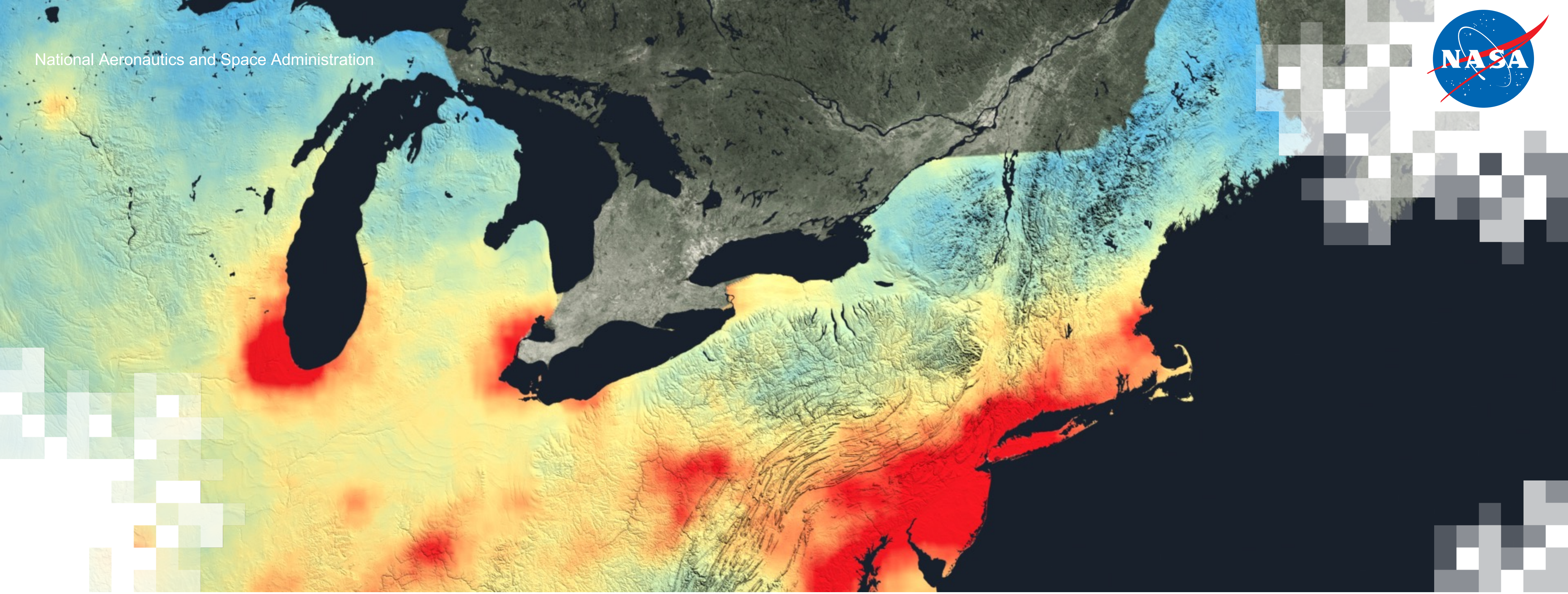


Estimation of Emissions and Surface Concentrations From Satellites: Trace Gases

Sarah Strode, Melanie Follette-Cook, Pawan Gupta, Carl Malings

NASA Air Quality Remote Sensing Training for EPA, March 21-21, 2023

Learning Objectives

By the end of this presentation, you will be able to:

- List several ways satellite observations of trace gases can be used to estimate surface concentrations or surface emissions
- Describe how temporal changes in satellite observations can relate to changes in emissions

Satellite Remote Sensing of Trace Gases for Air Quality

Overview

- With advances in the detection of atmospheric pollution from space, atmospheric composition can be measured at higher spatial and temporal resolutions.
- If chemistry and transport can be accounted for, satellite observations can be used to estimate emission rates.

Review Articles:
Streets et al. 2013, Atmospheric Environment
Emissions estimation from satellite retrievals: A review of current capability
Duncan et al. 2014, Atmospheric Environment (free)
Satellite data of atmospheric pollution for U.S. air quality applications: Examples of applications, summary of data end-user resources, answers to FAQs, and common mistakes to avoid

Bottom-Up Emissions Inventories

- Big undertaking
- Dependent on historical information from many sources
- Updated periodically, not usually real-time

Point Sources | Area Sources | Mobile Sources

→ Emissions Inventory

Power Plant Image: http://cbf.typepad.com/
Ship Image: http://www.un.org/
Cars Image: By User Minesweeper on en.wikipedia
Airplane: http://www.gettyimages.com/

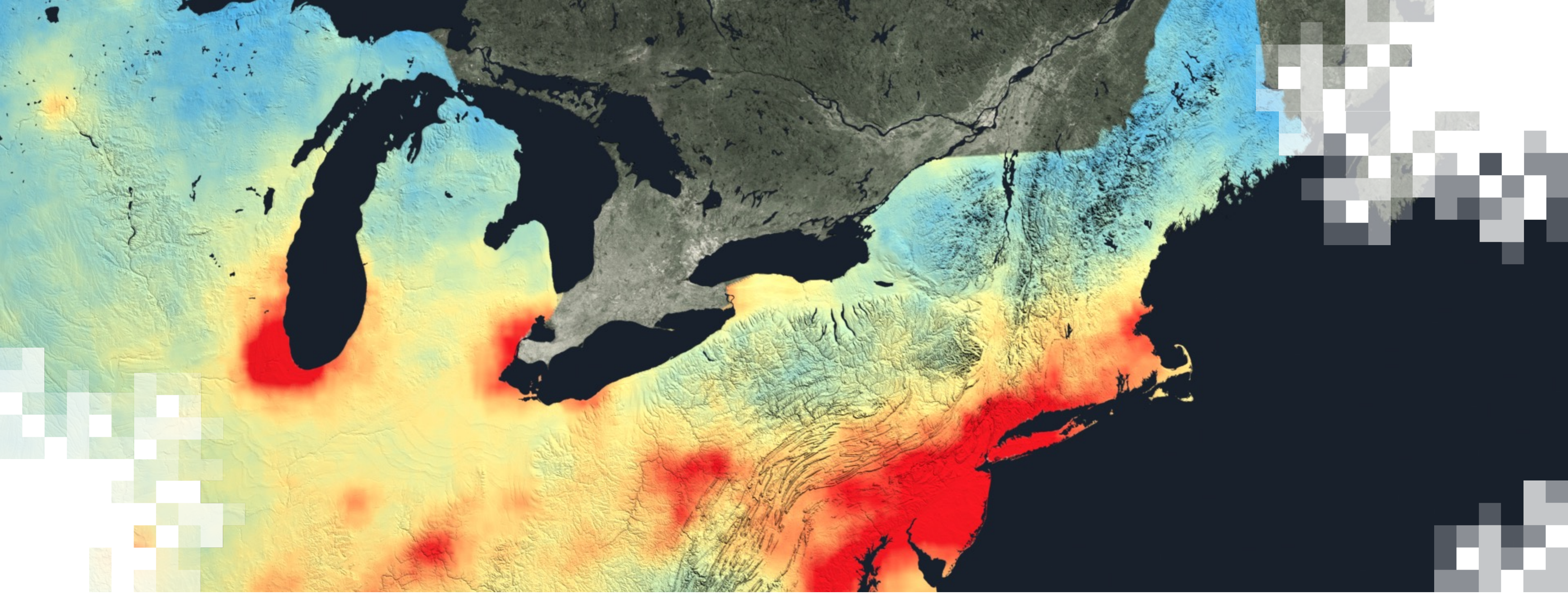
Satellite Remote Sensing of Trace Gases for Air Quality

Types of Emissions that Satellite Observations can Help Constrain

- Anthropogenic Point Source Emissions
  - Power Plants
- Natural Point Sources
  - Volcanoes
- Anthropogenic Area Sources
  - Energy Extraction, Shipping Emissions, Megacities
- Natural Area Sources
  - Biomass Burning, Soils, Lightning, Biogenic

Strengths and Limitations

- Up-to-date information can help infer how emissions are changing.
- Can update bottom-up emissions inventories until a new inventory is completed
  - Example: Lamsal et al. (2011)
- Detection of missing sources
- Also subject to uncertainties
  - Uncertainties in observations
  - Uncertainties as observations are converted to emissions



Methods for Constraining Emissions

Inverse Modeling

- Attribute changes in observed concentrations to changes in emissions
- "Top-down" constraint on emissions
- Constrains emissions using:
  - Observations (e.g., satellite measurements)
  - Background information (a priori)
  - Model simulation of the observed quantity with associated error estimates

[1]Streets et al. (2013) Atmos. Environ.

Inverse Modeling

- Becomes more complicated and computationally expensive as the number of observations increases

- Often uses Bayes theory, which is used to describe the probability of an event, given prior knowledge of other probabilities

- Most inversion methods seek to minimize a cost function or equivalently, use the pdf of the predicted values to find the value that represents the most likely choice (i.e., the maximum of the pdf)

Inverse Modeling

Usually….

$$y = F(x, b) + \varepsilon$$

Observations Model Errors (modeled and observed)

x = the variable we want to estimate
b = all other model parameters

Goal: Obtain x, given y
But errors are important.

Information on x from satellite observations is a *top-down* constraint.
Information on x from processes determining the flux is a *bottom-up* constraint.

