The promise of closing the spatial gap in O_3 monitoring with machine learning and satellite observations

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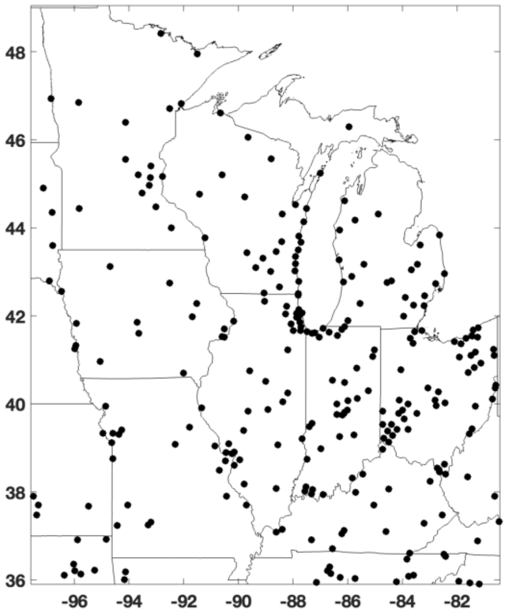
14 May 2026

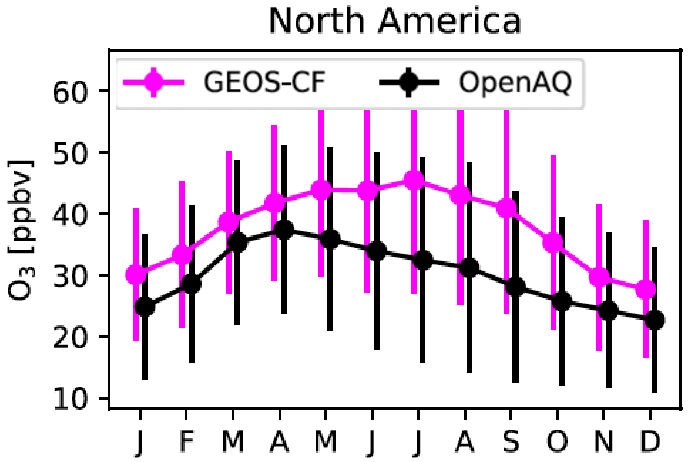
Limitations of the current surface ozone monitoring system

EPA O_3 Monitors



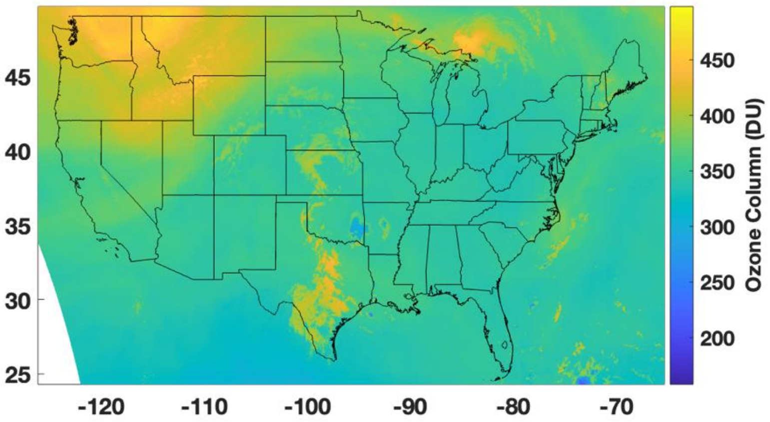
Tools are needed to constrain O_3 elsewhere.

Evaluation of the NASA GEOS-CF model with surface observations



Keller et al, 2021, Description of NASA GEOS CF, JAMES

TEMPO total column O_3 (15Z May 1, 2024)



O_3 monitors provide highly accurate observations but are sparsely distributed.

Air quality models often have significant biases

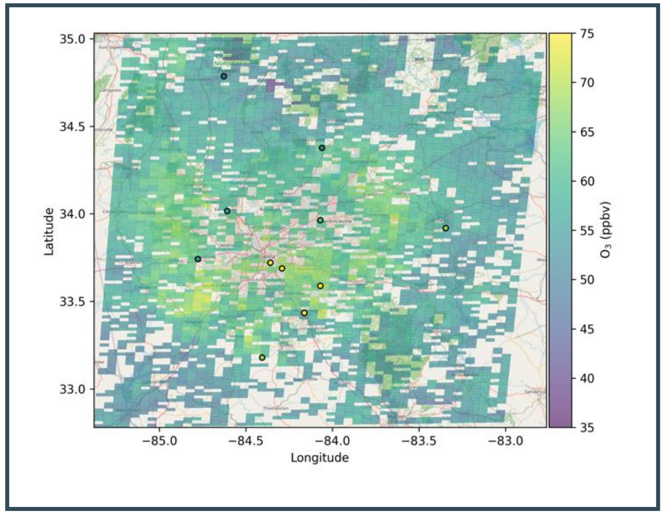
Satellites don't provide surface concentrations

A multi-pronged approach to understanding ozone

Recent advances in machine learning (ML) and the launch of TEMPO present an opportunity to improve our ability to constrain O_3 outside monitoring sites.

