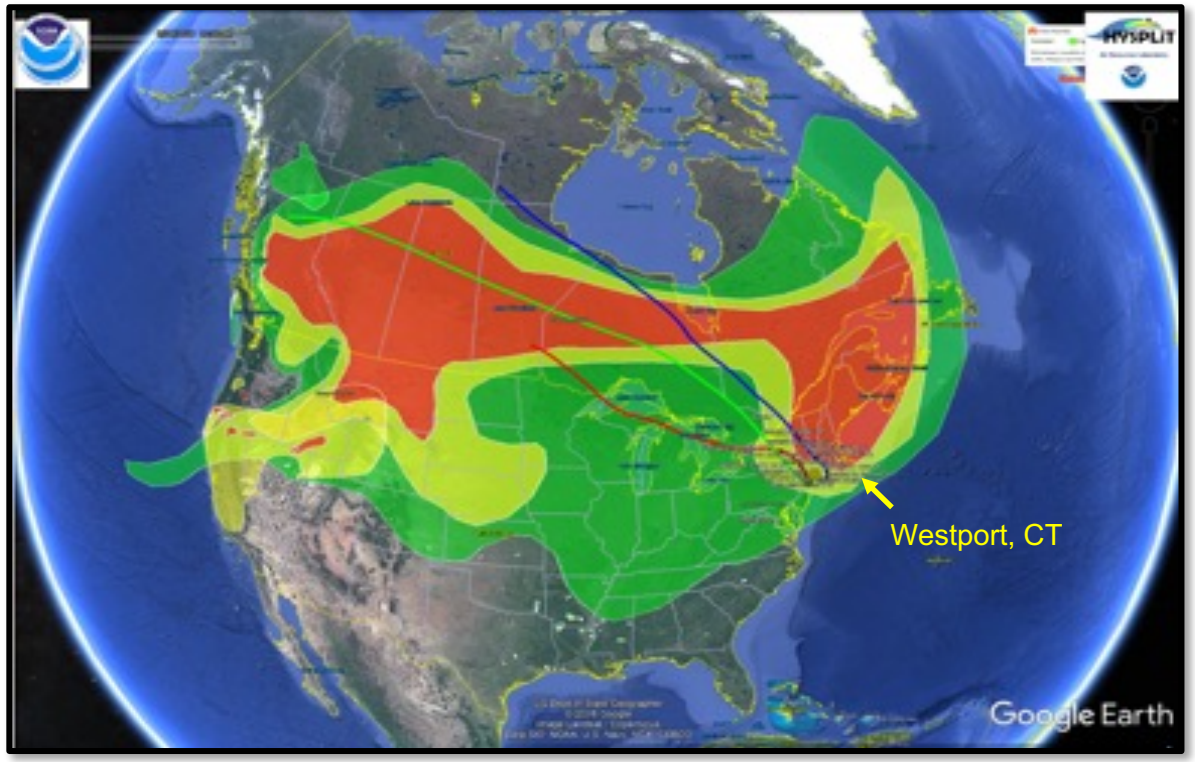
NASA Langley Mobile Ozone Lidar (LMOL)

Westport site, ~ 60 km NE of NYC
PI: Tim Berkoff, NASA LaRC
timothy.a.berkoff@nasa.gov 757-864-3684

Courtesy of Tim Berkoff (NASA)

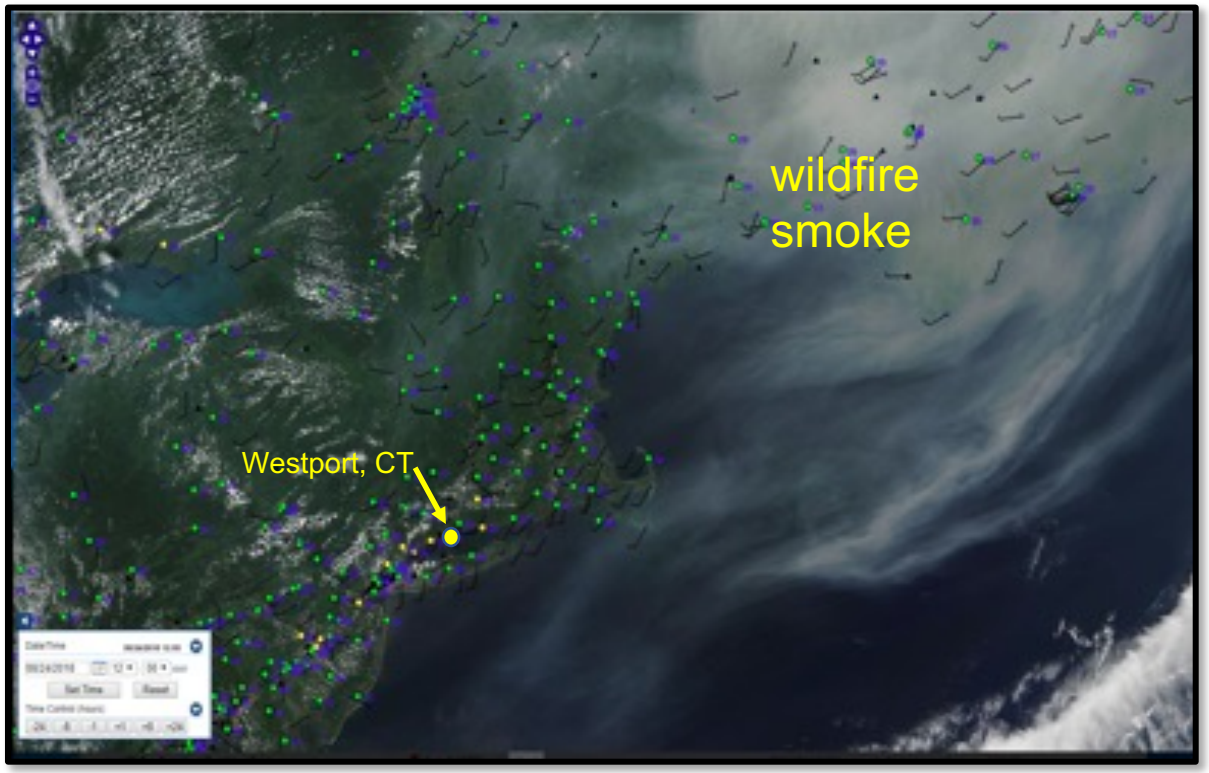
August 24-25 2018: airmass transport of wildfire smoke

HMS & HYSPLIT (1.0, 2.5, 4.3 km elevation)



NOAA Hazard Mapping System (HMS) reporting of satellite observed smoke over North America overlaid with HYSPLIT back-trajectories from Westport, CT