Inverse Modeling – Mass Balance

Basic Mass Balance Method

$$E_s = \alpha * \Omega_{observed}$$

Emission of Species, s

Observed Atmospheric Column

$$\alpha = \left(\frac{E_a}{\Omega_m}\right)$$

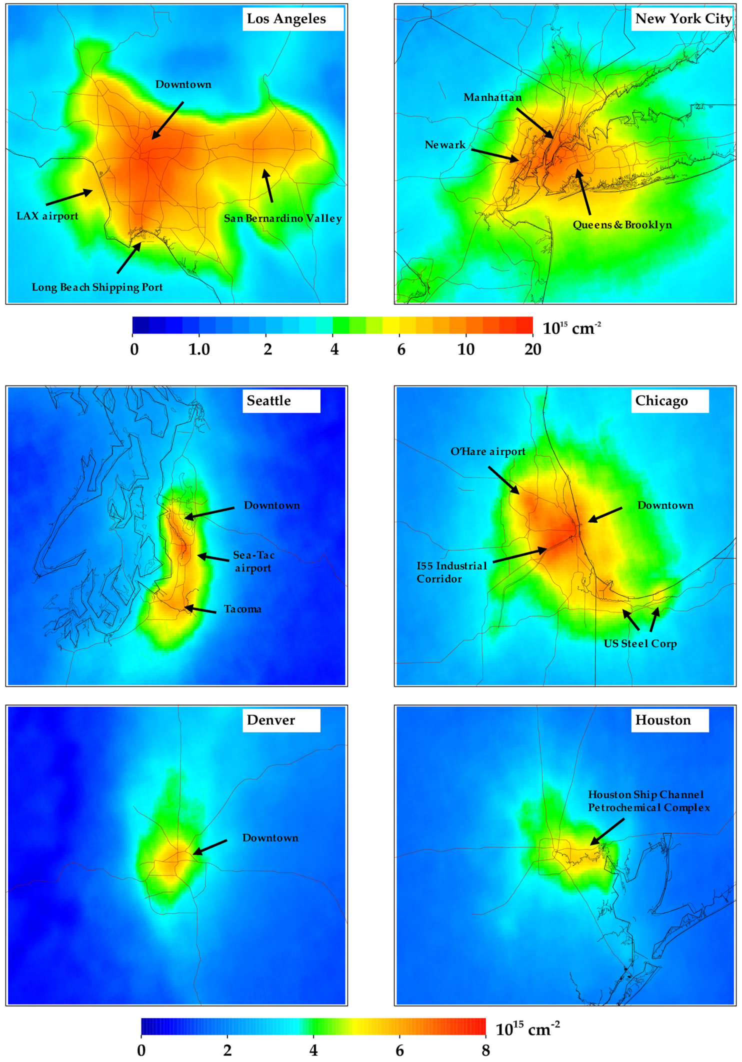
A Priori Emissions Inventory

Model Atmospheric Column

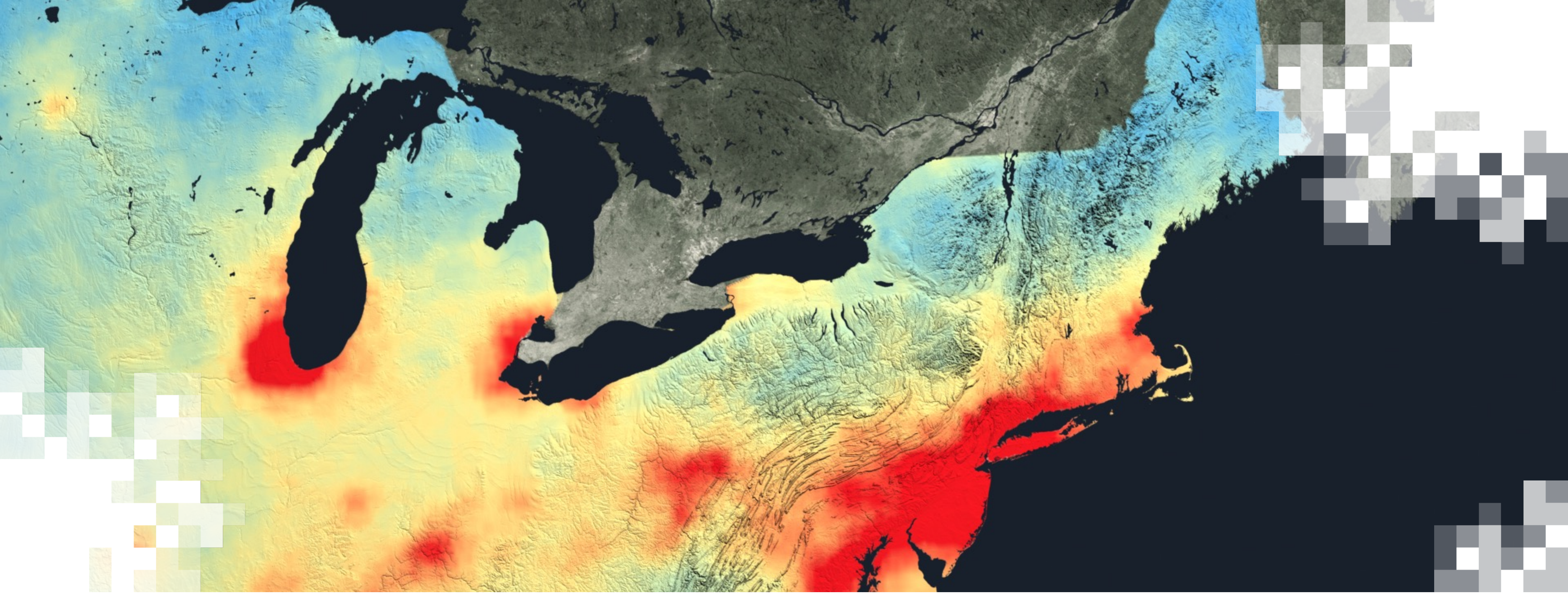
Oversampling

- Accumulating observations over a long time period can map satellite observations to finer resolution, trading temporal resolution for spatial resolution.
- Sometimes used in conjunction with emission estimation methods to reduce noise and improve plume definition
- Can reveal smaller sources
- Caveat: Not raw data and is subject to assumptions; verification is important

TROPOMI NO_2 Oversampled to 0.01°x0.01° Resolution



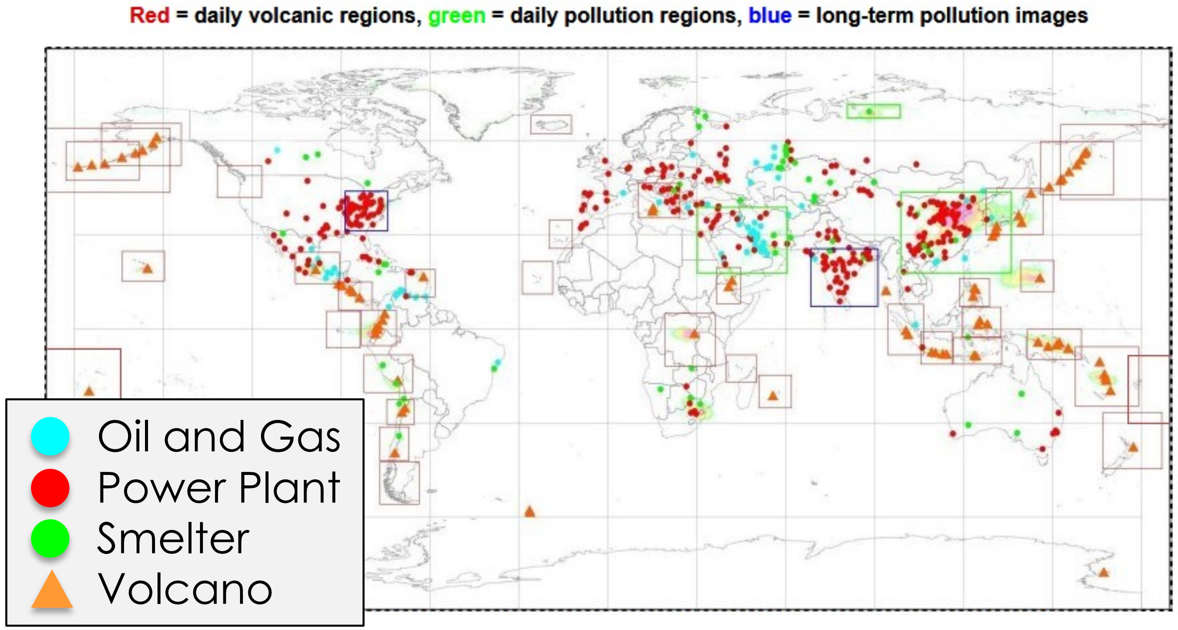
Goldberg et al (2021), "TROPOMI NO2 in the United States: A Detailed Look at the Annual Averages, Weekly Cycles, Effects of Temperature, and Correlation With Surface NO2 Concentrations", Earth's Future, doi: 10.1029/2020EF001665



Examples of Space-Based NO_2 and SO_2 Emission Estimates

Example: SO_2

- Observations available from multiple satellite platforms: OMI, TROPOMI, OMPS
- Sources: Volcanoes, Coal, and Oil Burning
- Why measure SO_2?
  - Linked to adverse respiratory effects
  - Contributes to acid deposition



https://so2.gsfc.nasa.gov/

Emissions Estimates from Space-Based SO_2 Observations

- Catalogue of SO_2 emissions derived from SO_2 observations (Fioletov et al, 2023)
- Available at https://so2.gsfc.nasa.gov/measures.html

Assuming Steady State:

Emission $$E = \frac{\alpha}{\tau}$$

α: Mass of SO_2

τ: Decay time

Emissions from OMI SO_2

Level 2 PBL SO_2
Oversampled to 0.04°

Winds from ECMWF

https://so2.gsfc.nasa.gov/measures.html

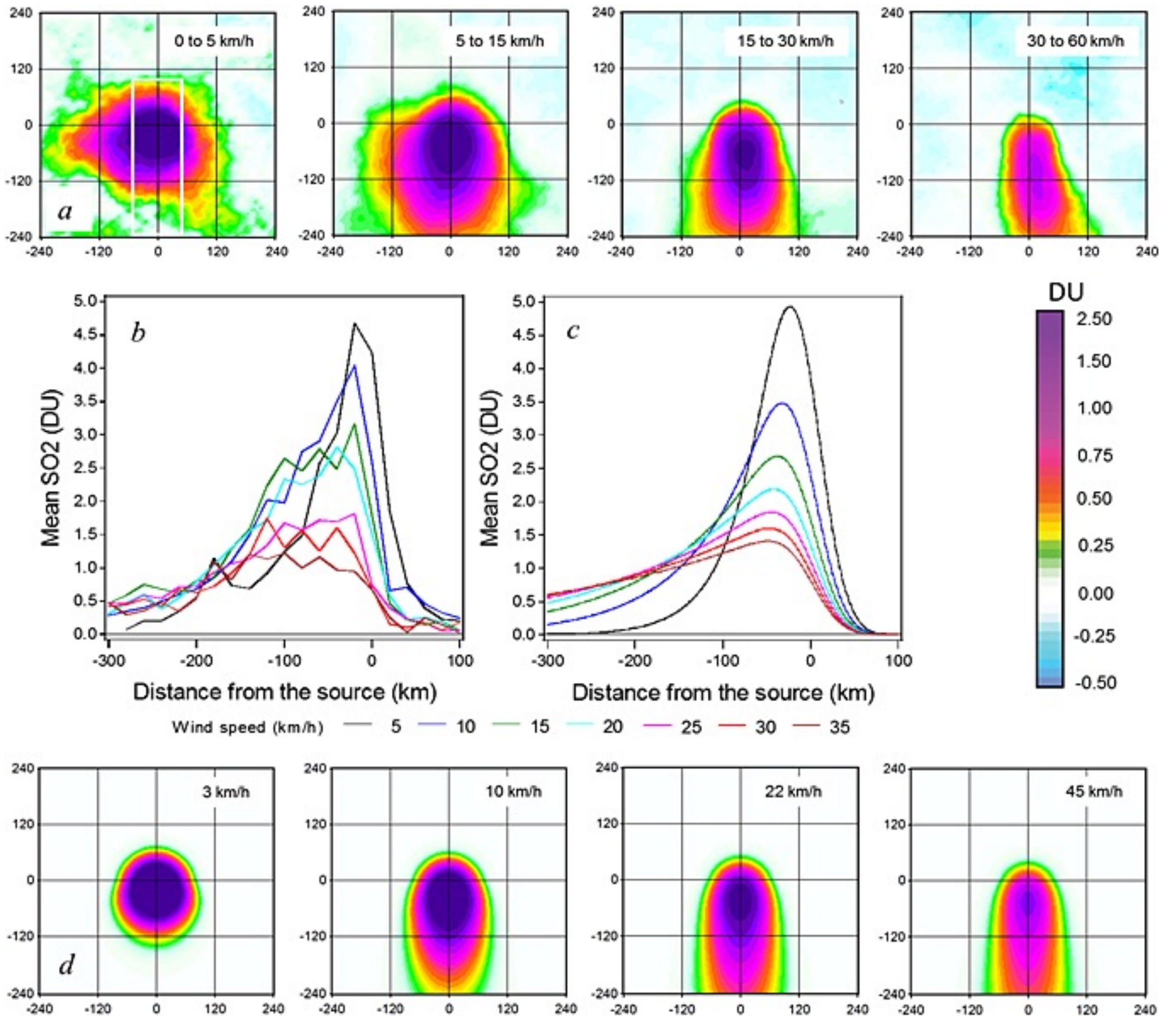
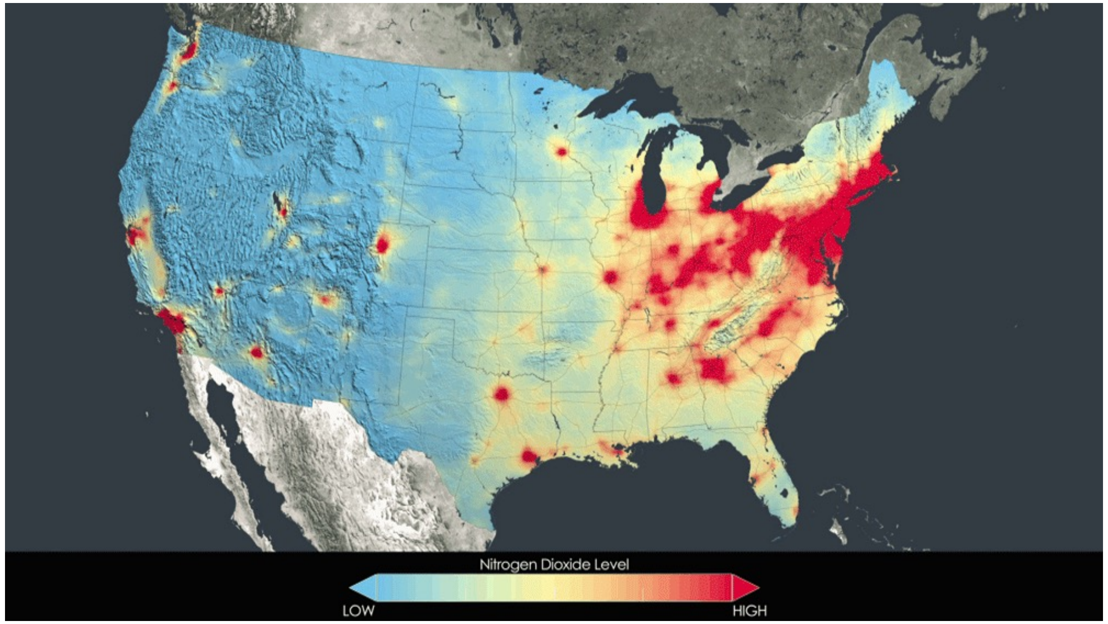