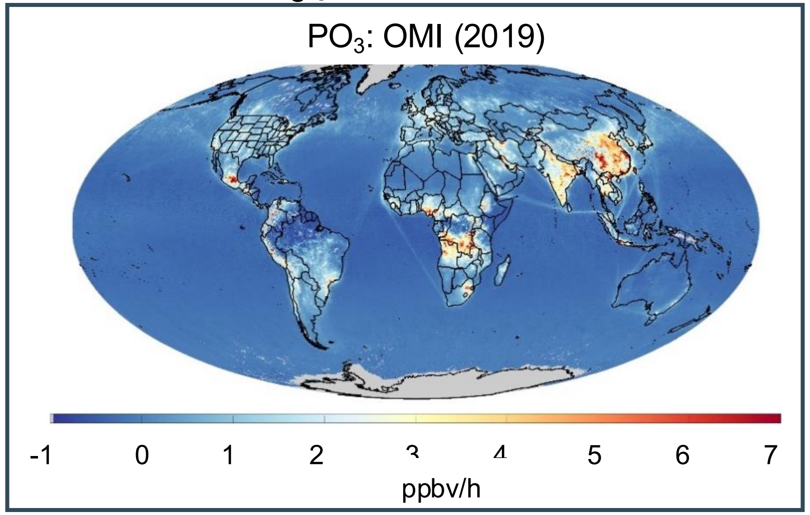
Approach facilitates development of multiple tools to inform understanding of O_3 events from multiple perspectives, to increase interpretability of results, and to complement existing tools.

Tool 1: Surface O_3 Mixing Ratios



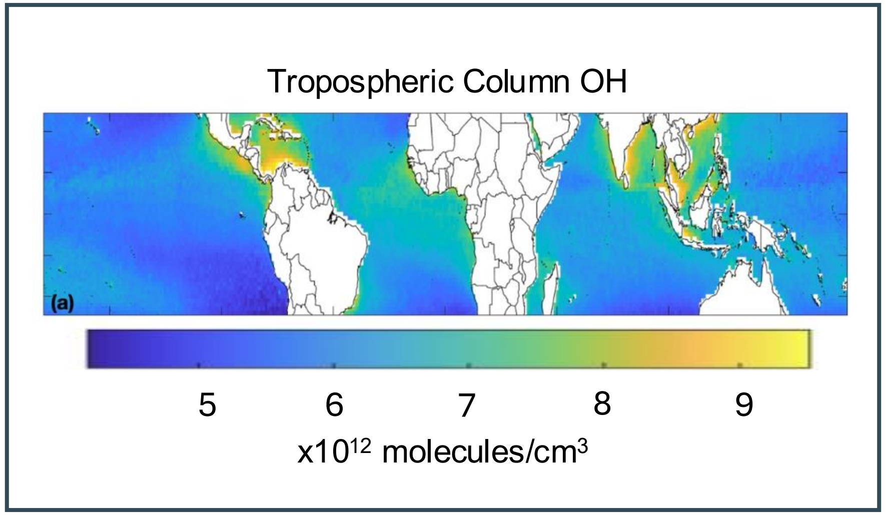
Results are preliminary and may change.

Tool 2: O_3 production rate



Souri et al, 2026, Beyond binary maps for $HCHO/NO_2$, ACP.

Tool 3: Constraining budgets



Anderson et al, 2024, Trends & Interannual Variability of OH in the Remote Tropics, GRL.

Tool1: Directly constraining ozone

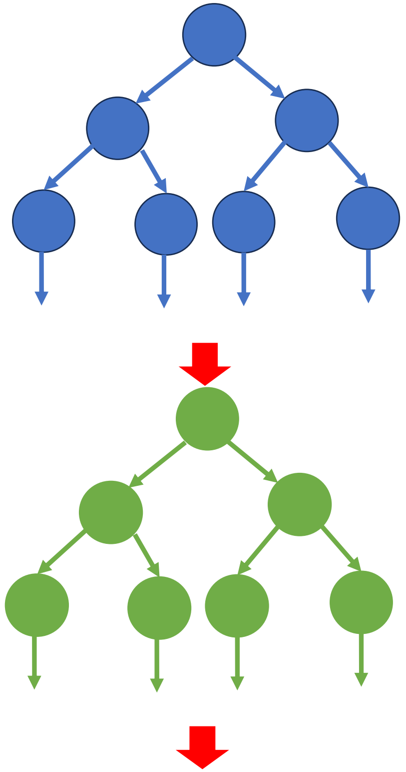
ML Model Inputs

TEMPO
- Trop. Column NO_2 & HCHO
- Total Column O_3
- Viewing Geometry
- Reflectivity

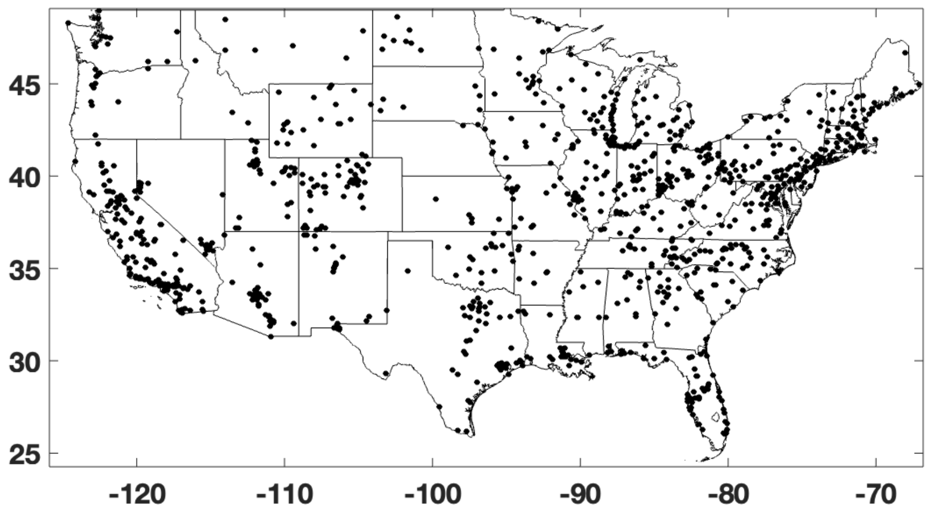
HRRR Meteorology
- T, P, Humidity
- Wind speed
- Wind direction
- PBL Height

Other
- Latitude
- Population
- Month, Hour
- Road Density
- Day of Week
- NDVI

Gradient Boosted Regression Tree Model Training



Training Targets (Surface O_3)