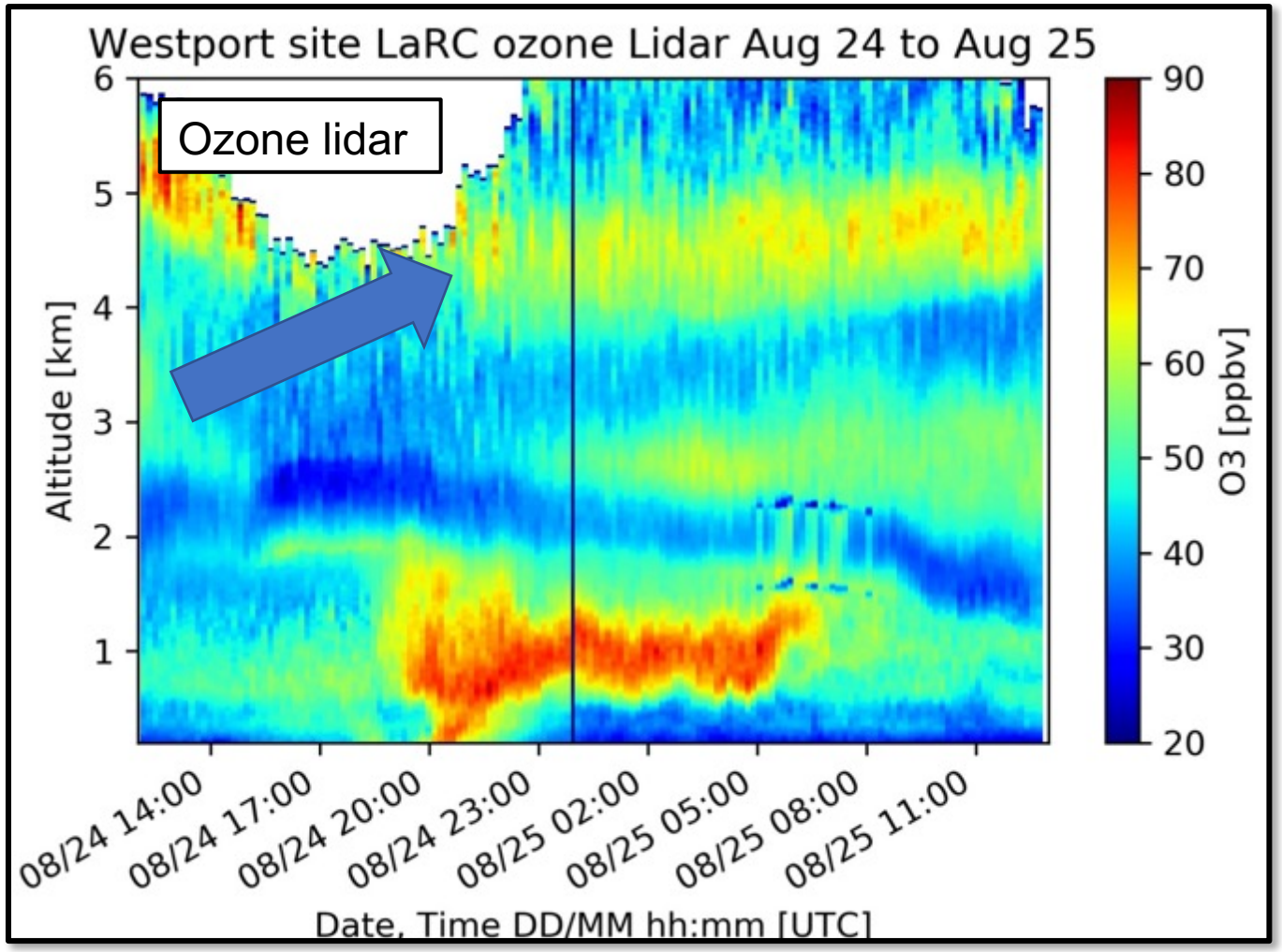
MODIS



Aqua/MODIS afternoon true color image showing wildfire smoke and Westport, CT LIDAR location

Courtesy of Tim Berkoff (NASA)