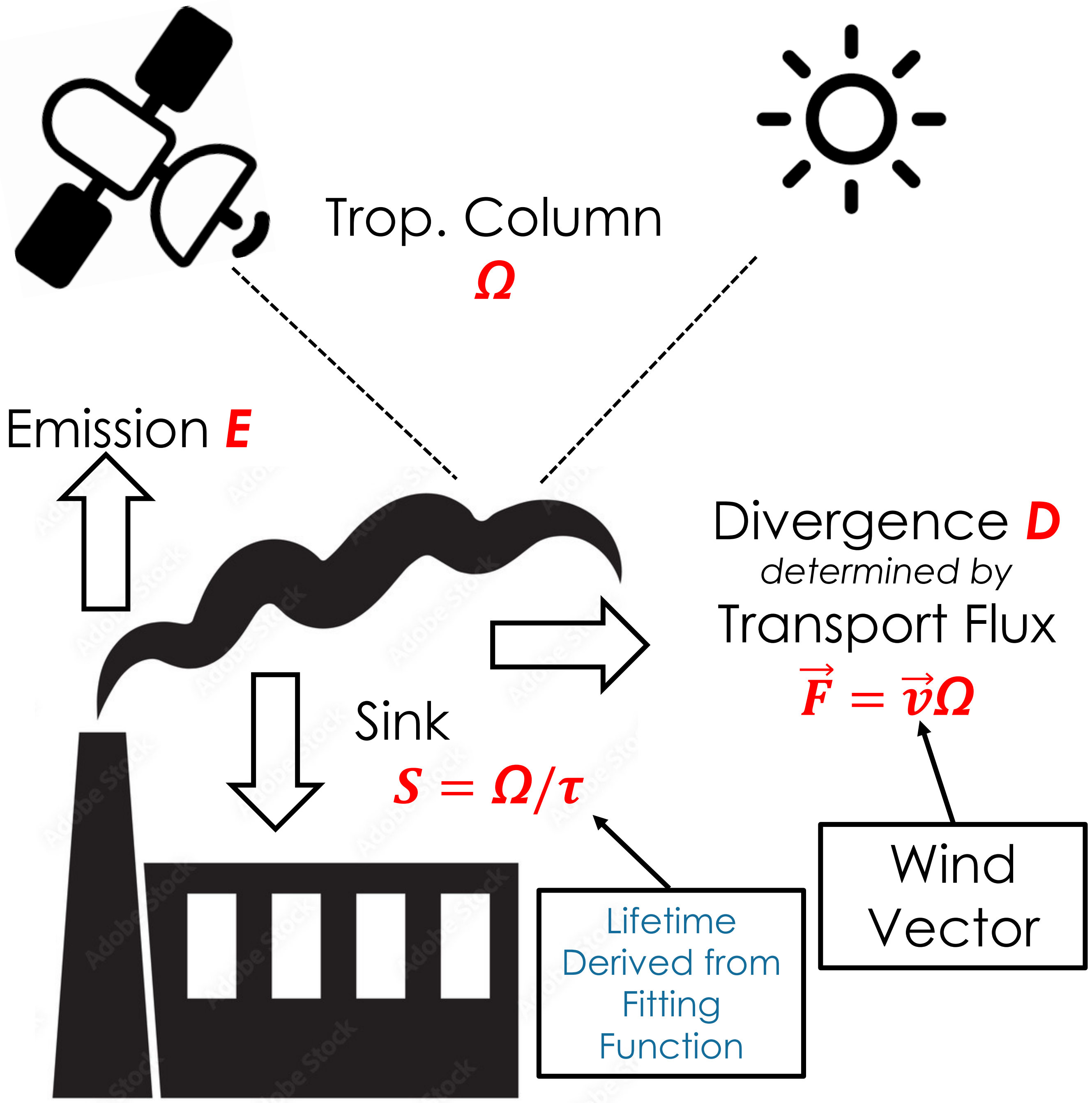
Figure 1, Fioletov et al. (2015), GRL, https://doi.org/10.1002/2015GL063148

Example: Nitrogen Dioxide (NO_2)

- Why measure NO_2?
  - NO_2 is an ozone precursor and health irritant.
  - Sources: Fires, Industrial and Transportation Sources, Stationary Sources (e.g., Power Plants), *but* emissions can vary depending on fuel type and conditions
  - Relatively short-lived, so large gradients and high concentrations within the Planetary Boundary Layer (PBL)
  - Satellite observations have been used in many inverse modeling studies



Source: Duncan, B.N. et al. (2016)



Continuity Equation

$$\frac{\partial \Omega}{\partial t} = E - S - D$$

Assuming Steady State:

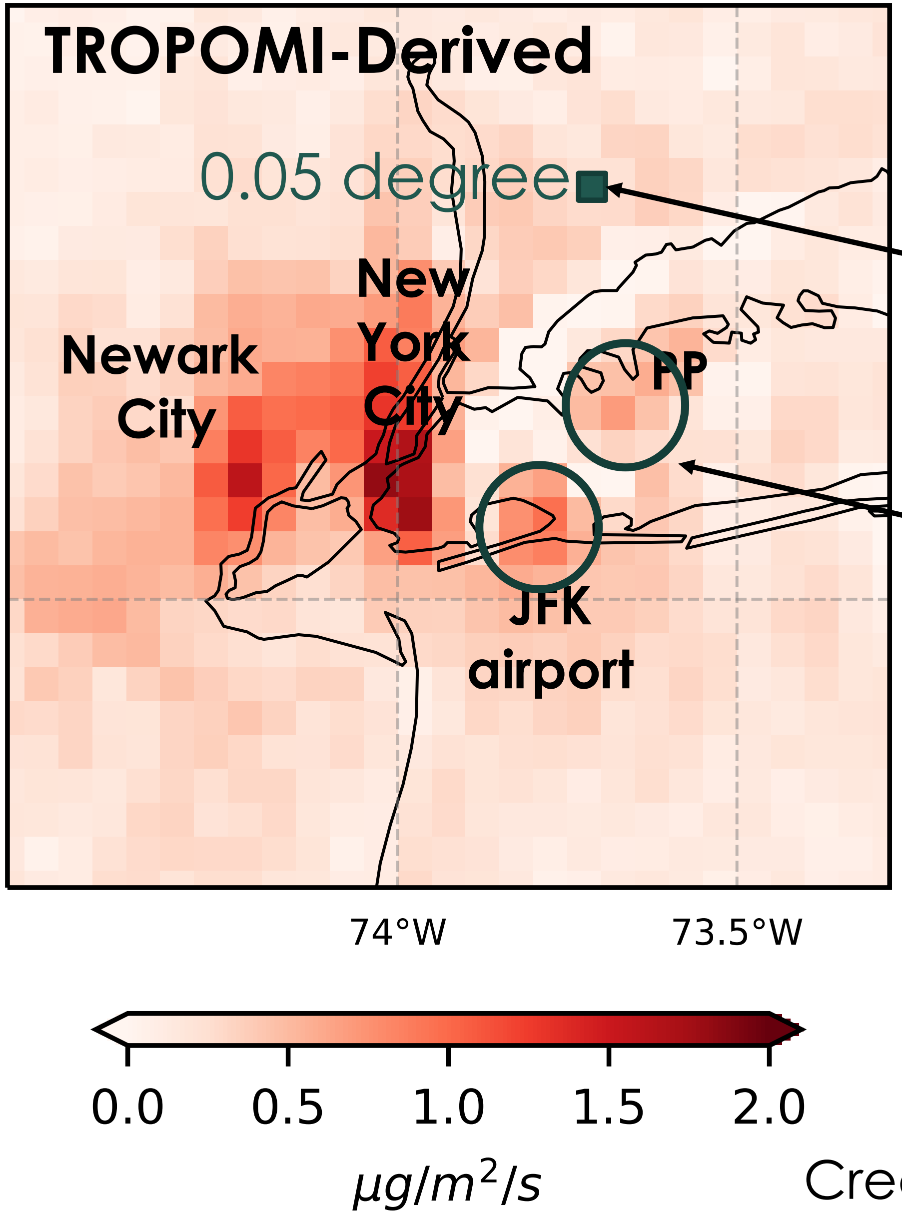
$$0 = E - S - D$$

$$E = D + S = \nabla \cdot \vec{F} + S$$
$$= \nabla \cdot \vec{v}\Omega + \Omega/\tau$$

$$mean(E) = mean(D) + mean(S)$$
$$= \nabla \cdot mean(\vec{F}) + mean(S)$$
$$= \nabla \cdot mean(\vec{v})mean(\Omega) + mean(\Omega)/\tau$$

