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Implementing satellite NO_2 data assimilation in CMAQ for identifying emissions biases and improving regional boundary conditions

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Progress for a Stronger Future

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Motivating Satellite NO_2 Data Assimilation

- How can we use fused CMAQ + satellite NO_2 estimates to QA or improve emissions?
  - Improved boundary conditions for regional air quality simulations
  - Constraints on international emissions
  - Fast first-pass estimates of NO_x emissions in response to unexpected emissions changes
  - NO_x emissions from some sources with uncertainty, such as soil NO_x

Today's results summarize:

- OMI NO_2 retrievals (Ω)
- CMAQ *a priori* VCD performance (Ω_{CMAQ})
- CMAQ VCD Sensitivity (β)
- Assimilation increment ($\Delta\Omega$)
- Emissions inference (ΔE)

Chemical data assimilation in CMAQ

- HAQAST implemented OMI NO_2 satellite assimilation.
  - Assimilation has been used in meteorology for a long time.
  - HAQAST applied the same tools updated to satellite NO_2 measurements.
- Gridpoint Statistical Interpolation (GSI) assimilation in CMAQ
  - Accounts for background error covariance.
  - Accounts for sensitivity of satellite at different altitudes.
  - Fused to estimate “updated” CMAQ field each timestep.
  - Updated simulation better agrees with satellite.

Ω = NO_2 *vertical column density (VCD)*

Updating emissions with CMAQ-GSI

1. CMAQ simulates the VCD (Ω_{CMAQ})
   - From standard inputs/outputs
   - Integrated within troposphere
2. Calculate the sensitivity (β)
   - via brute-force or DDM or adjoint
   - Monthly resolution
3. Assimilate satellite NO_2 ($\Delta\Omega$)
   - Account for satellite sensitivity and error covariance
   - Estimate increment to match satellite
4. Estimate ΔE using β from step 2 and $\Delta\Omega$ from step 3 and Ω from step 1

1. $$\Omega_{CMAQ} = M_{w,air}^{-1} \sum_z \rho_z \chi_z h_z$$

2. $$\beta = \frac{\partial e\%}{\partial \omega\%} \approx \frac{\Delta E}{E} \frac{\Omega_{CMAQ}}{\Delta\Omega_{CMAQ,dE}}$$

3. $$\Delta\Omega = \left(\Omega_{GSI} - \Omega_{CMAQ}\right)$$

4. $$\frac{\Delta E}{E} = \beta \frac{\Delta\Omega}{\Omega_{CMAQ}}$$

[Lamsal et al. 2011, GRL]