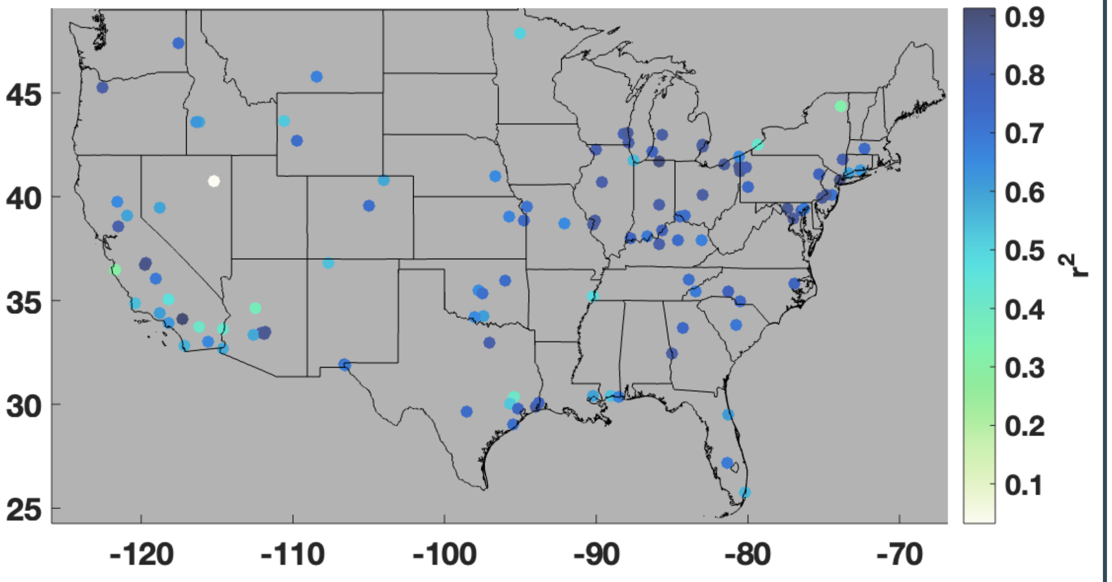


EPA Ozone Monitoring Sites

Test model performance at independent O_3 monitoring sites

TEMPO-derived surface O_3 reproduces variability of surface monitors

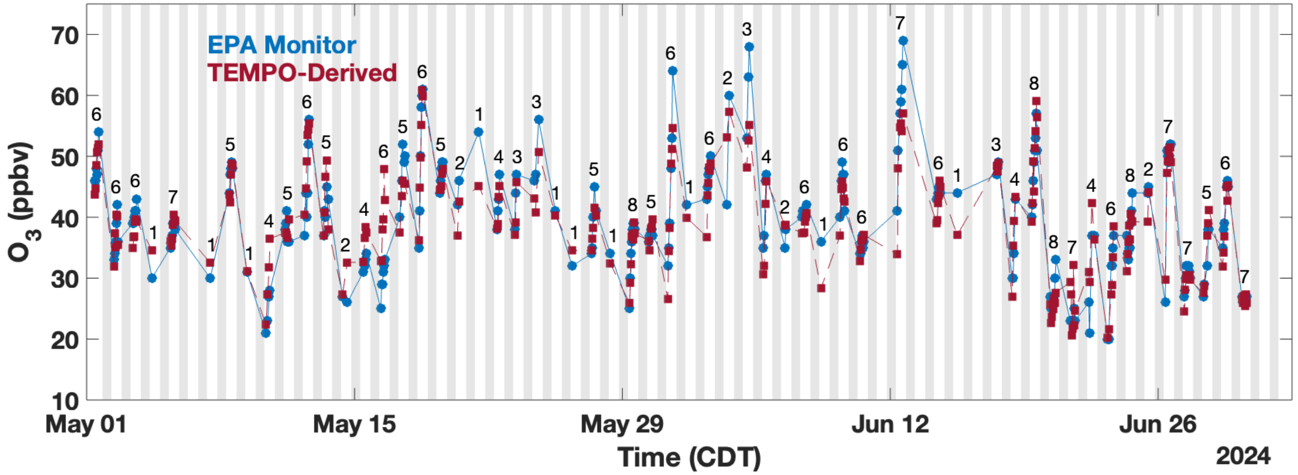
Correlation between EPA and TEMPO-Derived O_3



Satellite data can constrain surface O_3 variability over many regions of the continental US.

TEMPO-derived O_3 replicates the observed diurnal cycle, although it does underestimate O_3 on highest days.

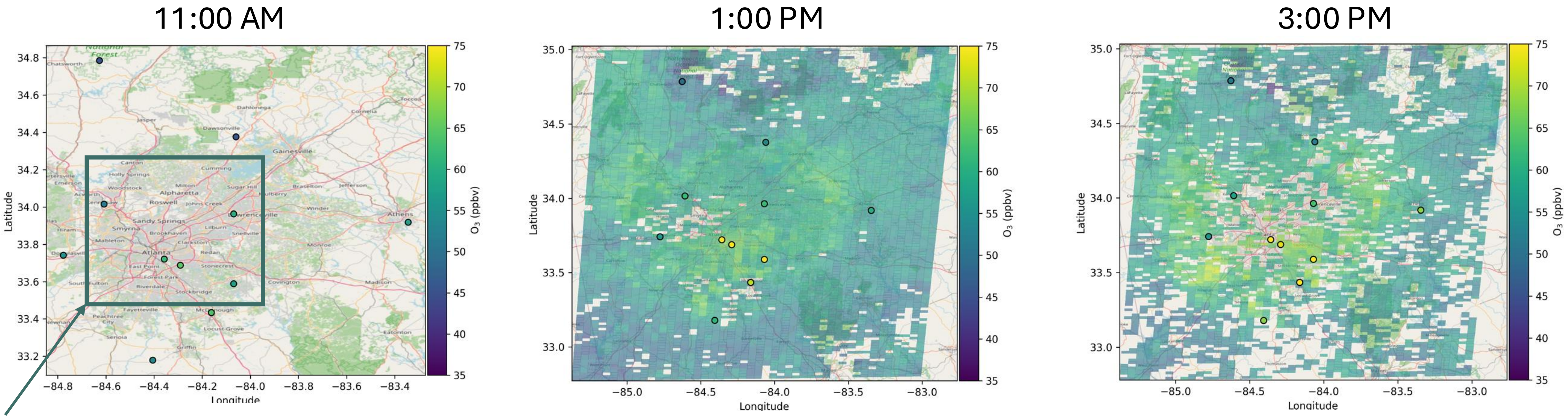
O_3 variability at UW – Milwaukee EPA site