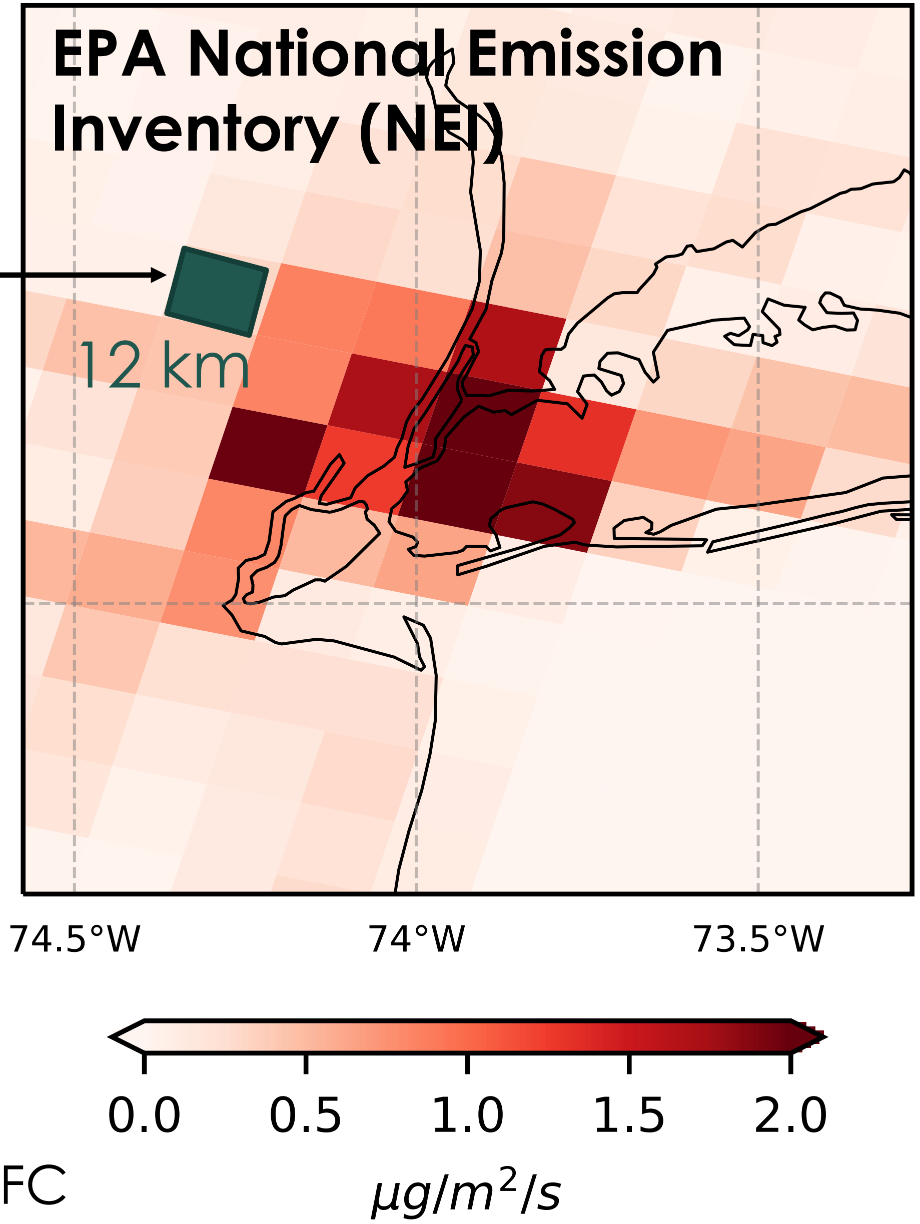
Courtesy of Fei Liu

CTM-Independent High-Resolution Mapping of Urban NO_x Emissions



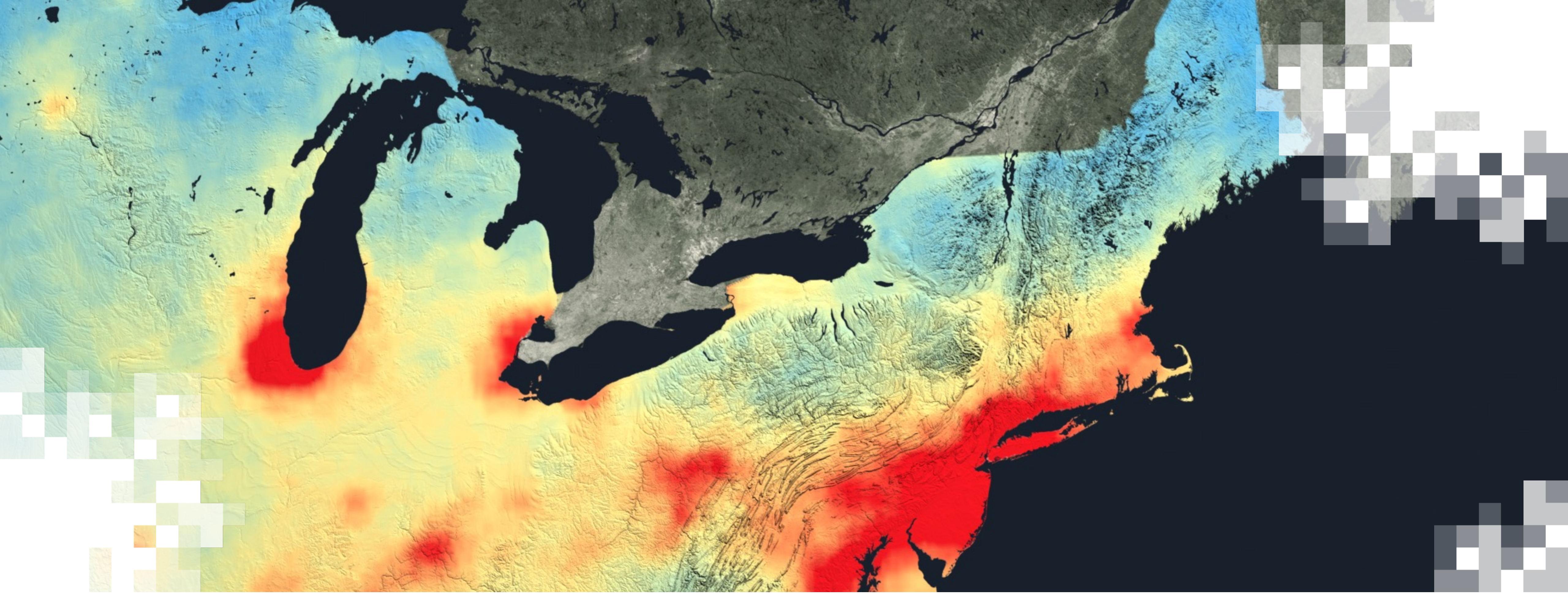
Feature:

- Higher Resolution
- Missing Sources
- Quicker Update (lag of days)



Credit: Fei Liu, NASA GSFC

Annual emissions from 2018-2021 are available upon request from Fei Liu (fei.liu@nasa.gov).



Estimating Surface Concentrations

What can NO_2 columns tell us about the surface?

- NO_2 is relatively short-lived, so it has large gradients and high concentrations within the Planetary Boundary Layer (PBL).
- Emissions, chemistry, and weather all affect how much NO_2 is present at the surface.

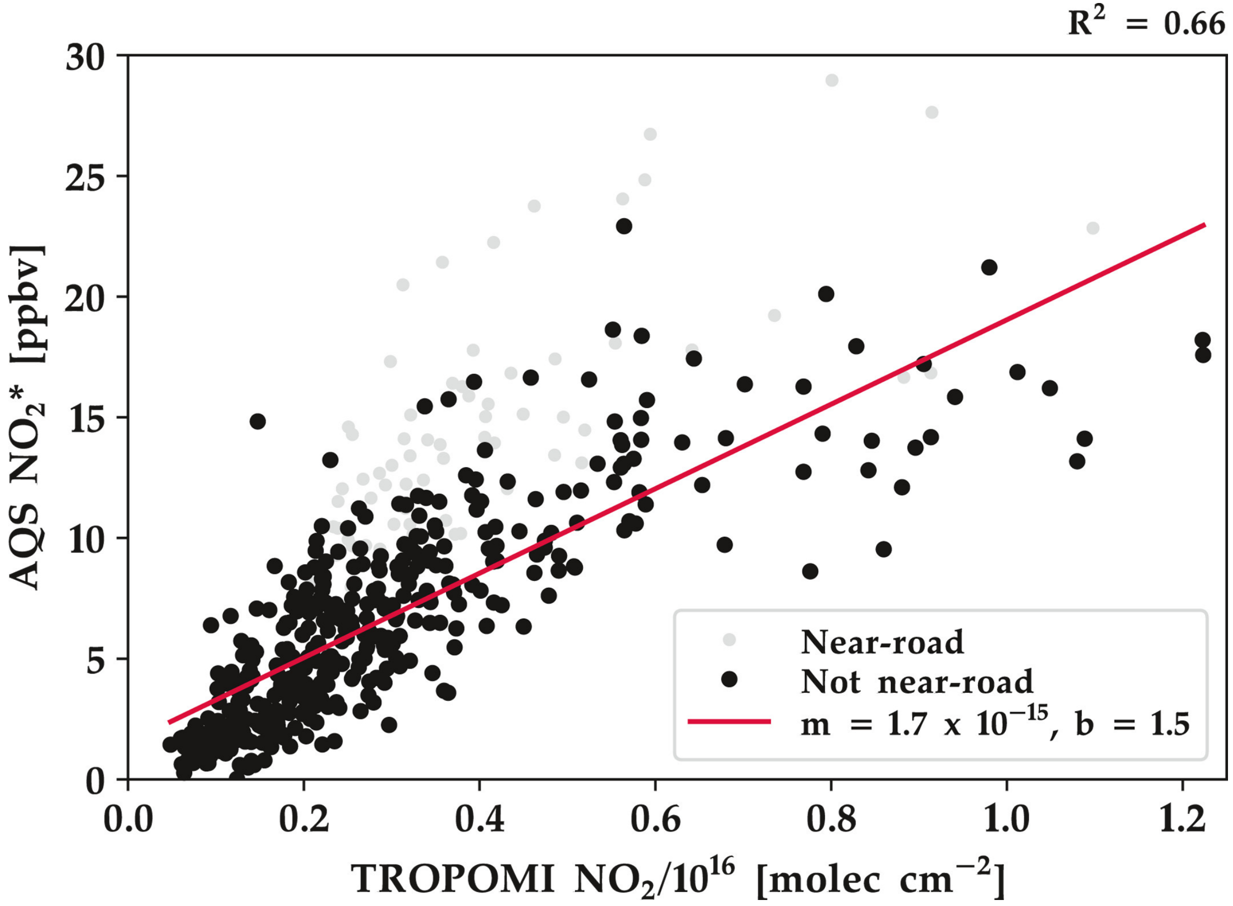
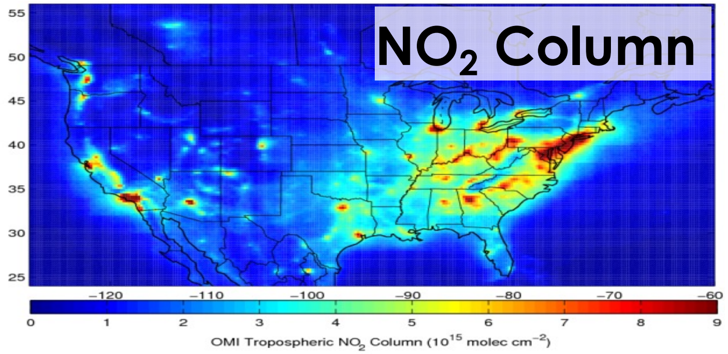


Figure: Goldberg et al, TROPOMI NO2 in the United States: A Detailed Look at the Annual Averages, Weekly Cycles, Effects of Temperature, and Correlation With Surface NO2 Concentrations, Earth's Future, Volume: 9, Issue: 4, First published: 23 February 2021, DOI: (10.1029/2020EF001665)