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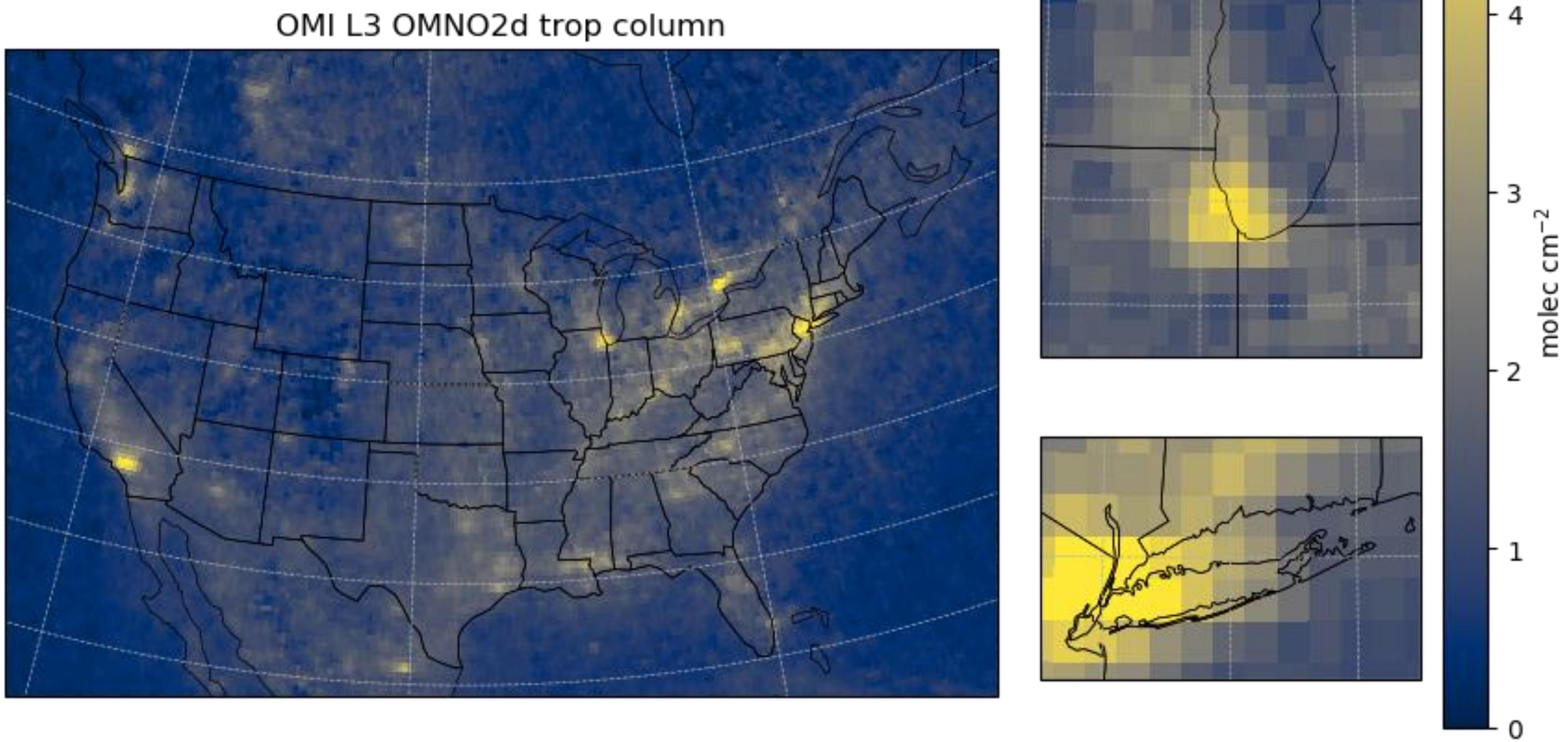
Proof of concept

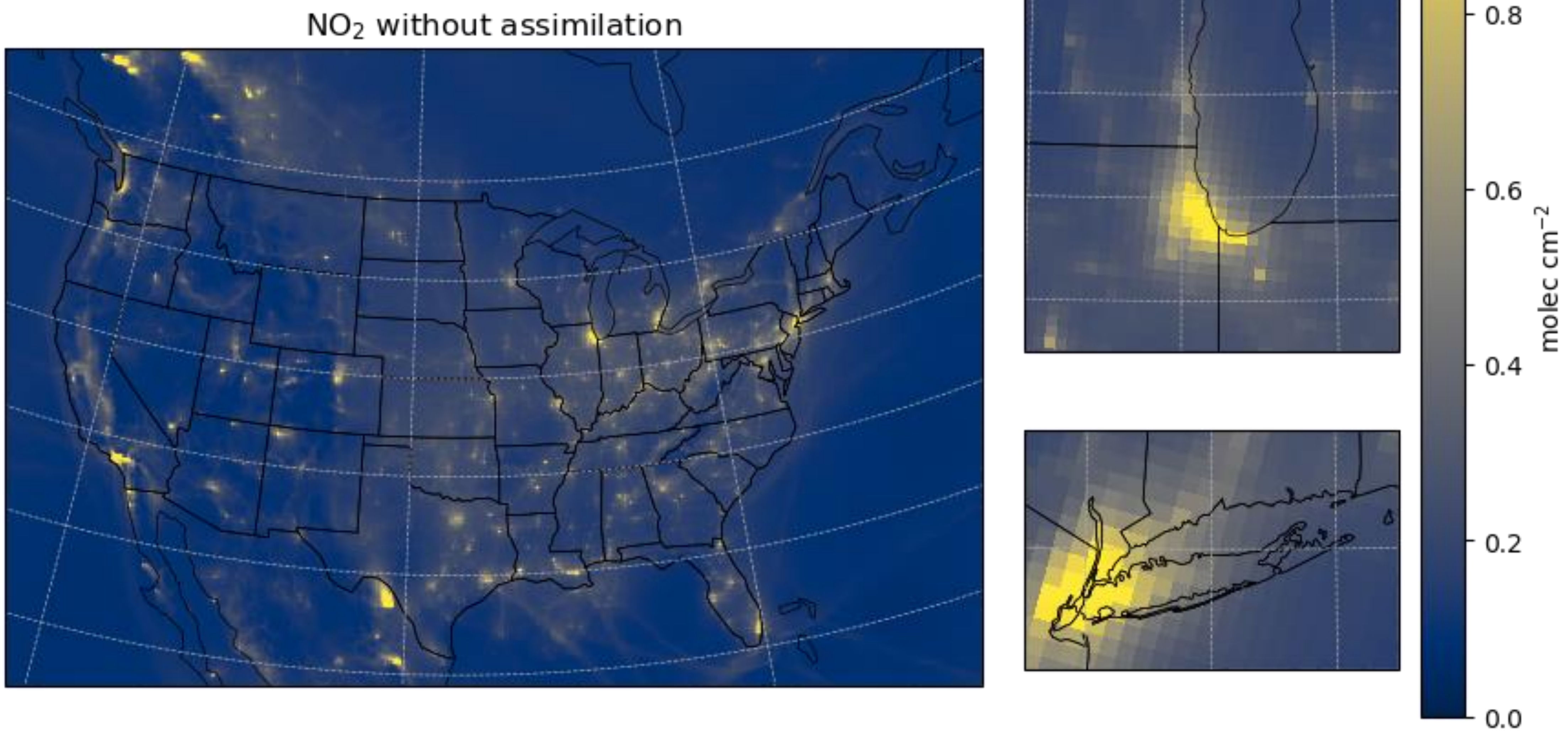
- Domain: CONUS
- Simulation: 9-31 July 2014
- Results show *successful implementation* of assimilation system
- Iterative emissions update
  - First, we update lightning emissions because OMI is sensitive to lightning NO.
  - Second, we update surface anthropogenic emissions.