Shading indicates nighttime (8pm – 7am), and numbers indicate number of TEMPO-Derived observations per day.

Results are preliminary and may change.

Capturing O_3 exceedances in metro Atlanta



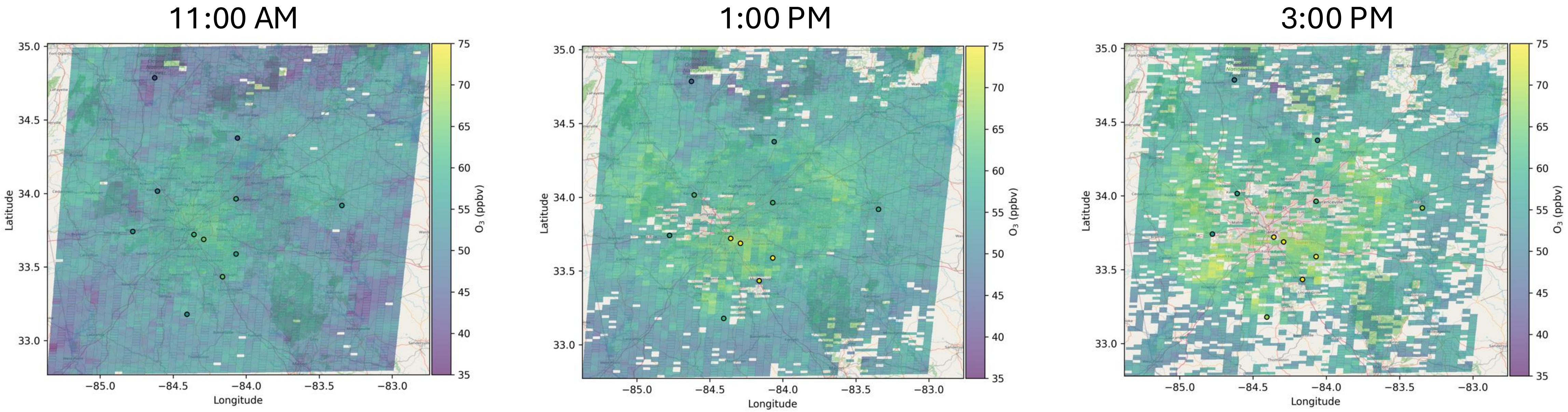
Metro Atlanta

TEMPO-Derived (background) and EPA monitor (circles) O_3 in northern Georgia on June 14, 2024, a day with several exceedances.

TEMPO-derived O_3 qualitatively captures the regional nature of air quality episodes.

Results are preliminary and may change.

Capturing O_3 exceedances in metro Atlanta



TEMPO-Derived (background) and EPA monitor (circles) O_3 in northern Georgia on June 14, 2024, a day with several exceedances.

TEMPO-derived O_3 qualitatively captures the regional nature of air quality episodes.

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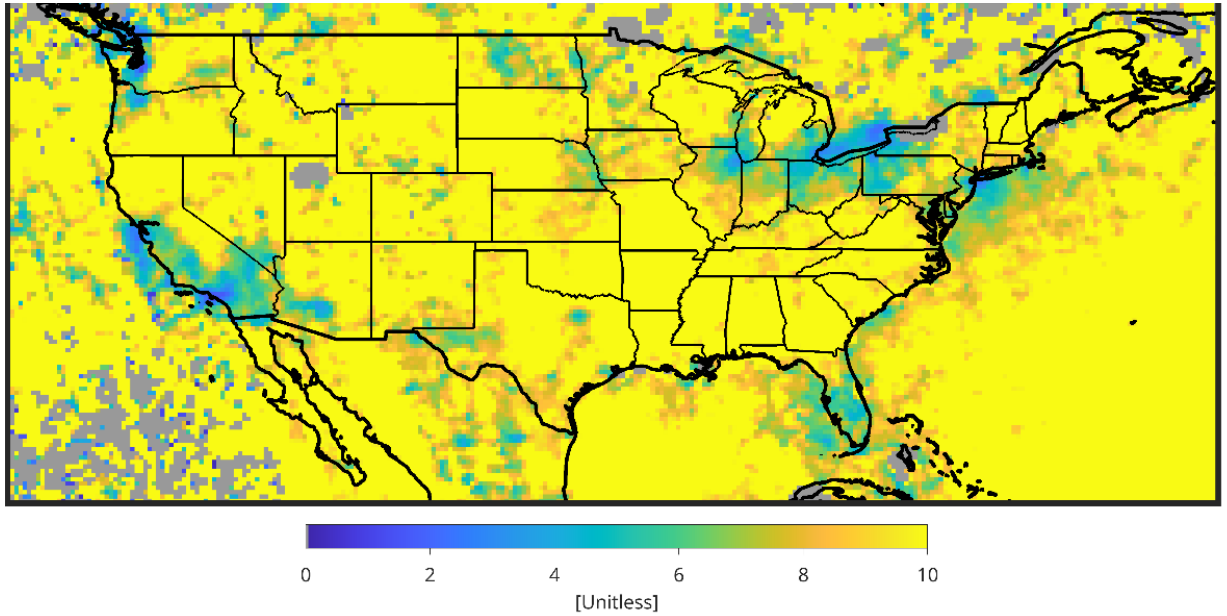
Tool 2: Constraining ozone production

A long-standing need for air quality (AQ) managers has been to infer surface ozone production (PO_3) with fine spatiotemporal coverage, which cannot be done with their sparse surface network of AQ monitors.