Estimating Surface NO_2 from the Tropospheric Column



$$v = \frac{\Omega_{Satellite}}{\Omega_{Model}}$$

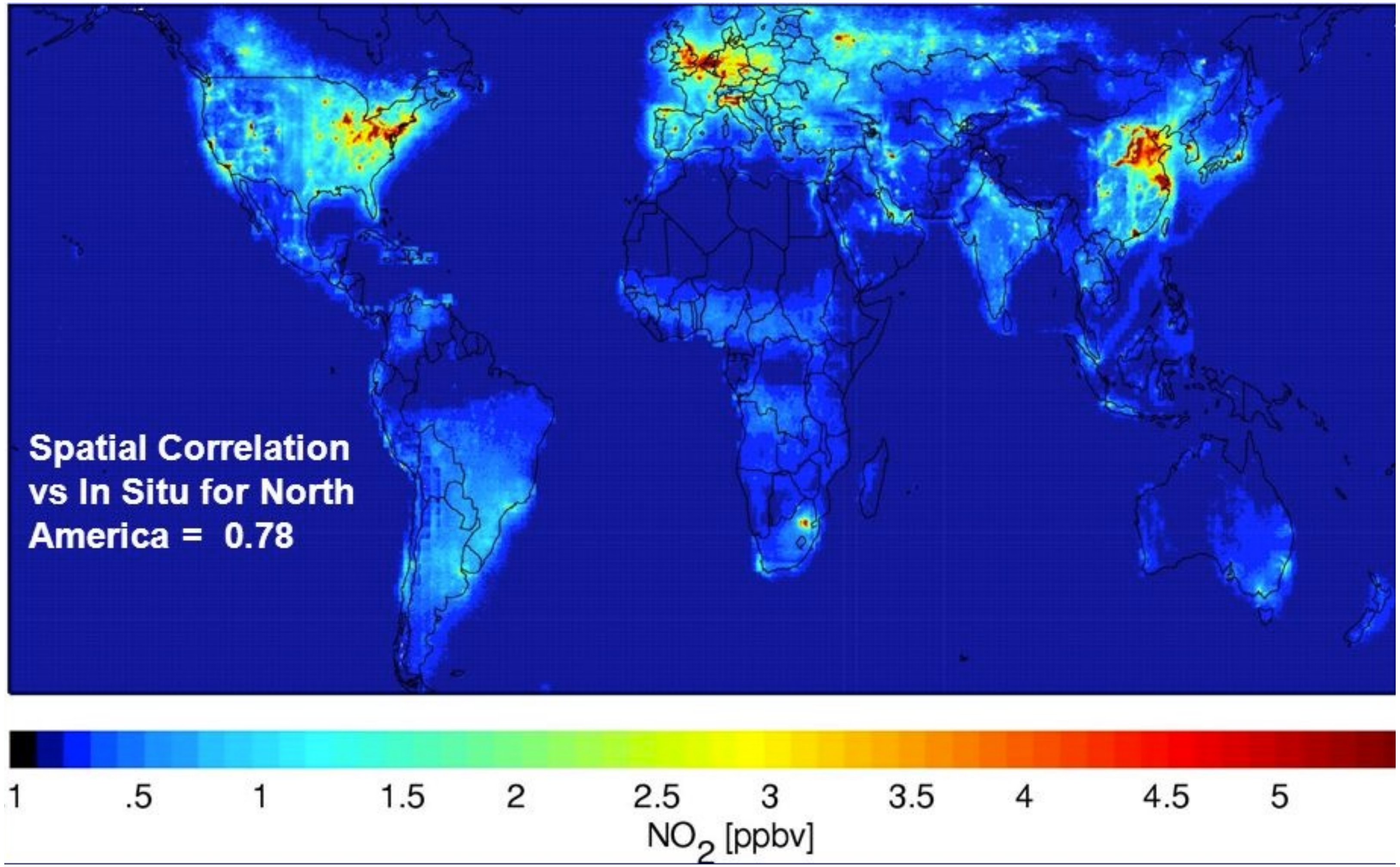
$$S = \Omega_{Sat} \, x \left[\frac{v S_{Model}}{v\Omega_{Model} - (v-1)\Omega_{FT\,(Model)}} \right]$$

Use vertical information from an atmospheric chemistry model to estimate the relationship between the column and the surface.

S = Surface Concentration
Ω = Tropospheric Column
FT = Free Troposphere

Courtesy of Randall Martin

Ground-Level Afternoon NO_2 Inferred from OMI for 2005



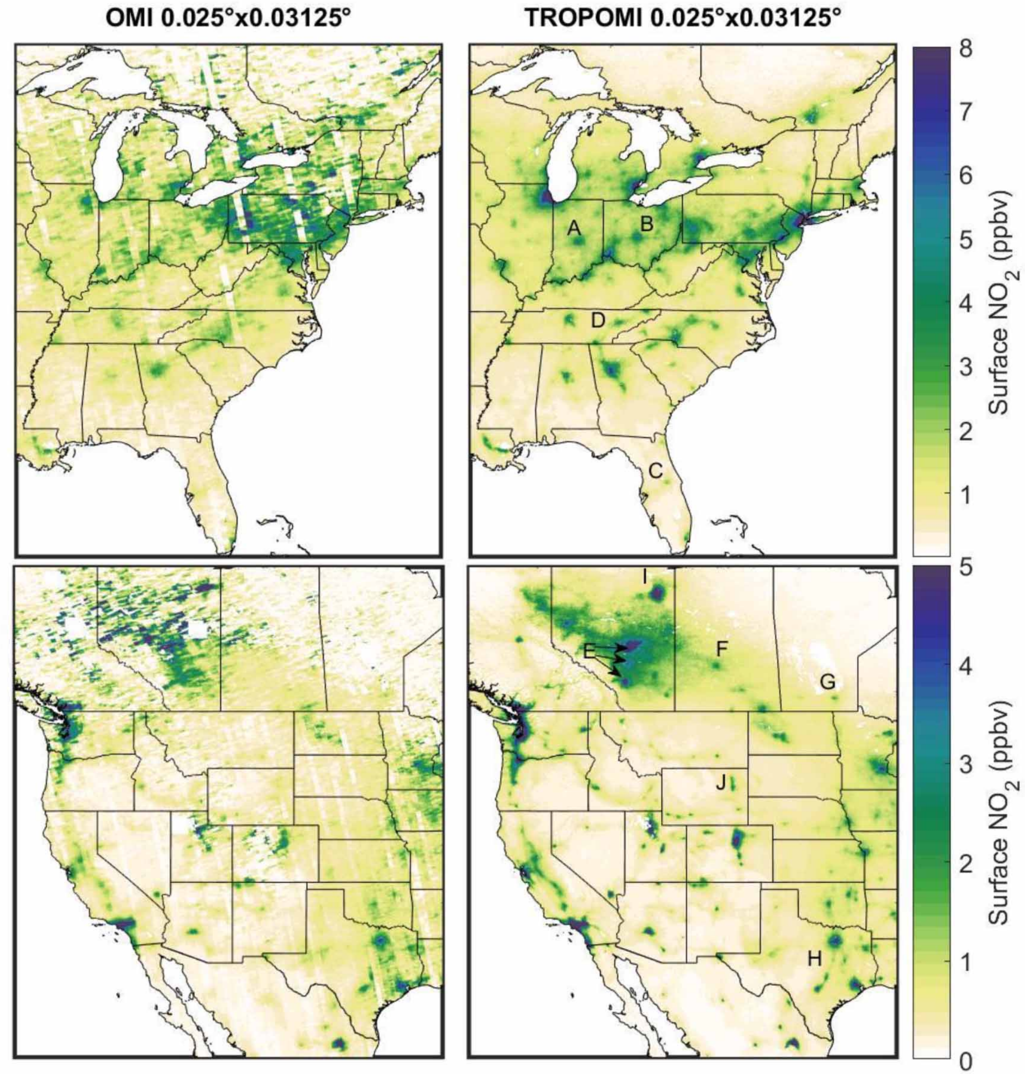
Note: This is a research product and not an official NASA product.

Source: Lok Lamsal

Surface NO_2 Inferred from OMI and TROPOMI

- Cooper et al (2020) estimated surface NO_2 from OMI and TROPOMI using the GEOS-Chem model.
- Differences depending on which satellite is used
  - Smaller cities/corridors resolved with TROPOMI

Annual Mean Surface Concentrations



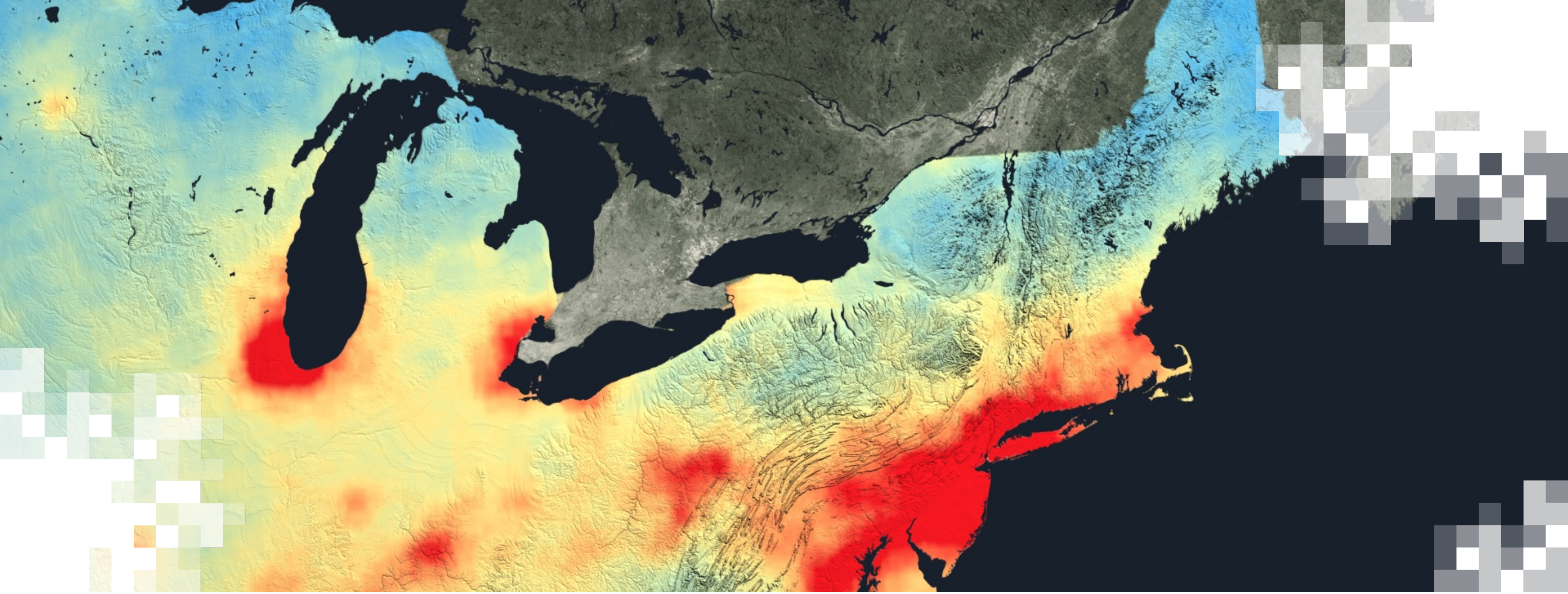
Cooper et al (2020), Inferring ground-level nitrogen dioxide concentrations at fine spatial resolution applied to the TROPOMI satellite instrument, *Environ. Res. Lett.* 15 104013DOI 10.1088/1748-9326/aba3a5

Land Use Regression Models

- Land Use Regression (LUR) models provide another tool for combining satellite observations and other data sources to estimate surface concentrations at fine spatial scales.
- Predictors could include satellite NO_2 observations, distance from roads/traffic, amounts or types of vegetation, population, distance from the coast, elevation, etc.
- Statistical models or machine learning relate predictors to surface concentrations, training on surface observations.