LIDAR detects ozone aloft in vertical transect

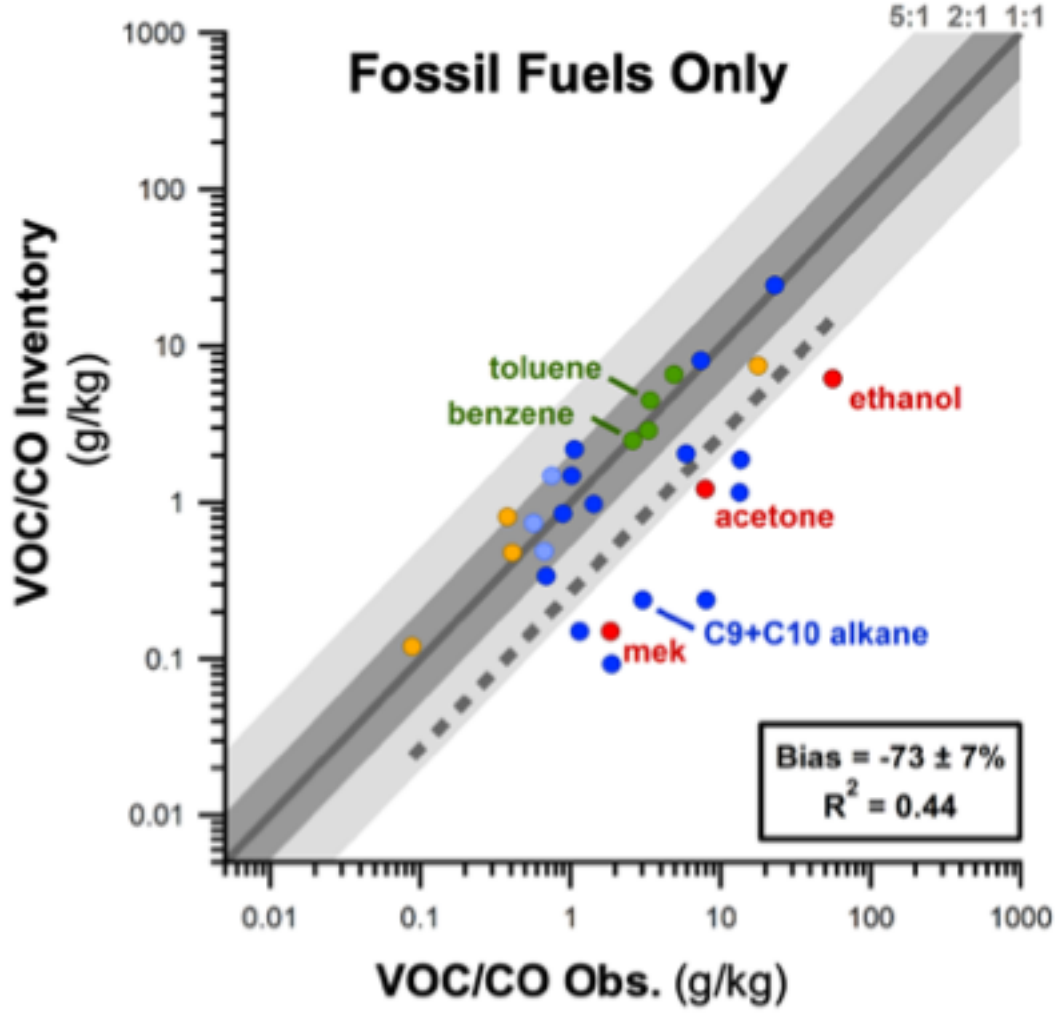


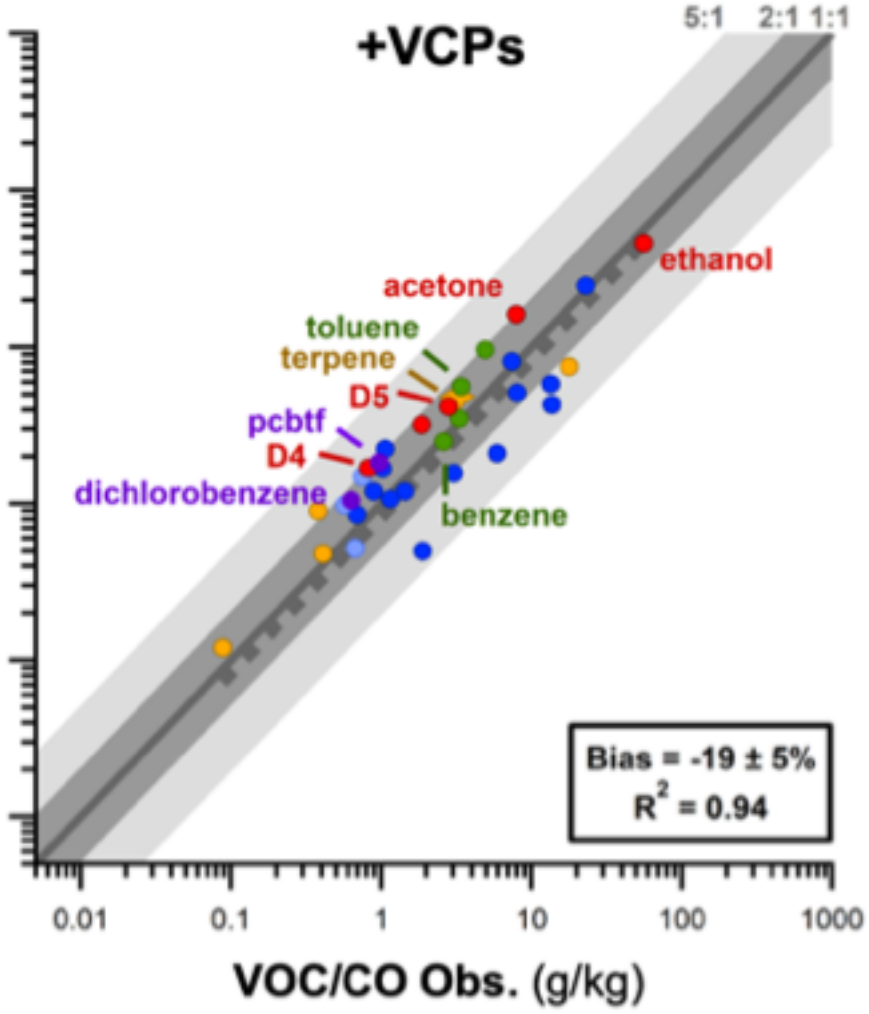
- Aug 24-25, 2018 wildfire transport event during LISTOS
- O_3 curtain time series measured by the NASA LaRC lidar (Westport, CT) showing aloft O_3 layers as a result of wildfire emission transport.

Courtesy of Tim Berkoff (NASA)

4. Winter-time Speciated VOCs and VCPs

Volatile chemical products (VCPs) needed to reflect ambient VOC levels in Manhattan





From B. McDonald (NOAA)

Long-term measurements of VOCs/VCPs

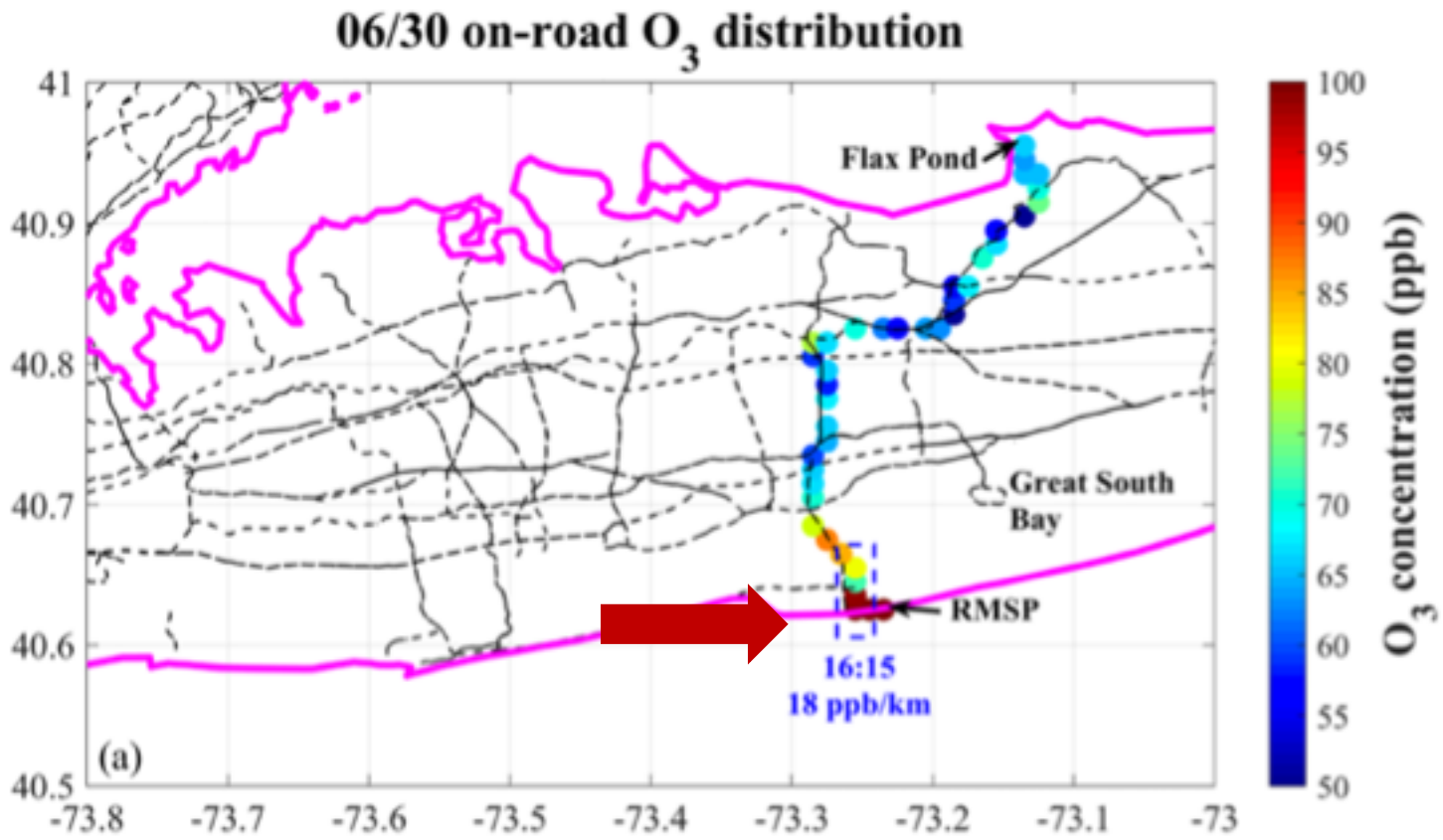
Sampling & Analysis Methods	Pollutants
High resolution proton transfer time of flight mass spectrometer (PTRTOFMS)	High-time resolution VOCs (1 minute)
Active collection on custom adsorbent tubes, analyzed via thermal desorption (TD) with GC and high-res MS	Short-duration chemically-speciated gas-phase organic compounds (VOCs, IVOCs, SVOCs) (3 hour samples)
Collection on PM filters analyzed via solvent extraction with GC/LC and high-resolution tandem MS	Chemically-speciated organic compounds in PM (periodic day-long samples)
Vocus R2 PTR-TOFMS	High-time resolution hard-to-measure VOCs (1 minute averages)