AQ managers have used satellite data of formaldehyde (HCHO) and nitrogen dioxide (NO_2) to serve as a proxy for VOC/NO_x, an indicator of PO_3 sensitivity to NO_x and VOC concentration changes.

However, $HCHO/NO_2$ is not PO_3 and has inherent limitations. Also, a more robust estimate of PO_3 sensitivity would account for other factors that determine sensitivity (e.g., sunlight and water vapor).

OMI $HCHO/NO_2$ (July-August 2019)



The ratio of OMI $HCHO/NO_2$, where values <1 indicate VOC-limited, 1–2 indicate mixed, and >2 suggest NO_x-limited regimes. Image courtesy of Amir Souri.

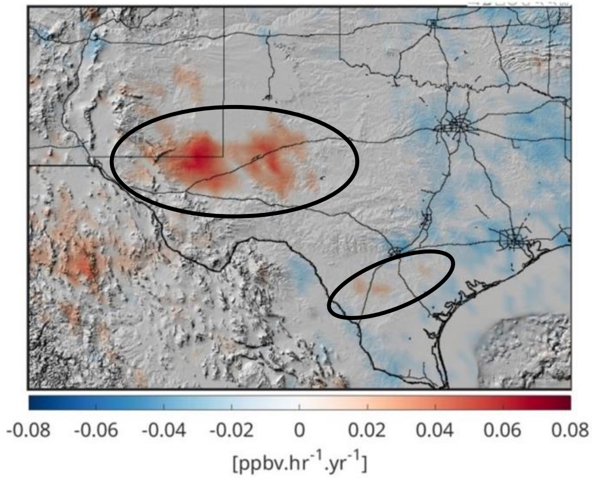
PO_3 from OMI and TROPOMI provide constraints on long-term trends

ML Technique: Used Deep Neural Net (DNN) to parameterize surface ozone production rates (PO_3) rates and chemical sensitivities with fine spatiotemporal resolution.

Training datasets: Trained on millions of NASA/NOAA airborne data points.

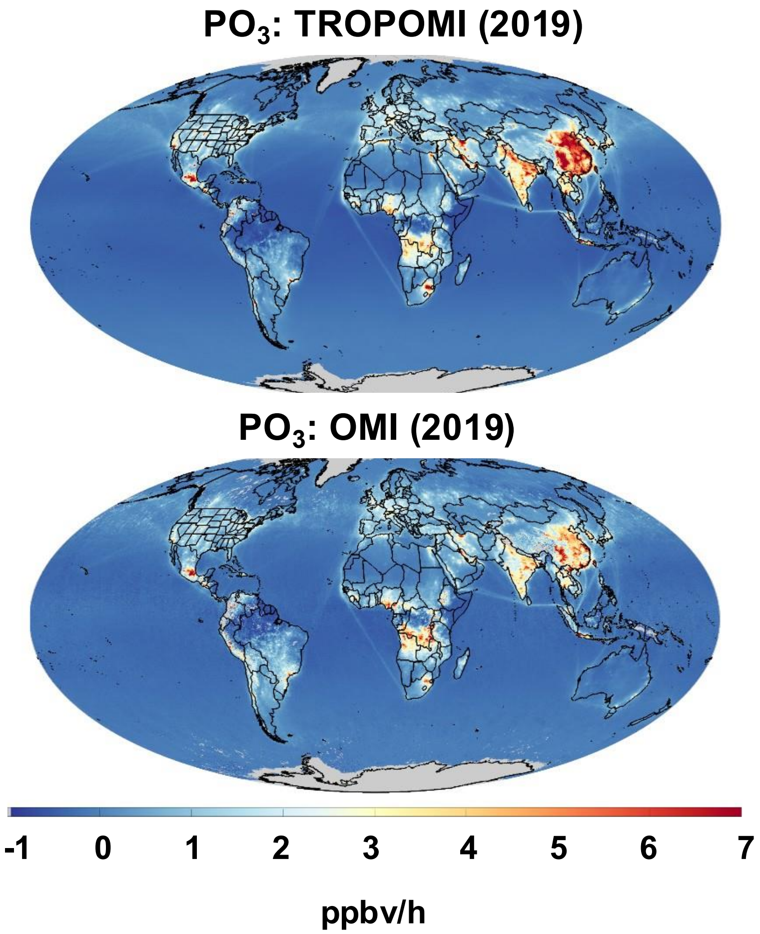
PO_3 Product: In the ML model, observations of O_3 drivers (i.e., NO_2, HCHO) were input from the multi-decadal NASA and international satellite record (e.g., OMI and TROPOMI NO_2 and HCHO; TROPOMI surface albedo).

Trends of PO_3 (2005-2020) Inferred using OMI Data



PO_3 increases (red) are primarily associated with increased pollutant emissions from oil and natural gas extraction activities.

PO_3 decreases (blue) are primarily associated with NO_x emission reductions from automobiles and power plants.