OMI NO_2 VCD (Ω)

OMI observations here are screened for cloud fraction <30%

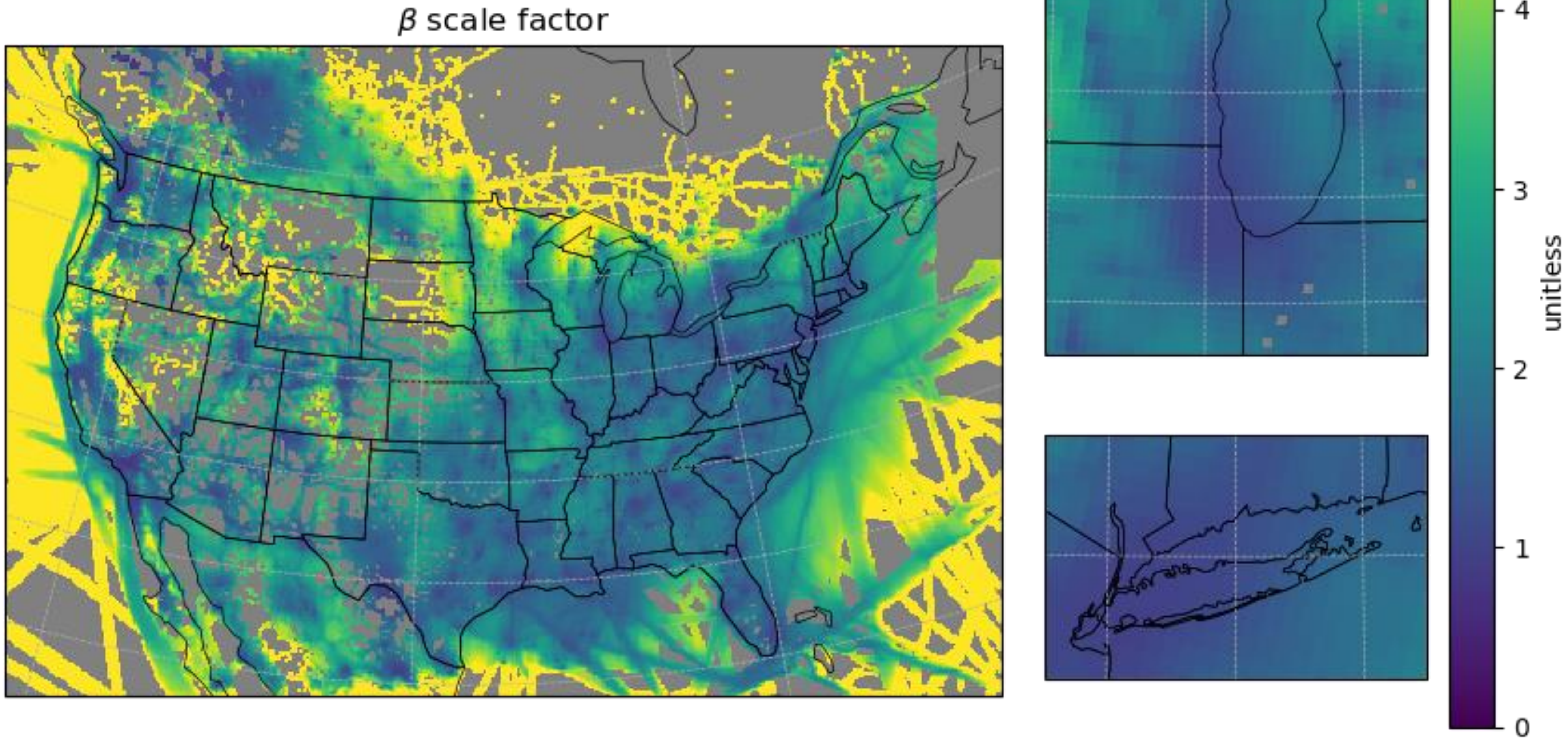


CMAQ NO_2 VCD (Ω_{CMAQ})



Sensitivity of NO_2 column to NO_x emissions (β)