VOCs/SVOCs Compound Classes Collected

Single-ring aromatic VOCs
PAHs
Oxygenated VOCs
Other oxygenated compounds
Phthalates
PDBEs
PCBs
Alkanes
Terpenoids
Siloxanes

- Research team led by Prof. John Mak (Stony Brook University) and Prof. Drew Gentner (Yale University)
- Spatially distributed cartridges measuring a variety of VOCs in New York City
- Ongoing measurements since December 2019 including during COVID-19 related shelter-in-place orders
- Goals of providing a comprehensive chemical characterization of VOCs-SVOCs

5. Long Island south shore monitoring site

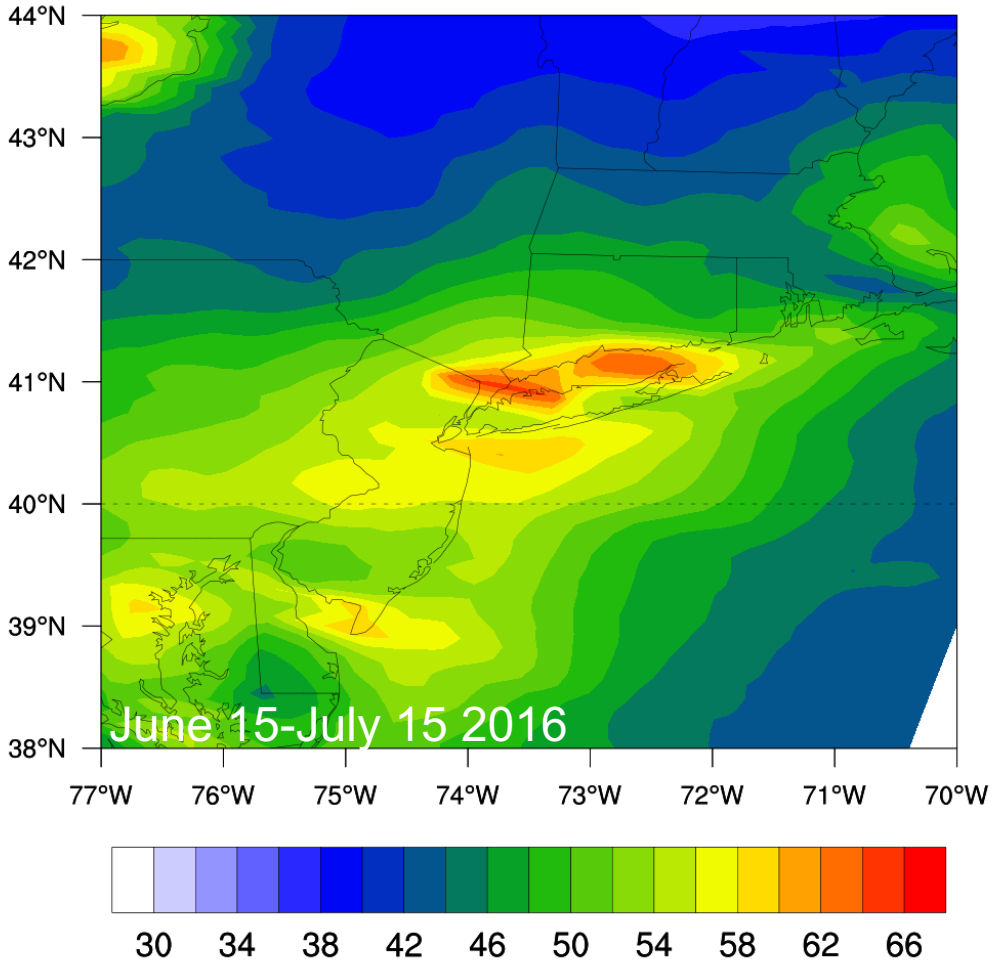


- O_3 measured with mobile van instruments during LISTOS led by Prof. Jim Schwab (SUNY-Albany)
- Rapid shift in O_3 concentration measured at south shore Long Island
  - Increase in concentration of 18 ppb/km near Robert Moses State Park
- LISTOS evidence for monitoring at strategic locations like this one to better understand sources of O_3 along south shore Long Island