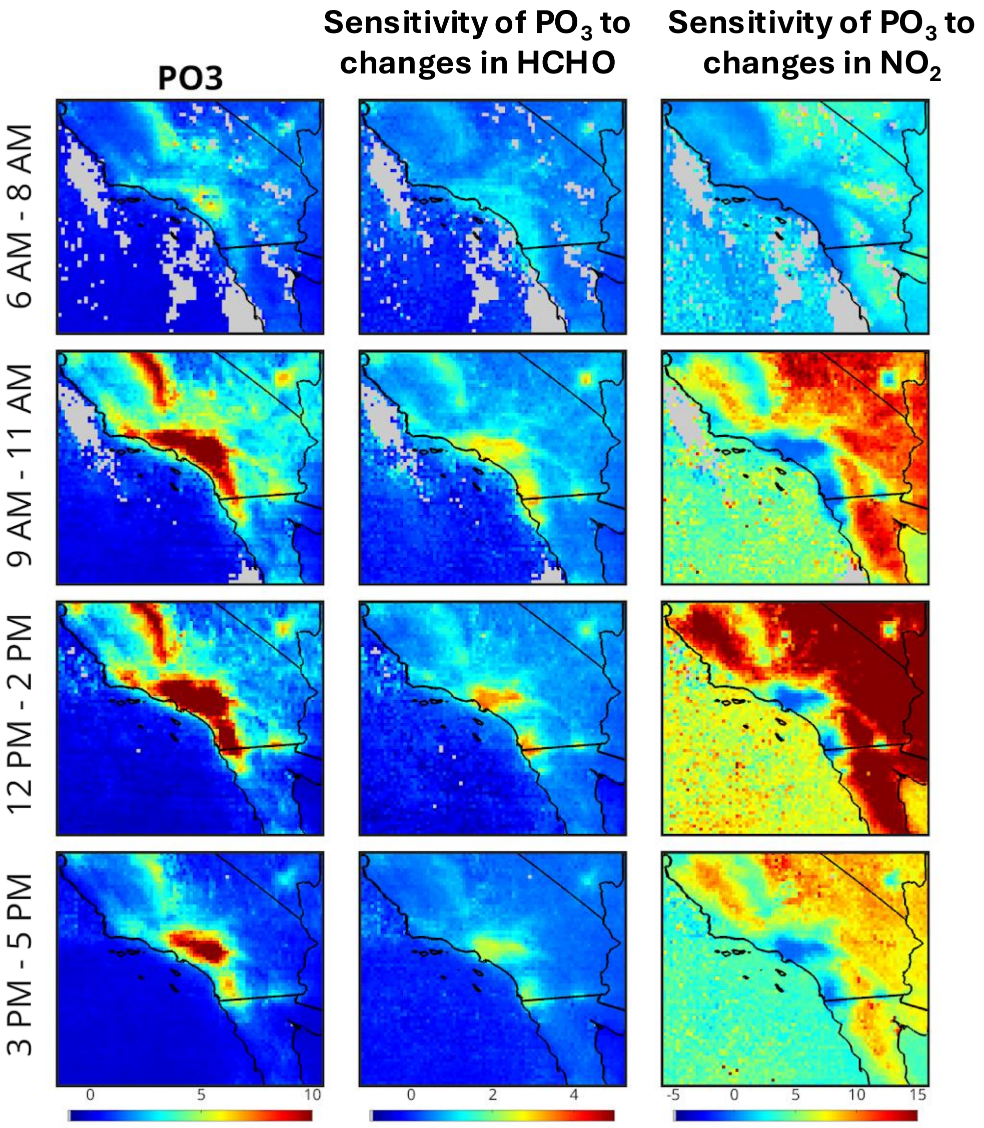


Global PO_3 maps derived from TROPOMI (top) and OMI (bottom) datasets based on the PO_3DNN algorithm in 2019. These near-surface values are estimated at ~13:30 LST.

https://www.ozonerates.space

Souri et al, 2026, Beyond binary maps for HCHO/NO_2, ACP.

PO_3 from TEMPO reveals diurnal changes in drivers of production



Southern California, July 2024

Machine learning allows for a new approach in determining observationally constrained sensitivities of PO_3 to HCHO and NO_2, complementing the HCHO/NO_2 ratio approach for determining O_3 production regimes.

- Can use a similar methodology with TEMPO data, facilitating analysis on the diurnal variability of PO_3.
- In addition to NO_2 and HCHO, ML approach also constrains relative importance of photolysis in driving PO_3.
- PO_3 sensitivity to HCHO and NO_2 is substantially smaller in the early morning and after 3 PM.

Tool 3: Constraining pollutant budgets

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Background Information

The hydroxyl radical (OH) is the atmosphere's primary oxidant as it chemically reacts with many gases, influencing the residence times of pollutants, such as ozone, NO_x and VOCs.

Despite its pivotal role, the spatiotemporal distributions and variations of tropospheric OH are poorly constrained.

- Tropospheric OH isn't observed from space and in situ observations are very sparse and uncertain.
- Models disagree on OH abundances and thus do not serve as a useful constraint.