Example References:

- Novotny et al (2011), doi: https://doi.org/10.1021/es103578x
- Larkin et al (2017), doi: https://doi.org/10.1021/acs.est.7b01148



Temporal Changes

Temporal Variations

Satellite observations can be used to monitor changes in emissions over time. This movie shows changes in OMI NO_2 from 2005-2022.

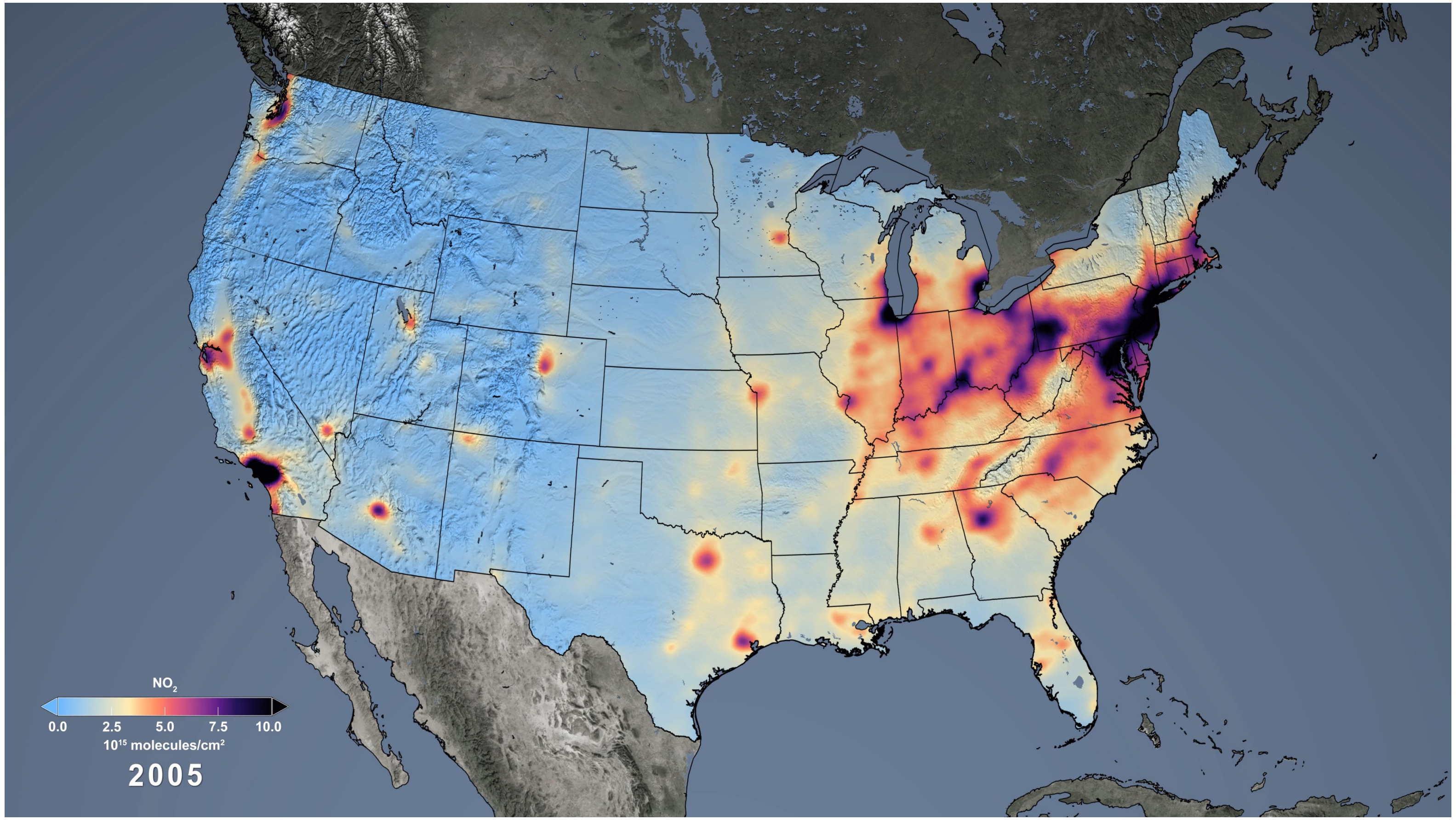
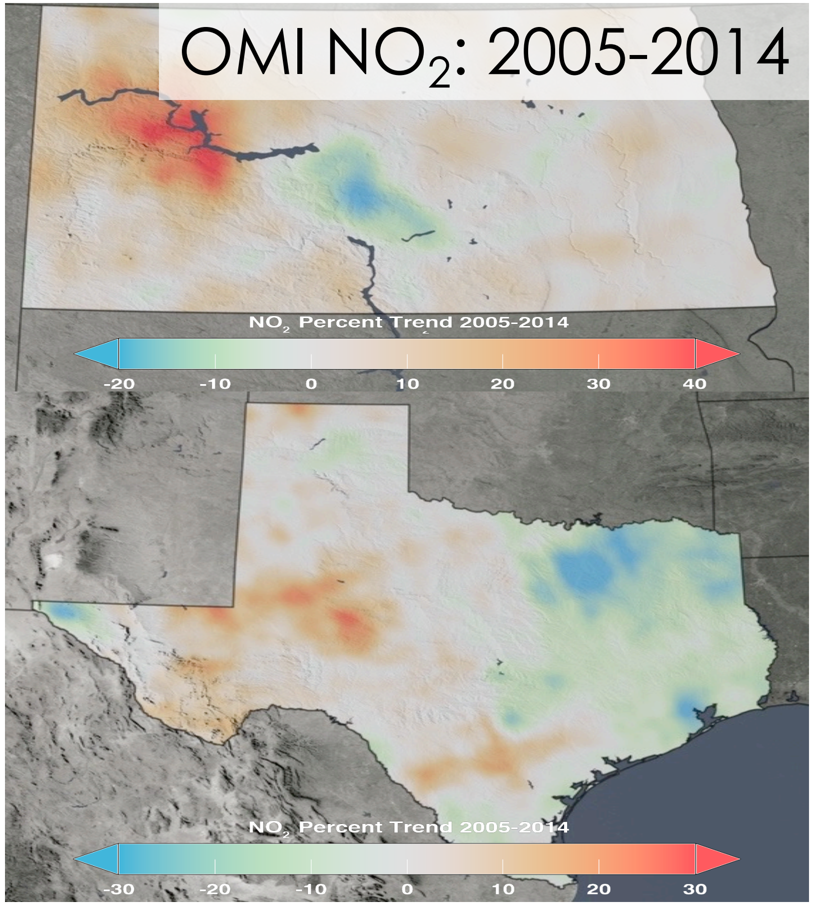


Image Credit: NASA's Scientific Visualization Studio https://svs.gsfc.nasa.gov/5070