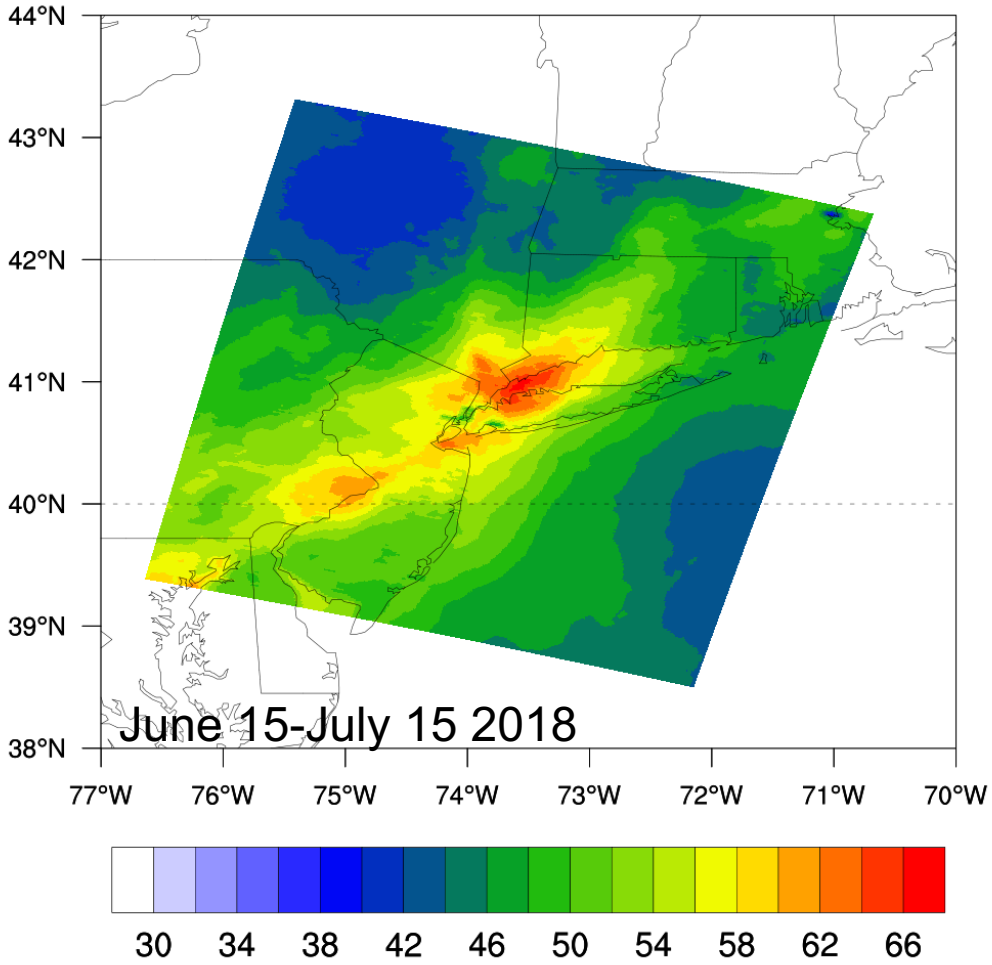
Zhang et al., 2020 *JGR Atmospheres*

6. CMAQ: Using LISTOS Data to Inform Modeling

CMAQv5.3.1 2016v1: 12 km

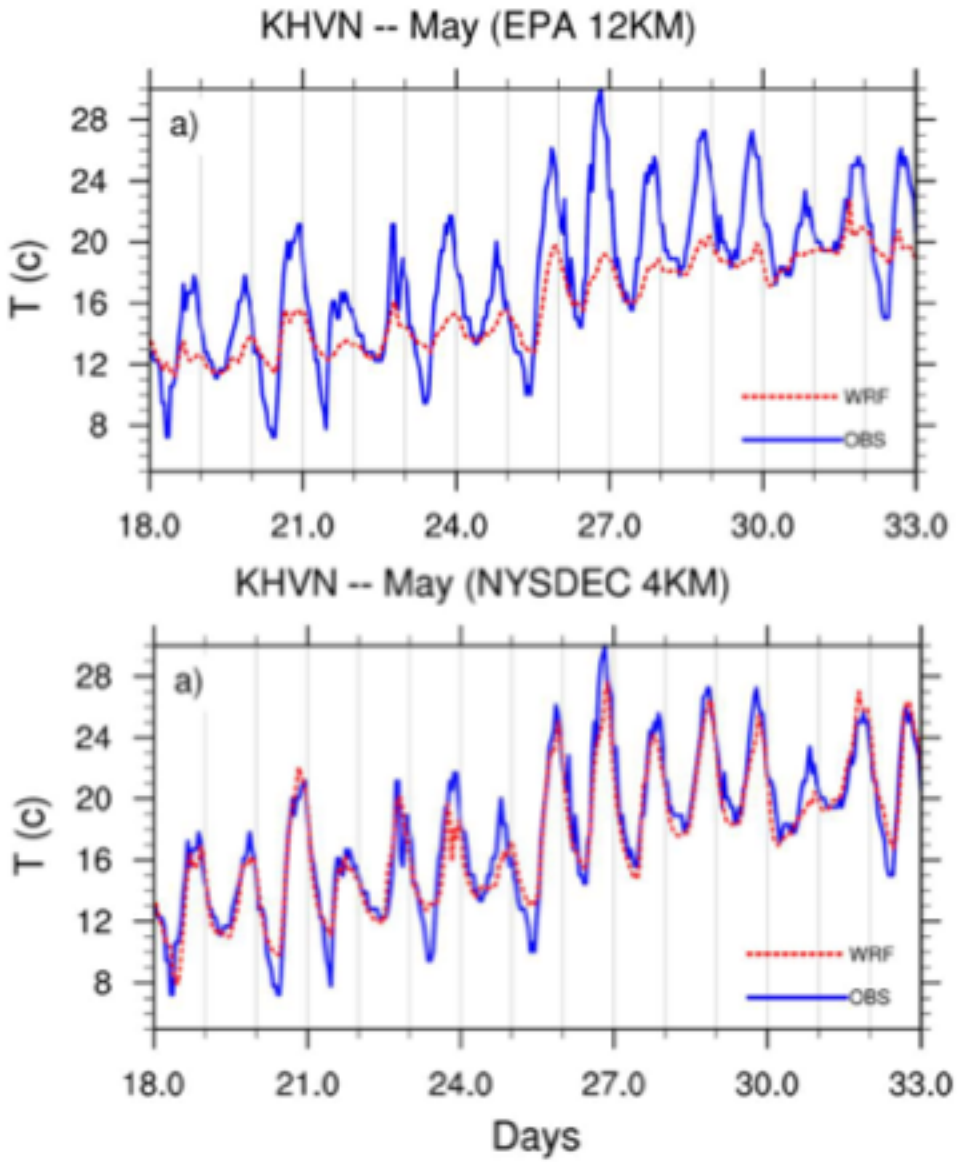


WRFv4.11-CMAQv5.3.1 LISTOS: 1.33 km



Urban-Scale Modeling for the NYC and LIS Region

- Develop a practical high-resolution urban-scale modeling platform
- Coarse resolution simulations may underestimate O_3 concentrations, misallocate emissions, or not represent well land-sea breeze
- Use 1.33 km x 1.33 km horizontal resolution in LIS region to assess control strategy effectiveness