Simplified Schematic of OH Chemistry

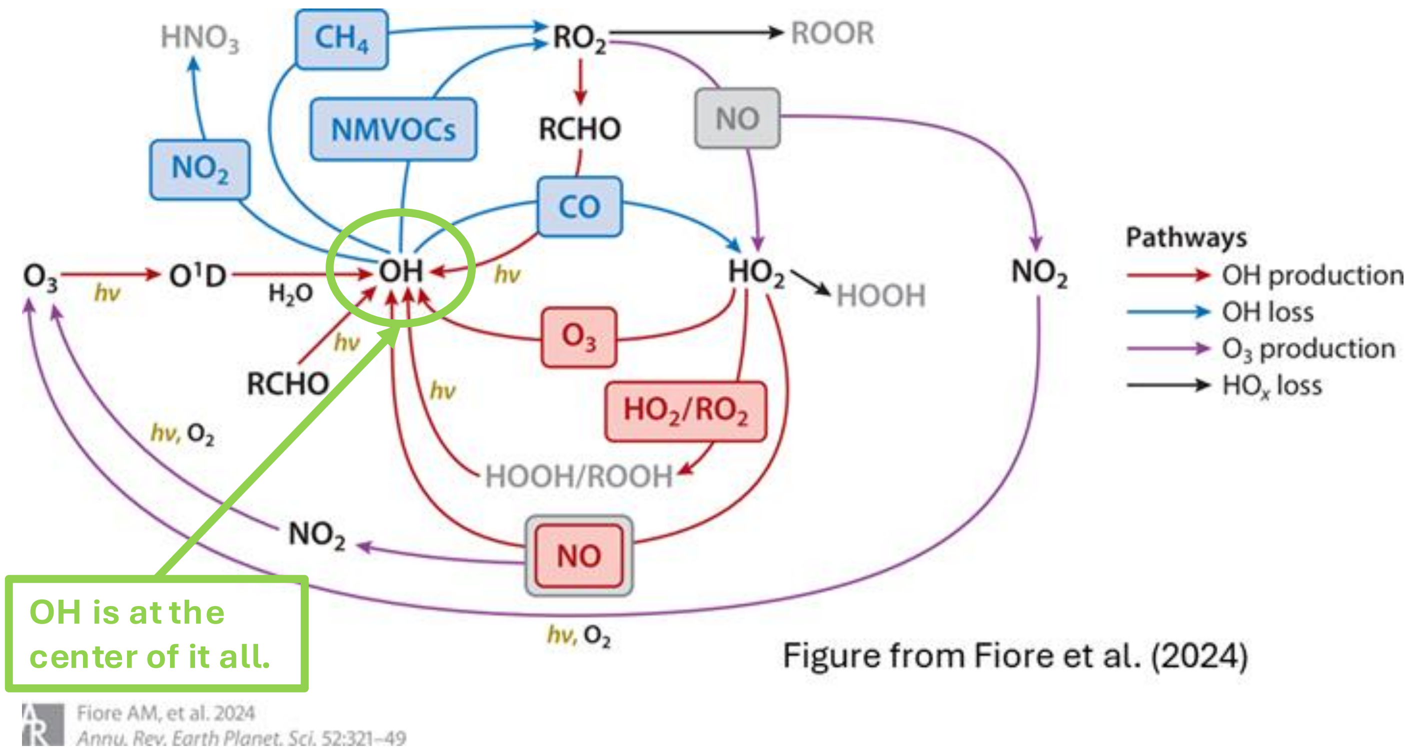


Figure from Fiore et al. (2024)

Constraints on the oxidative capacity would help stakeholders to better quantify the residence times of key pollutants influenced by OH (e.g., improve AQ and atmospheric composition models; inform policy makers).

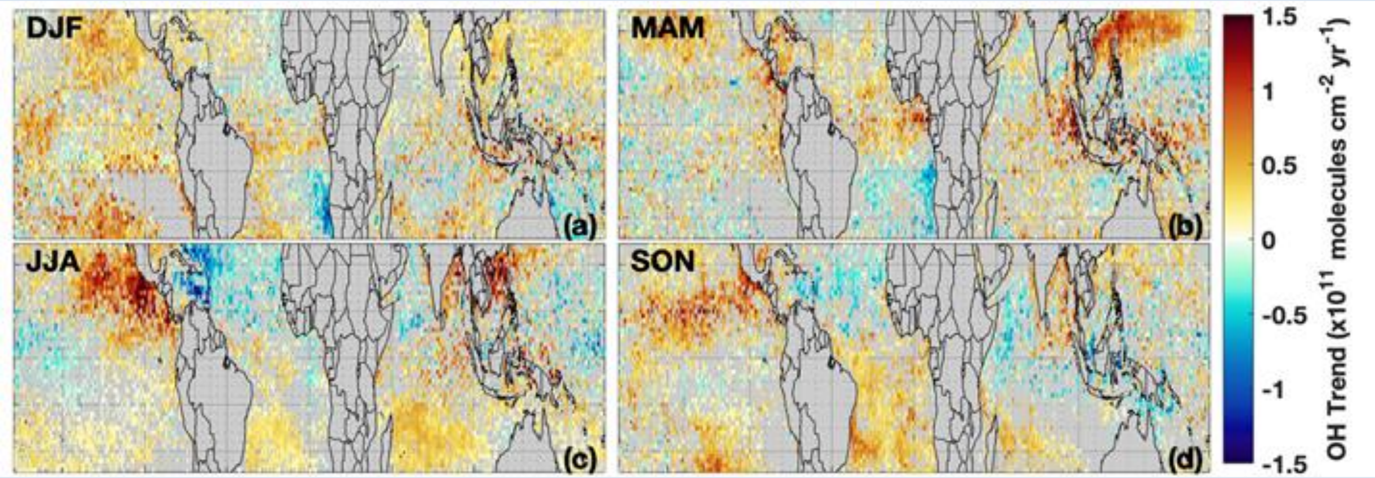
Novel constraint of OH with satellite data and machine learning

ML Technique: Use Gradient Boosted Regression Trees (GBRT) to create a model to predict tropospheric column OH (TCOH) with fine spatiotemporal resolution.

Training Dataset: Train with output from a NASA GEOS atmospheric composition simulation of satellite-observed quantities for 2005 – 2019.

Sat-OH Product: Into the ML model, input observations of OH drivers from the multi-decadal NASA EOS satellite record (e.g., OMI NO_2, HCHO, & O_3, MOPITT CO, AIRS H_2O).

OH Trends (2005-2019) over Tropical Oceans



Statistically significant trends in OH from 2005 – 2019 as determined from Sat-OH. This product allows for the determination of spatially resolved trends in OH variability, representing a significant advance over traditional methods of inferring OH. Figure from Duncan et al. (2024)

A similar methodology applied over land could provide constraints on VOC loss and O_3 production regime.

Increasing interpretability of results

Combining machine learning and satellite data offers multiple new, complementary pathways to constrain surface O_3. Because the models are not process based, however, interpretation of results should be approached cautiously.