Temporal Variations



North Dakota

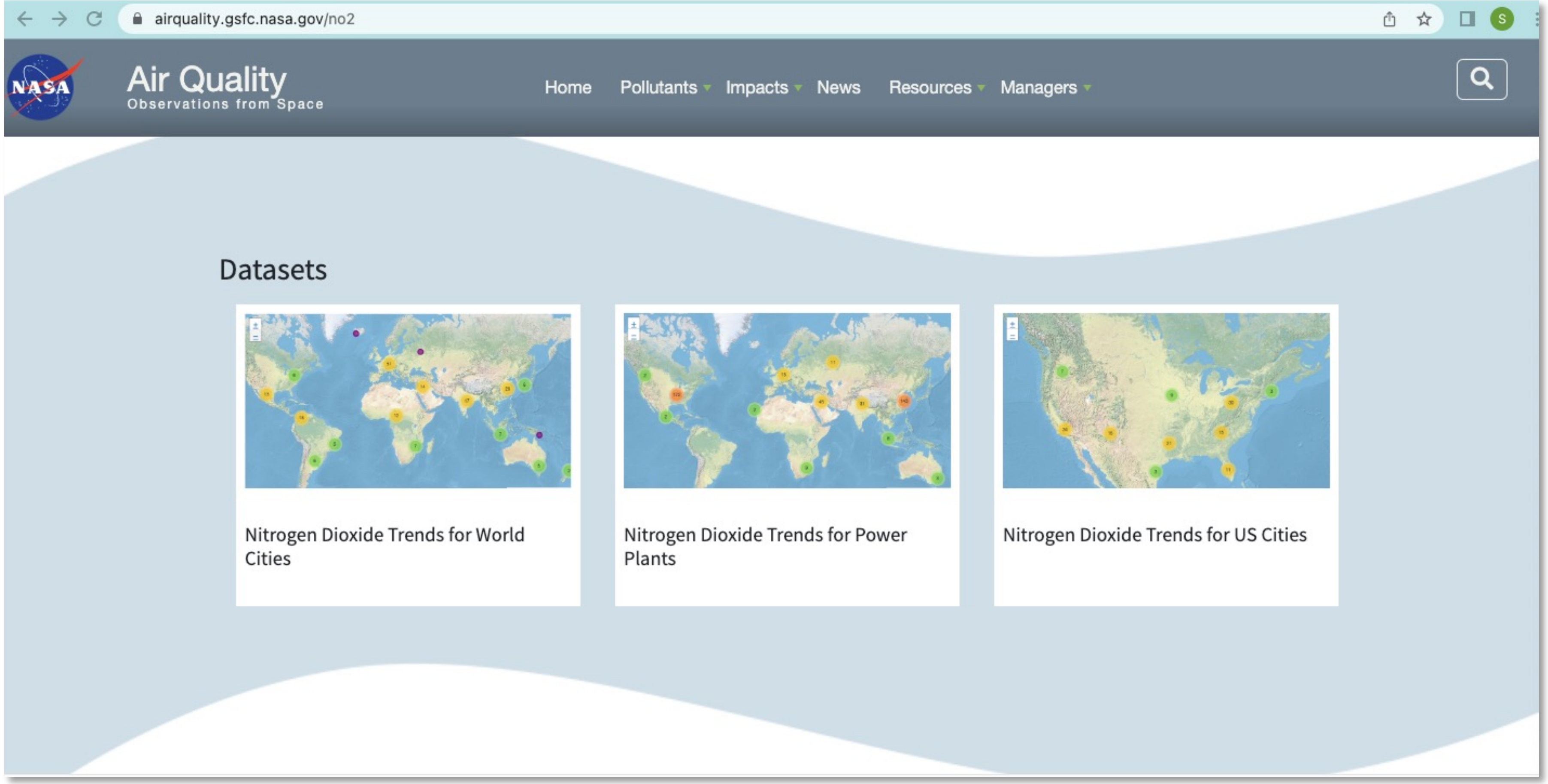
Texas

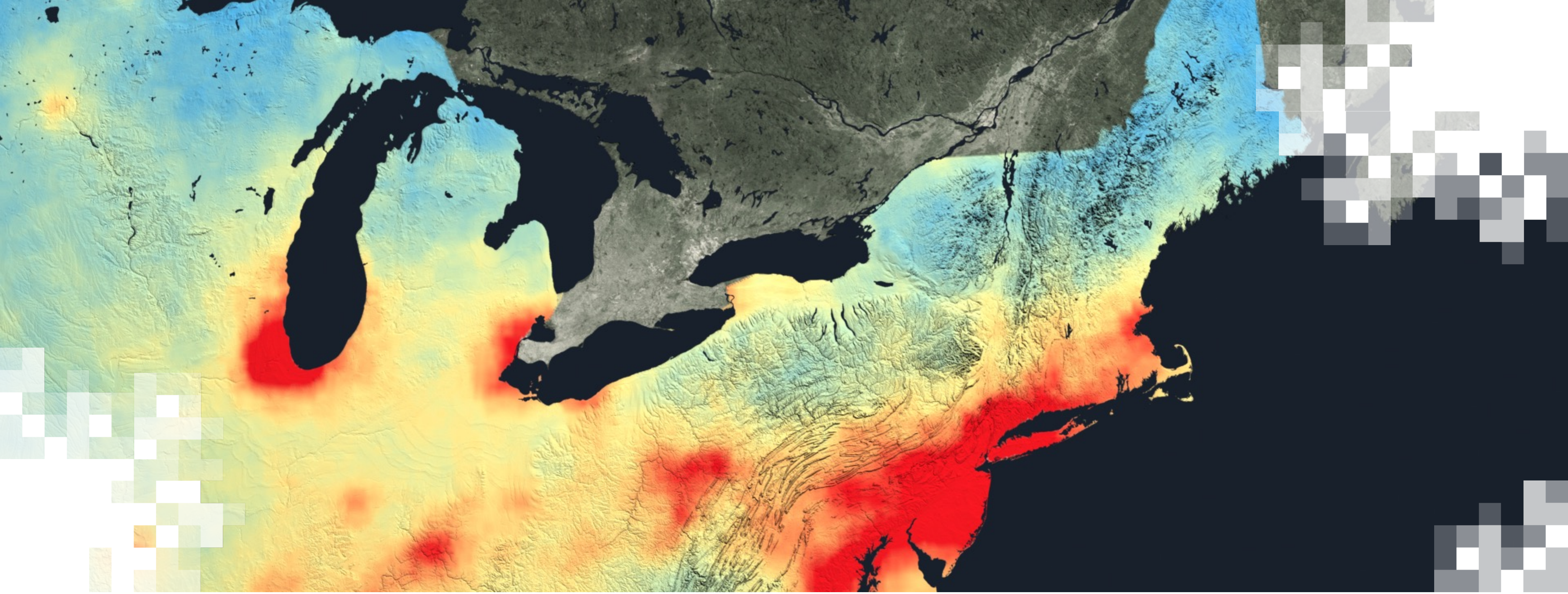
Suomi NPP VIIRS Lights at Night

Courtesy of: Bryan Duncan

Temporal Variations

NASA's Air Quality website shows trends for individual cities and power plants: https://airquality.gsfc.nasa.gov/no2.





Case Study: Emission Changes during COVID-19

What determines the amount of NO_2 at ground level?

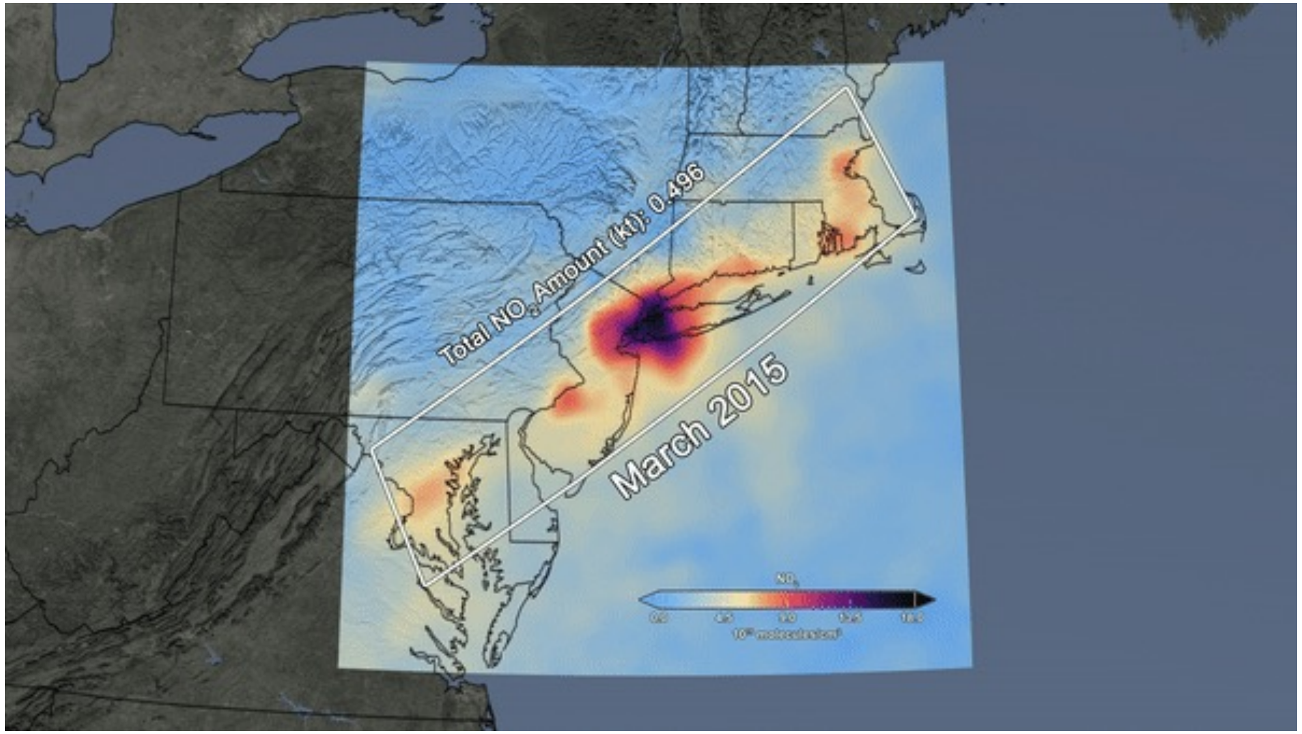
Emissions

+

Chemistry

+

Weather



What determines the amount of NO_2 at ground level?

Emissions

Emissions can vary depending on fuel type and conditions and have both natural and man-made sources.

- Gasoline, Diesel (Vehicles)
- Coal and Natural Gas (Electrical Generation)
- Lightning and Fires

What can change emissions?

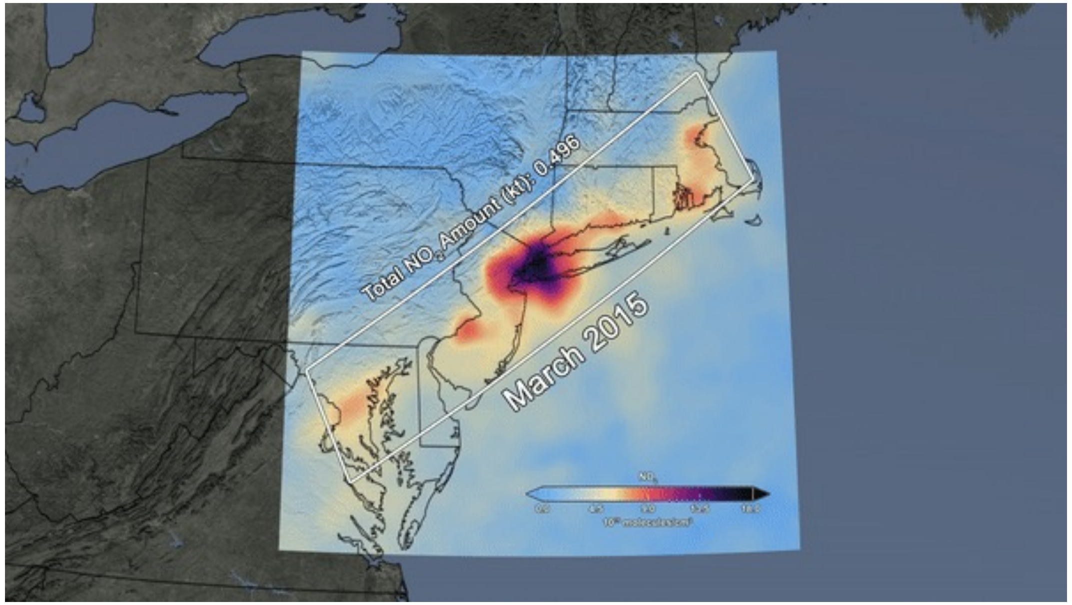
- Increased Use of Renewable Energy
- Air Quality or Climate-Change Policy or Regulation
- Unexpected Changes
  - Economic Recession
  - Natural Disasters
  - Lockdown due to COVID-19
  - Sudden Policy Interventions (e.g., Beijing Olympics)

What determines the amount of NO_2 at ground level?

Chemistry

There are always emissions of NO_2 and other pollutants into the atmosphere, but after they are emitted, they undergo chemical reactions that determine their lifetimes (how long they stay in the atmosphere). The speed of these chemical reactions can change depending on factors such as the temperature and amount of sunlight.

One way we account for seasonal changes in temperature is by looking at the same period over different years.



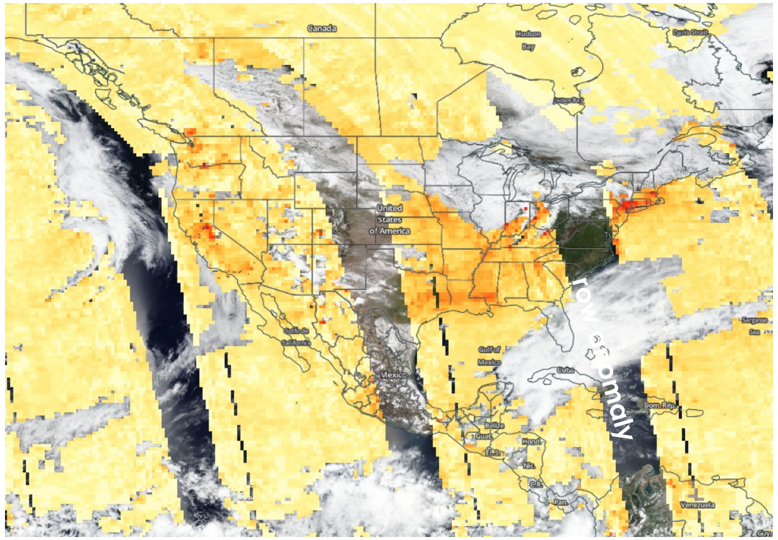
What determines the amount of NO_2 at ground level?

Weather

Weather varies from year to year and can impact the amount of NO_2 at the surface.