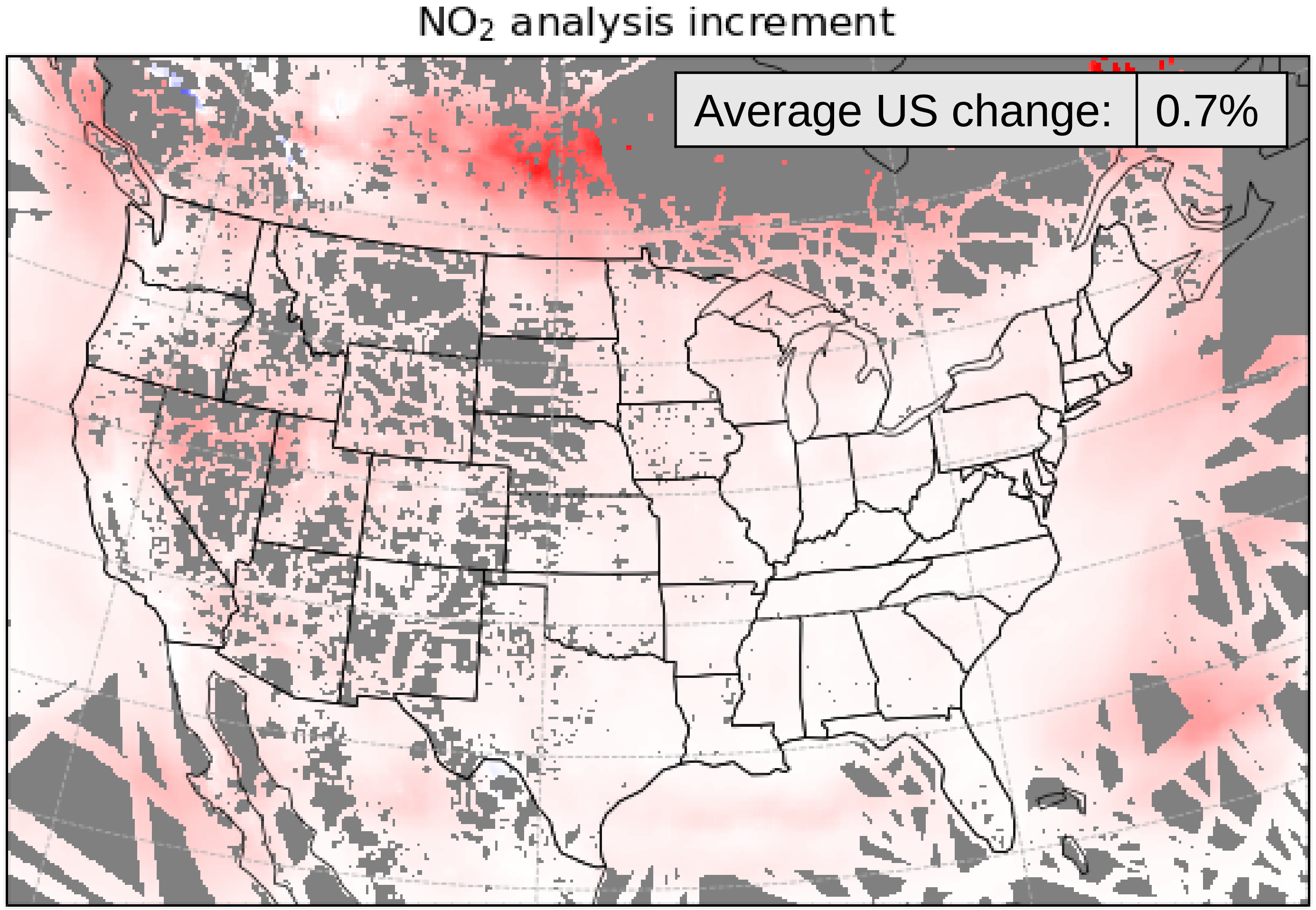
$$\beta = \frac{\partial e\%}{\partial \omega\%} \approx \frac{\Delta E}{E} \frac{\Omega_{CMAQ}}{\Delta\Omega_{CMAQ,dE}}$$