- Potential pathways to increase interpretability:
  - Constraining O_3 with multiple tools, as we demonstrated here.
  - Using newer ML approaches, such as process informed Neural Networks.
  - Constraining budget terms with a similar approach (e.g., O_3 loss to OH/primary OH production). See Anderson, et al. 2026, Towards closing the OH budget, JGR.

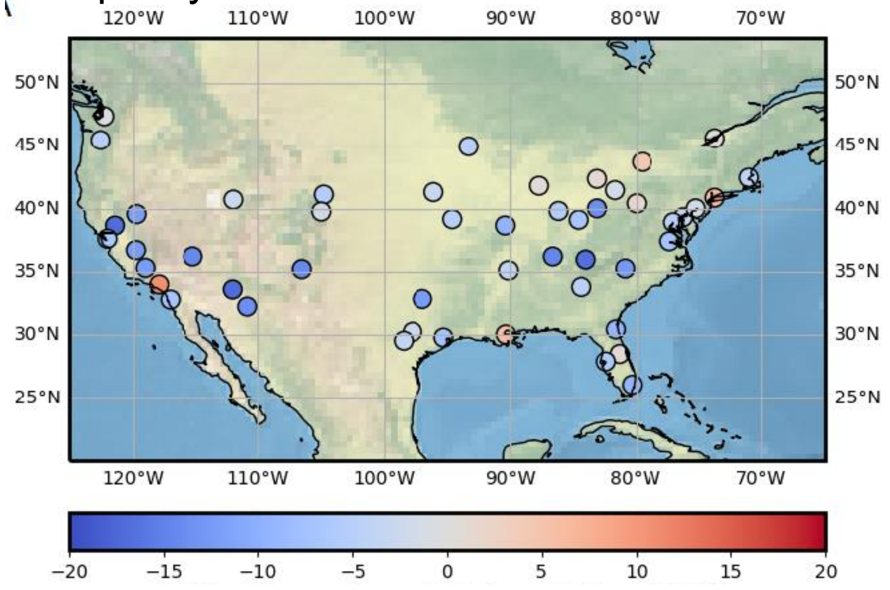
The path forward

- Surface O_3:
  - Improving performance at higher O_3 values
  - Development of a short-term (~24 hr) forecast
- O_3 Production:
  - Further development of TEMPO-based product
  - Analysis of relative importance of VOCs, NO_x, and photolysis in driving diurnal variability
- Satellite-Constrained OH:
  - Expansion of product over global oceans
  - Establishing feasibility of approach over land
  - Application of methodology to TEMPO
- Contact: daniel.c.anderson@nasa.gov (OH and surface O_3) and a.souri@nasa.gov (PO_3)

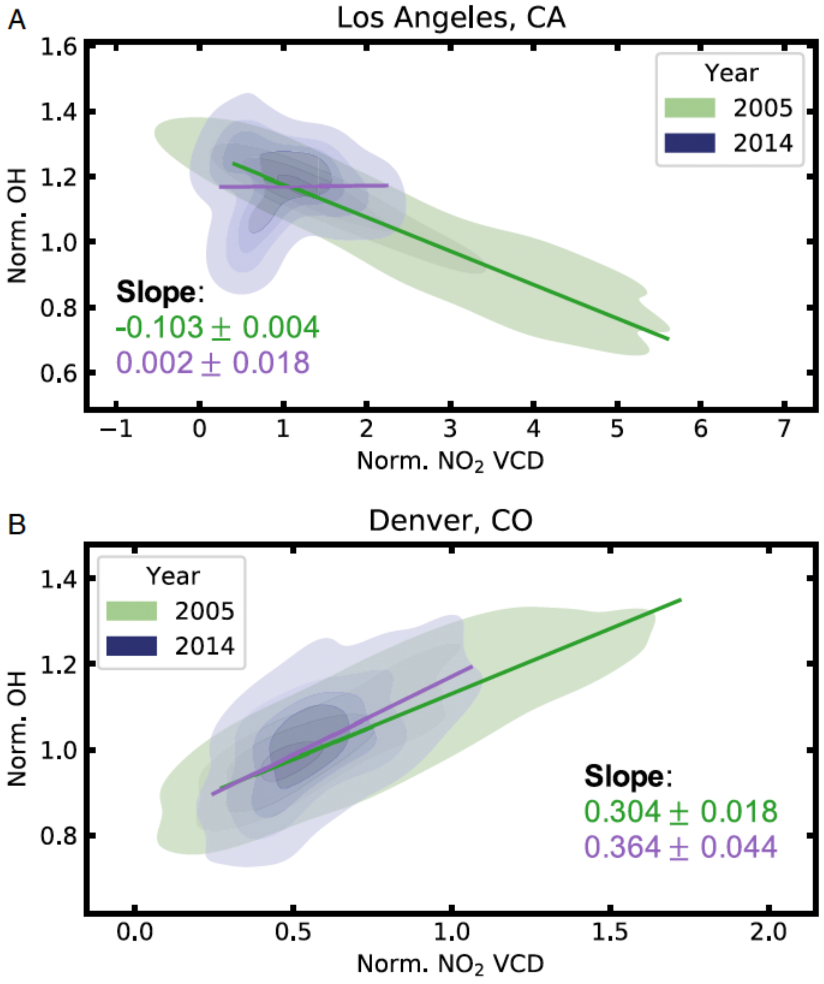
Backup

Using OH trends to infer O_3 production regime

- Zhu et al (2022) used ML, WRFChem, and OMI NO_2 and HCHO to estimate trends in OH over US urban areas.
- OH decreased over most areas from 2005 to 2014, suggesting a reduction in the oxidation capacity.



Difference of annual OH between 2005 and 2014 (%)



- Relationship between OH and NO_2 can provide insight into the O_3 production regime.
- Change in the slope in LA from 2005 to 2014 suggests a transition from NO_x saturated to NO_x limited conditions.
- Little change in Denver over the same time period.

Zhu et al, 2022, Estimate of OH trends over one decade in North American cities, PNAS