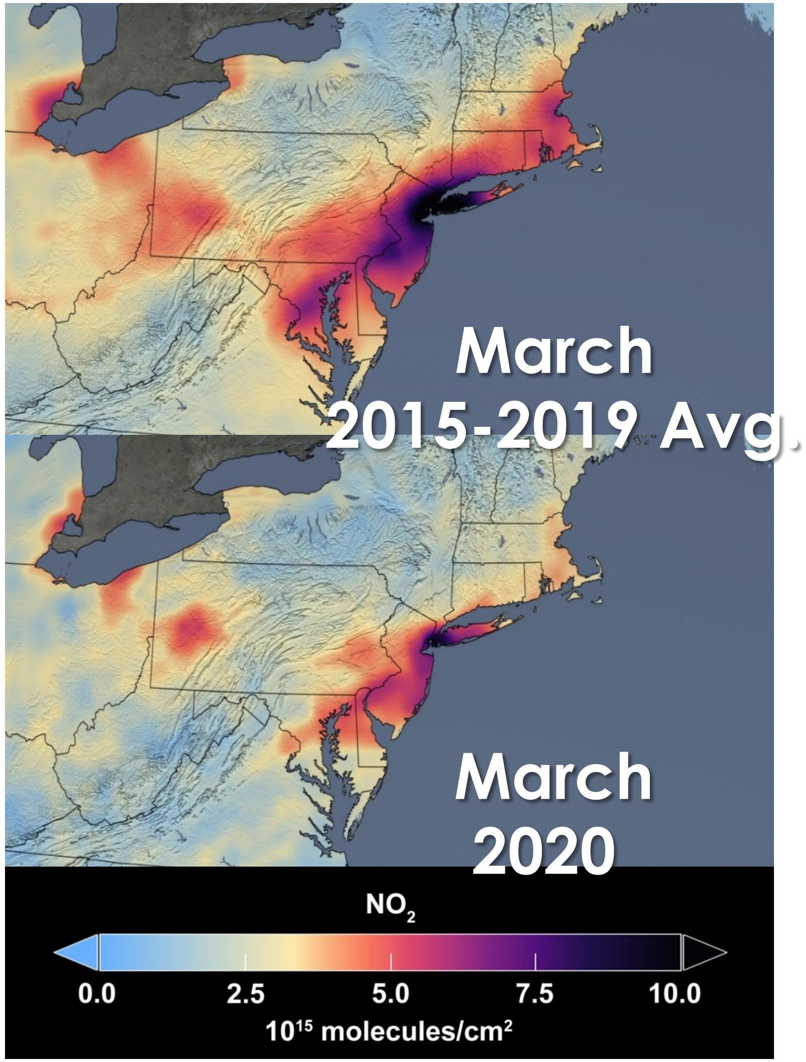
- ***Wind:*** Winds can disperse emissions, changing NO_2 levels depending on wind direction and speed
- ***Temperature, Clouds:*** Higher temperatures and/or more sunlight can speed up NO_2 chemistry in the air.
    - Clouds can also interfere with an instrument's ability to "see" all the way to the surface.
- ***Rain:*** Rain can wash away pollutants, cleaning the air and lowering pollutant levels.

OMI Tropospheric Column NO_2
May 10, 2020



(+ VIIRS true color imagery)

So, what can we see from this image?



So, what can we see from this image?

What quantity are we looking at?

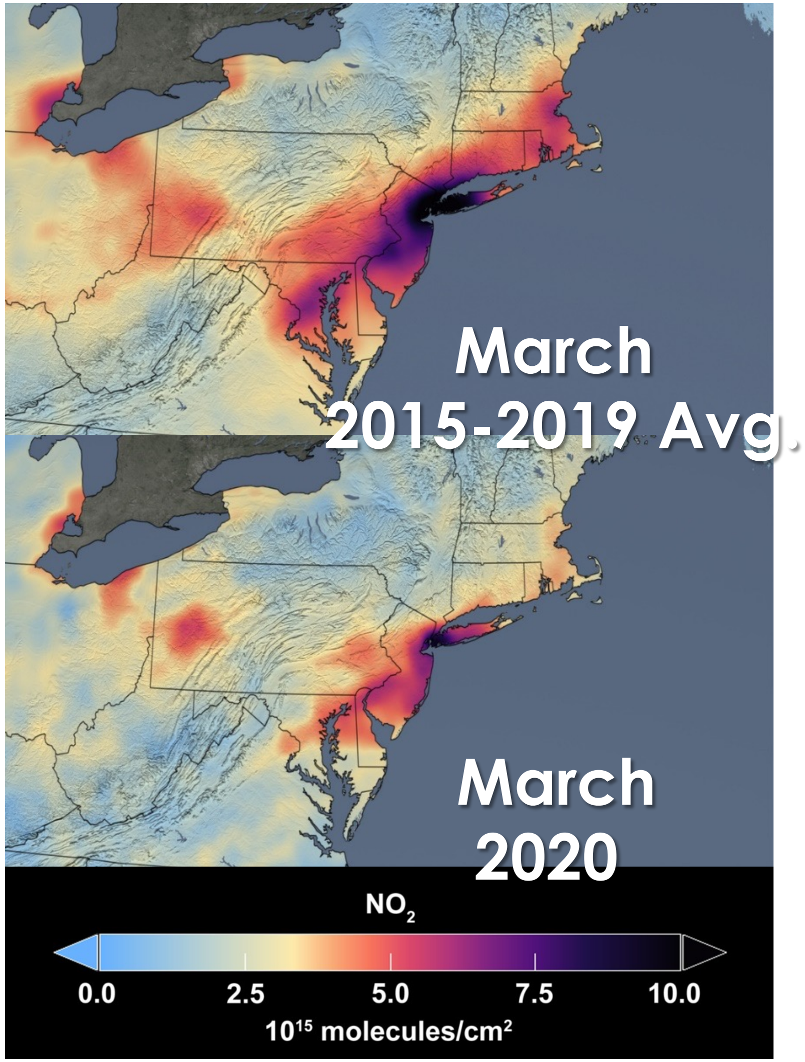
Tropospheric Column NO_2

Is this image for one day?

No, these images show averages of daily data over a month.

Is this data gridded? Or at the native resolution of the satellite?

This image was made using gridded data. This data is produced by NASA and involves carefully averaging and filtering the native resolution data from the satellite.



So, what can we see from this image?

Is this a map of NO_2 at the surface, where people breathe?

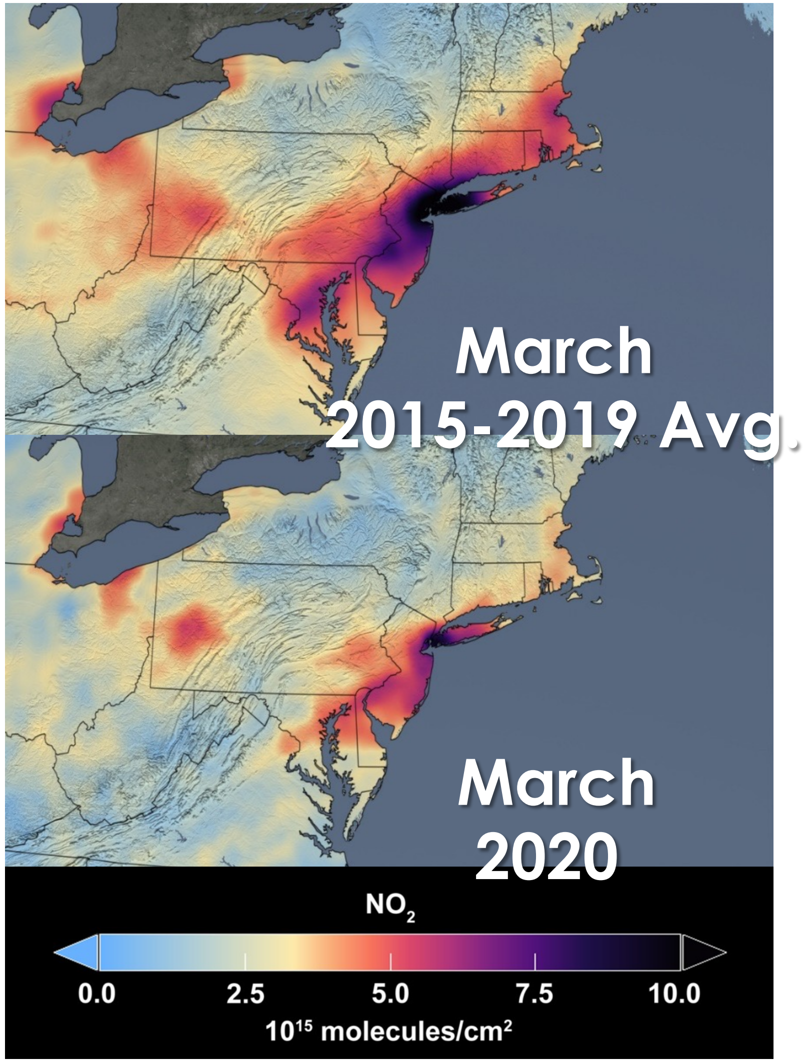
No, this is a map of tropospheric column NO_2, which is the total amount of NO_2 from the surface to the top of the troposphere.

Can changes in the tropospheric column tell me information about changes at the surface?

Yes, sources of NO_2 are primarily at the surface, and its lifetime is short, leading to high values near sources.

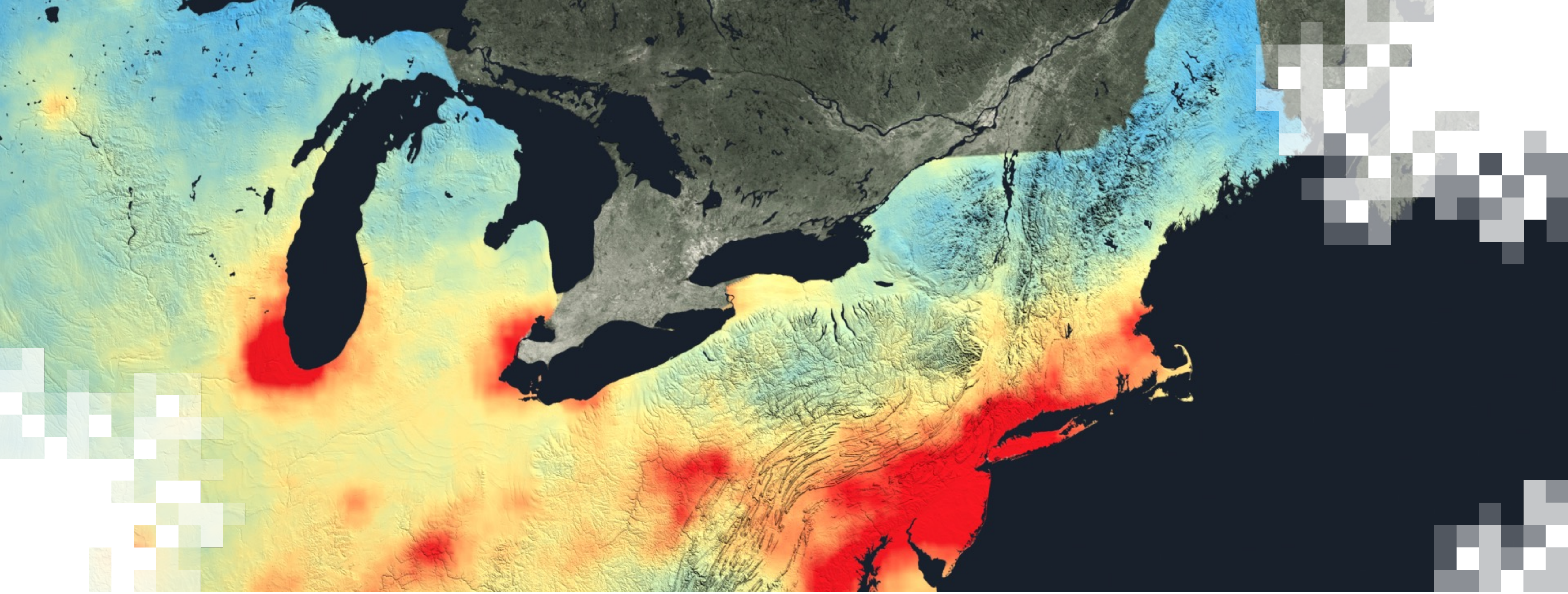
Are all the changes between the top and bottom image due to the lockdown in response to COVID-19?

No, the amount of NO_2 depends on:
emissions + chemistry + weather
Calculating the change in NO_2 from the lockdown requires careful and rigorous scientific analysis.



Questions & Discussion Prompts

- Name one way satellite observations can supplement an emissions inventory.
- What are some advantages of using satellite data to estimate surface concentrations?
- What are some uncertainties in estimating emissions or surface concentrations from satellite data?



Questions?