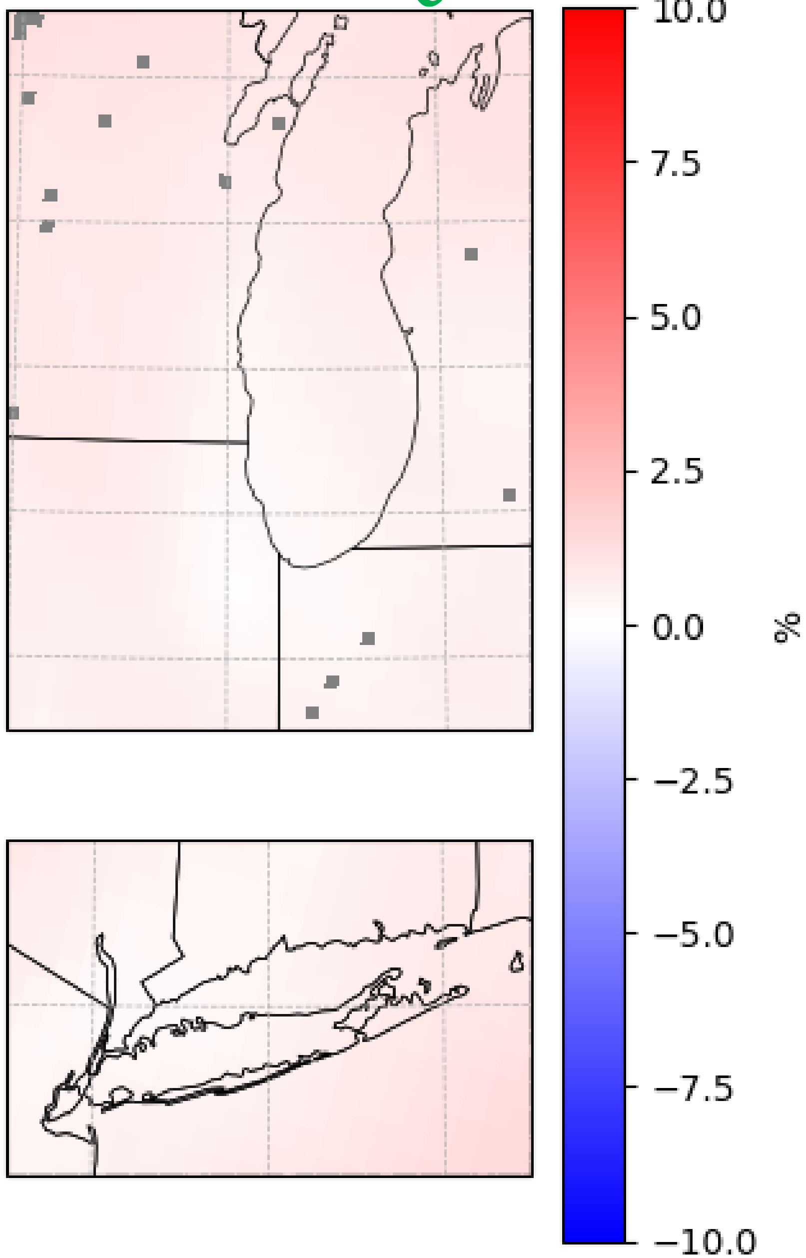


NO_2 change due to assimilation ($\Delta\Omega / \Omega_{CMAQ}$)

$$\frac{\Delta\Omega}{\Omega_{CMAQ}} = \frac{(\Omega_{GSI} - \Omega_{CMAQ})}{\Omega_{CMAQ}}$$