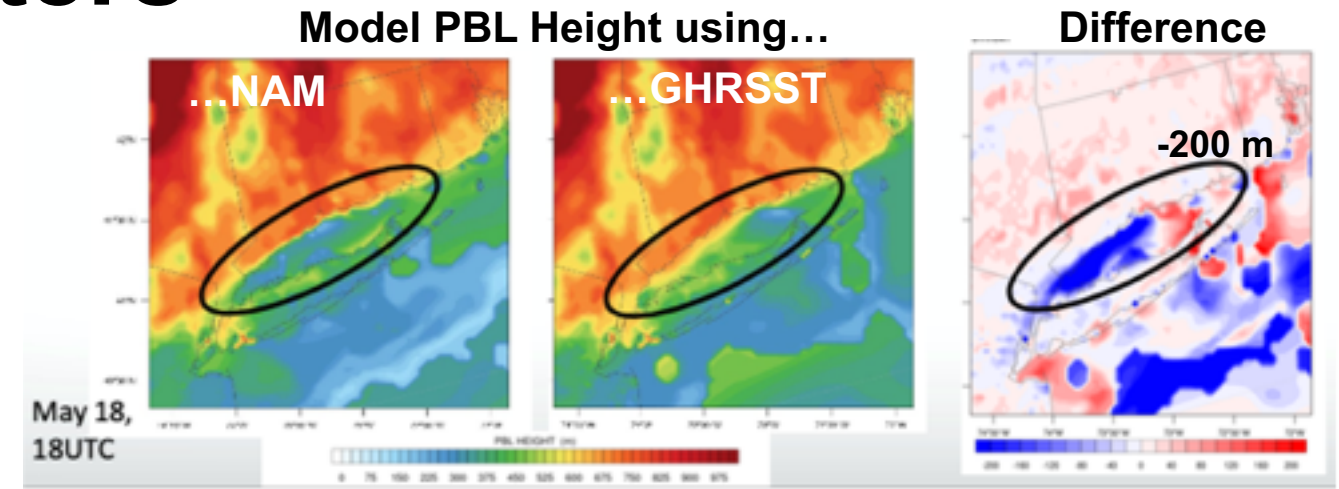
WRF model output
Observations

Model resolution may result in improved model performance against observations

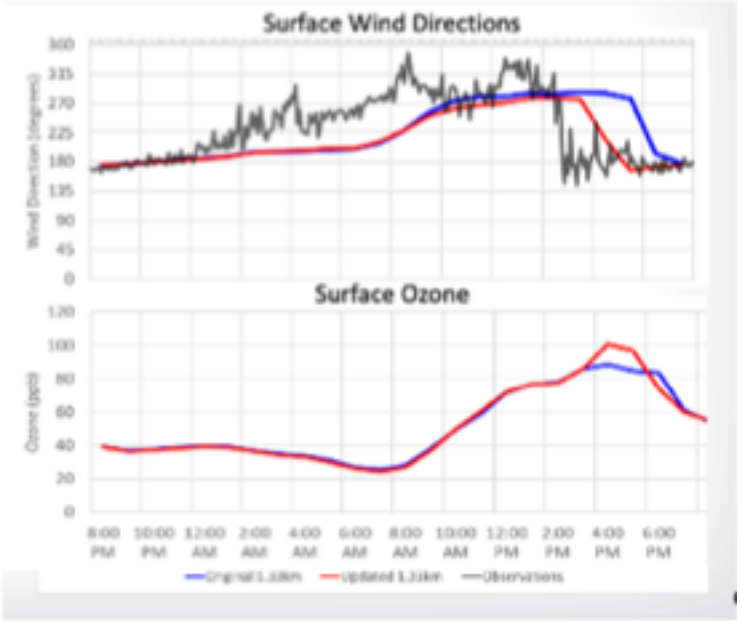
Credits: Margaret LaFarr (NYSDEC)

High Resolution Modeling with Region-Specific Meteorological Parameters

- Land-sea interface is currently not well captured in regulatory air quality models
- Test land cover and sea surface temperature inputs, wind field, PBL dynamics, in WRF and CMAQ to better represent complex meteorology in the LIS
- Get guidance from ongoing modeling from other land-water field studies (e.g., OWLETS, LMOS)
- Evaluate with LISTOS measurements and compare against baseline EPA-recommended WRF parameters



Using different SST inputs can dramatically affect modeled PBL height

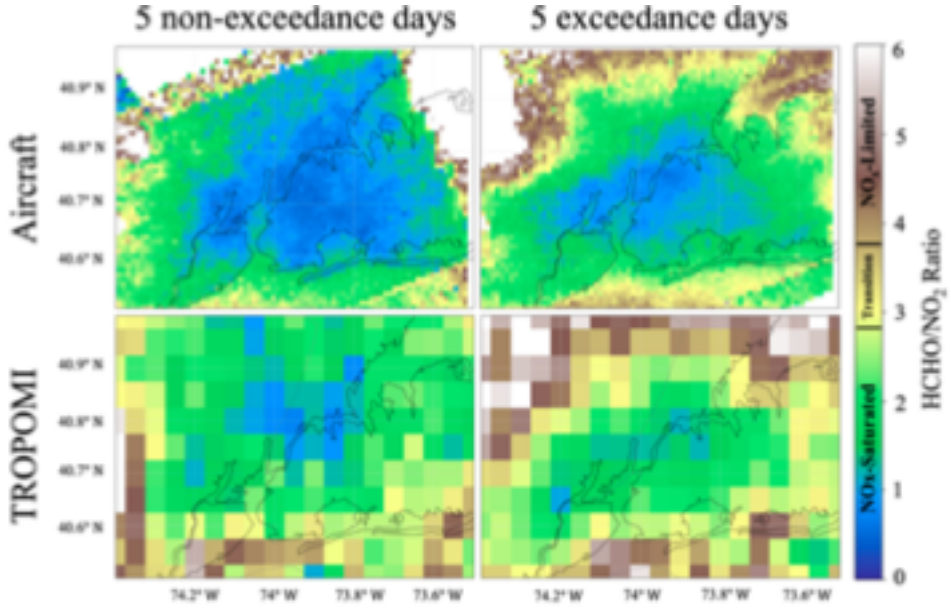


Updating SST diurnal signal improves modeled surface wind directions @ Port Jefferson

Credit: J. Pleim (USEPA)

Leverage observations of formaldehyde to NO_2 to for sensitivity analysis

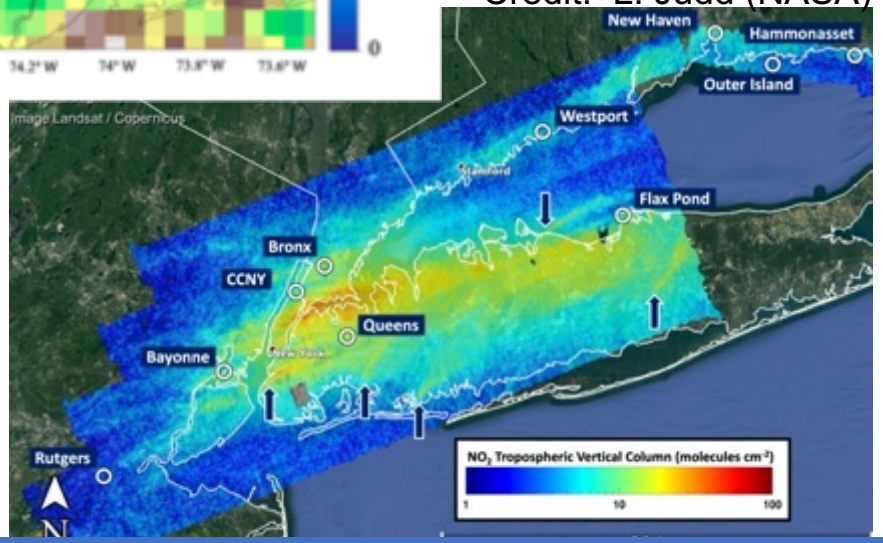
- Use LISTOS observations to identify possible VOC sensitivity areas in the NYC region
- Use results to inform possible complementary VOC strategies with NO_X strategies
- Compare formaldehyde/NO_2 ratios from:
  - *Satellites (TROPOMI and OMI)*
  - *Aircraft (GeoTASO/GCAS)*
  - *WRF-CMAQ*



Credit: M. Tao (Columbia University)

Highly localized NO_x saturated environment during high O_3 periods

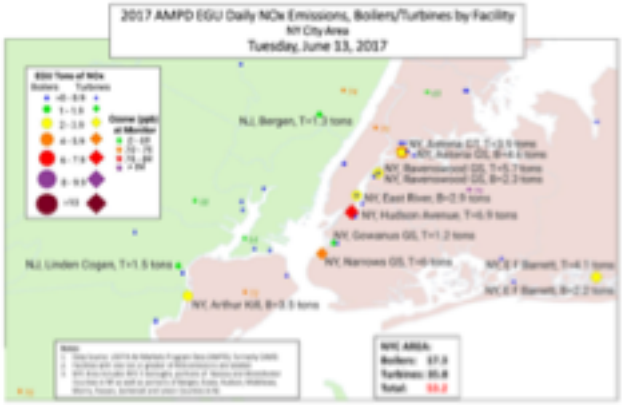
Credit: L. Judd (NASA)



Local NO_X Emissions Inventory Adjustment

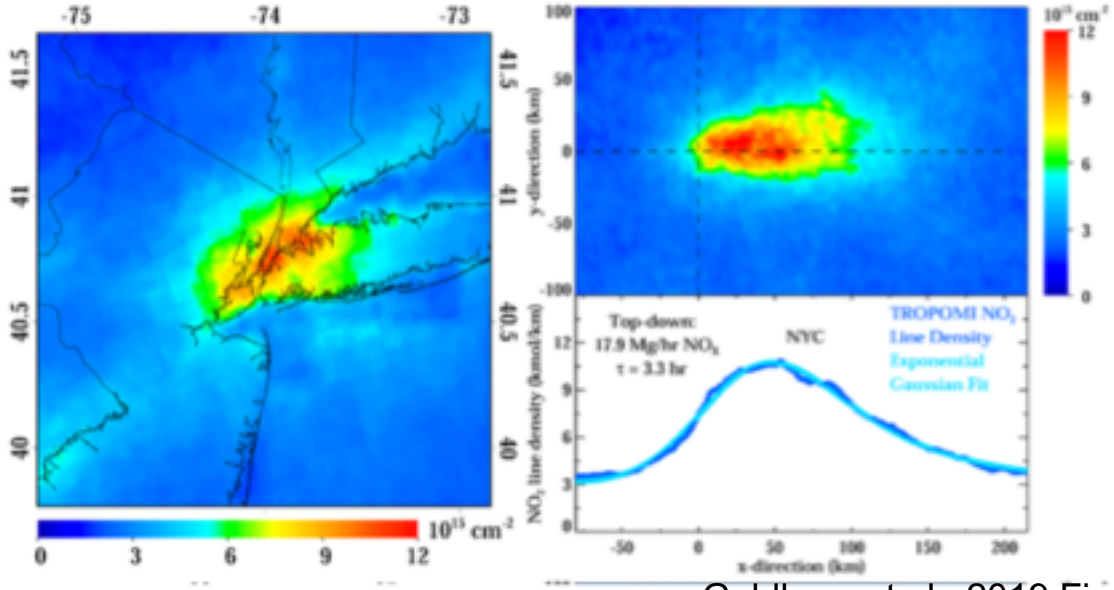
- Use high-temporal and spatial resolution remote sensing observations to inform and improve local emissions inventories used in modeling
- Provide constraints on the NO_X emissions inputs to air quality models on high O_3 days
- Model changes in control strategy effectiveness from changes to an observation-constrained inventory
- Example application: how to account for hard-to-predict “high demand” electric generating units in NYC region?

EGU locations



Credit: NJ DEP

Pandoras NO_2 measurements provide good spatial comparison and validation with TROPOMI



Goldberg et al., 2019 Figure 2

LISTOS provided a platform for researchers to build capacity to measure ozone, precursors in NYC and downwind

- Breadth of monitoring across the region reveals new regions of isolated sources (e.g., Northern New Jersey) and isolated impacts (e.g., South Shore Long Island)
- LISTOS opened the door for continuously measured speciated VOC and VCP, including during COVID-19 related shutdowns
- Continuous HCHO in-urban monitoring network helps understand local and transported precursor concentrations
- O_3 LIDARs capture elevated concentrations at surface and aloft due to air mass transport
- Many modeling projects in the pipeline to improve inputs and model performance
- Dense observations in the area provide great tool for evaluating TROPOMI and other remote sensing observations and in preparation of TEMPO launch in 2022

Acknowledgements

Thank you to LISTOS supporters
Connecticut Department of Energy and Environmental Protection
National Aeronautics and Space Administration
National Fish and Wildlife Foundation
National Oceanic and Atmospheric Administration
New Jersey Department of Environmental Protection
New York State Department of Environmental Conservation
U.S. Environmental Protection Agency Office of Research and Development
U.S. Environmental Protection Agency Region 1 (New England)

More about LISTOS: https://www.nescaum.org/documents/listos
Data: https://www-air.larc.nasa.gov/missions/listos/index.html

Contact: Alex Karambelas
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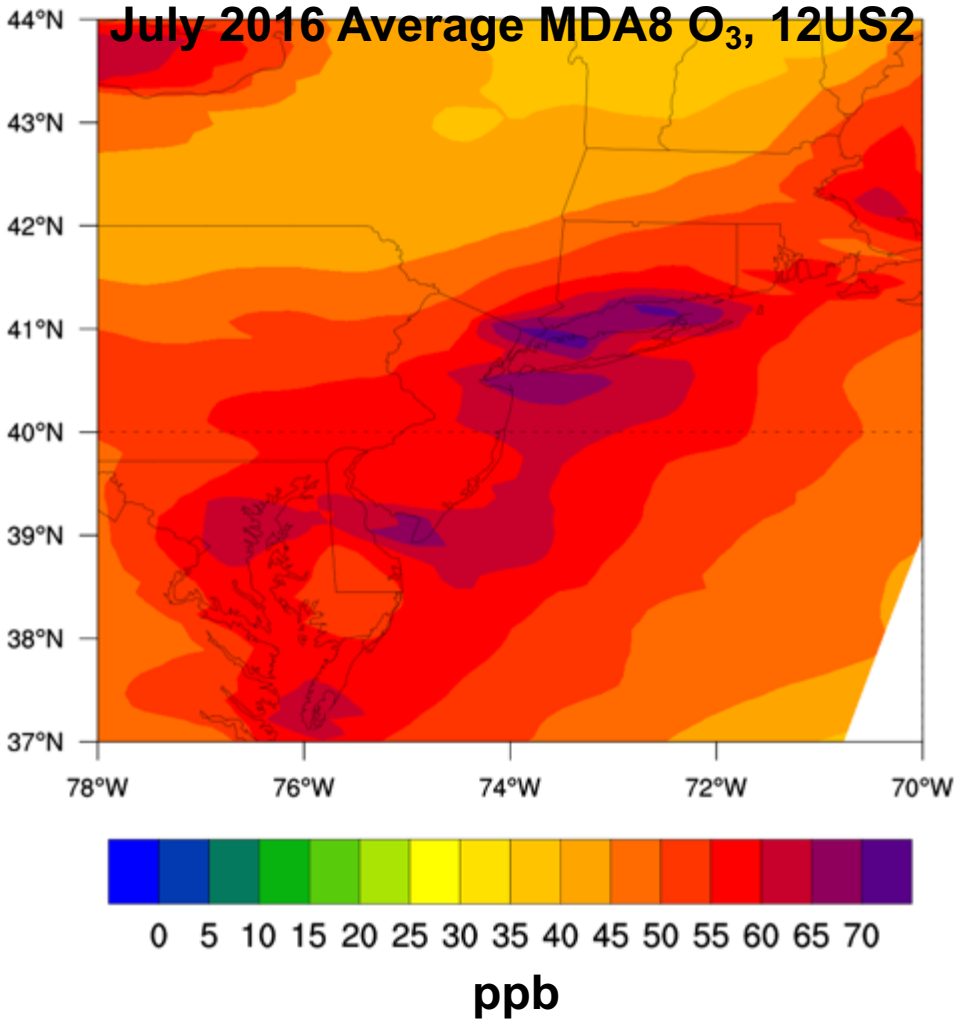
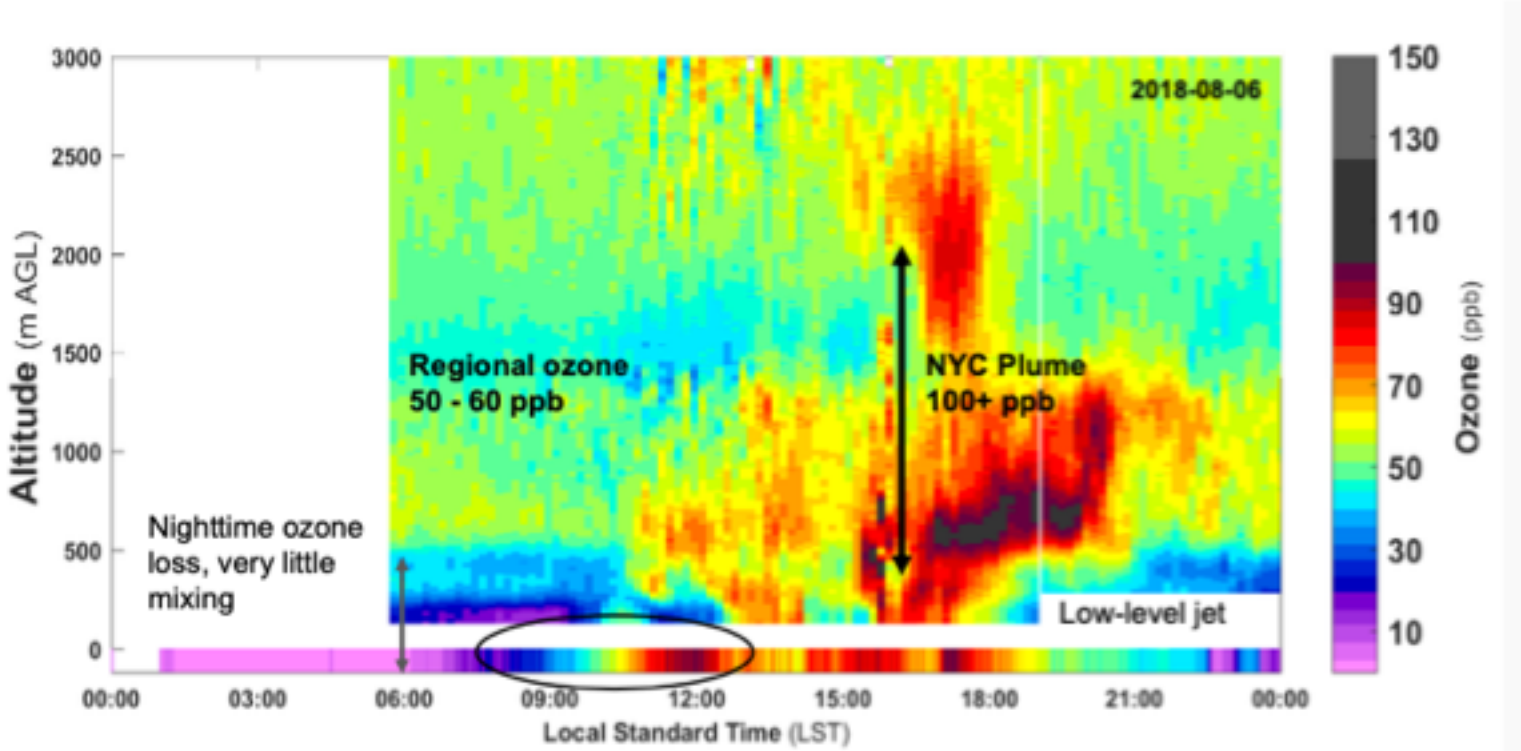
Extra Slides

Modeling Platform

- CMAQv5.3.1 at a variety of spatial domains and resolutions (12 km x 12 km 12US2, 4 km x 4 km NE, 1.33 km x 1.33 km LISTOS)
- WRF meteorology for 2018
  - CMAQ-ready with MCIP processing
- Emissions for 2018
  - Processing with SMOKE as necessary
- Model evaluation with LISTOS and EPA AQS observations
- Simulations focused on summer 2018, specifically O_3 episodes with co-located measurements



High local ozone generated in shallow marine layer seen at Westport, CT



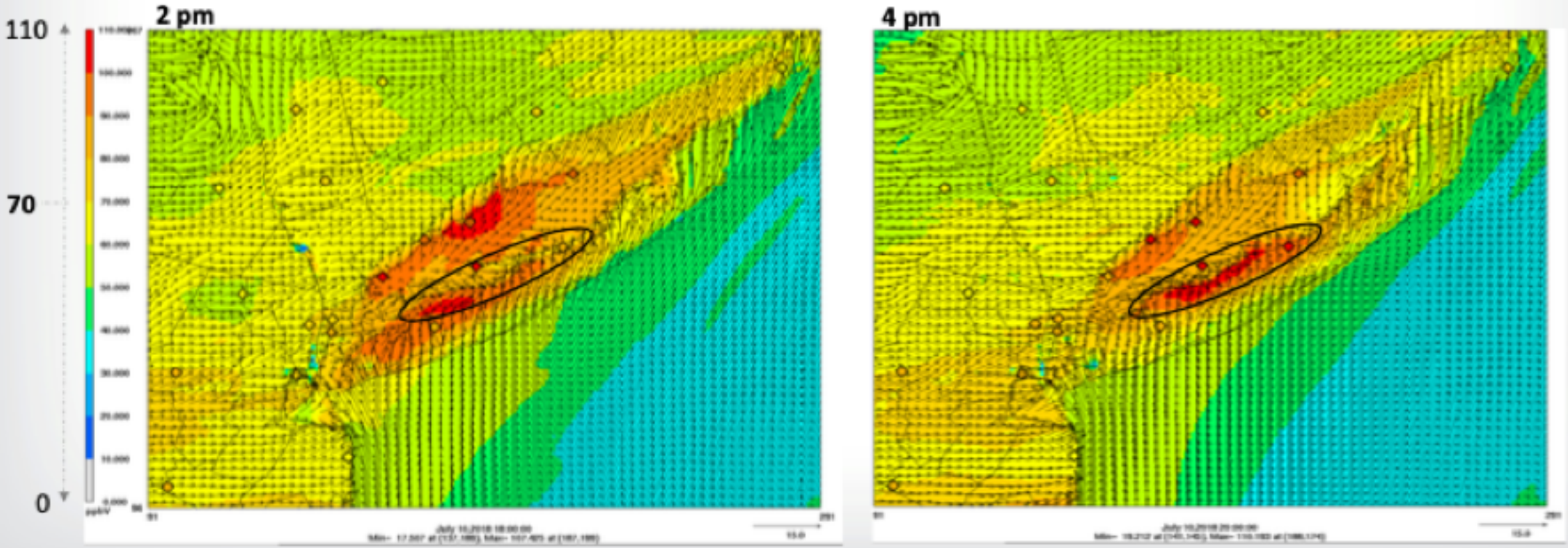
There is rapid growth in ozone in very shallow layer (<100m) from 8AM to 12PM ~90ppb

31

Data courtesy of Tim Berkoff (NASA LaRC), CT DEEP

Capturing the sea breeze and convergence fronts that form in the summer afternoons is critical to capturing localized ozone concentrations.

Modeled Surface Ozone (shaded) compared to AQS ozone (diamonds)



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Credit: Jon Pleim (USEPA)