← Difference between assimilated and standard CMAQ





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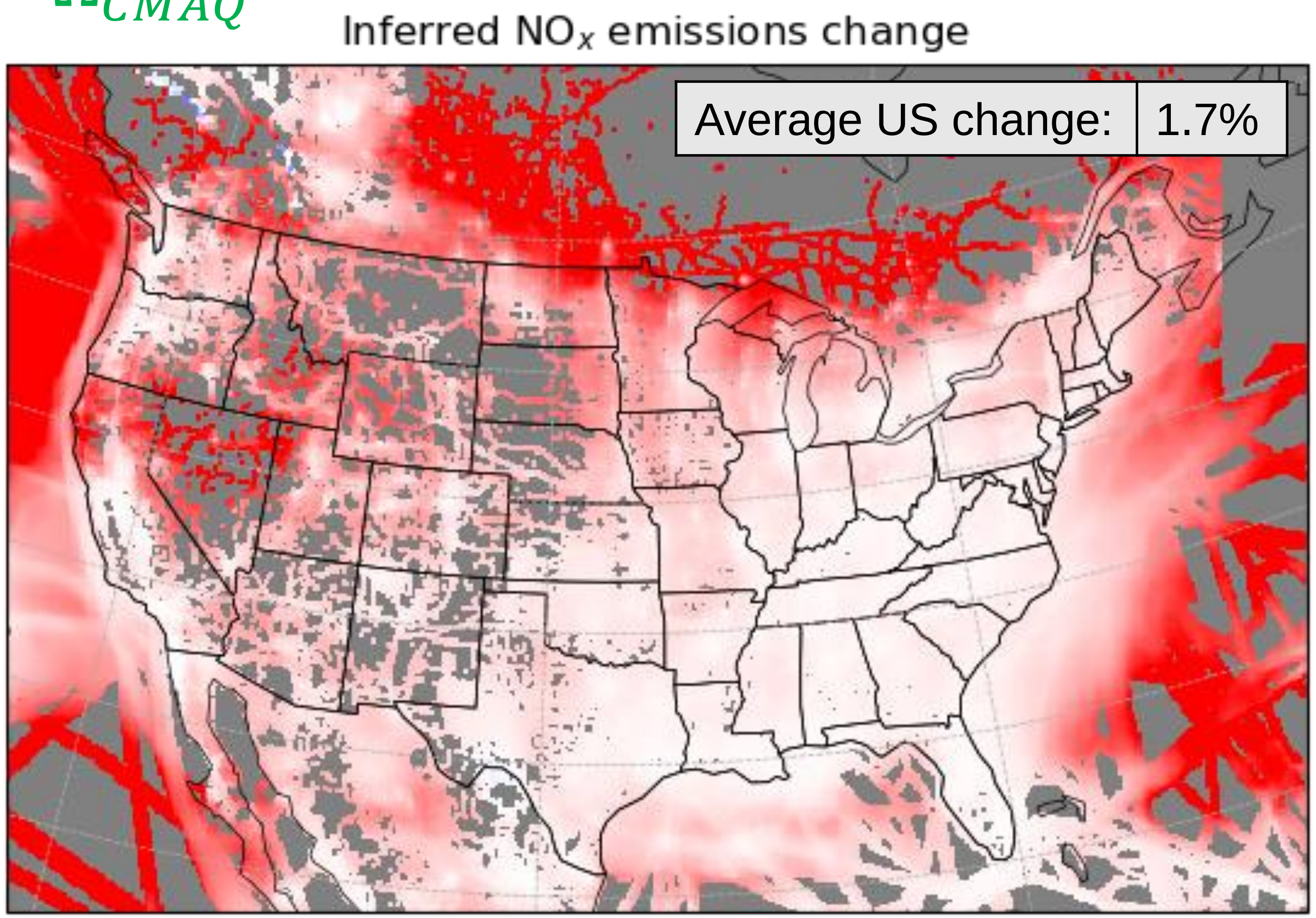
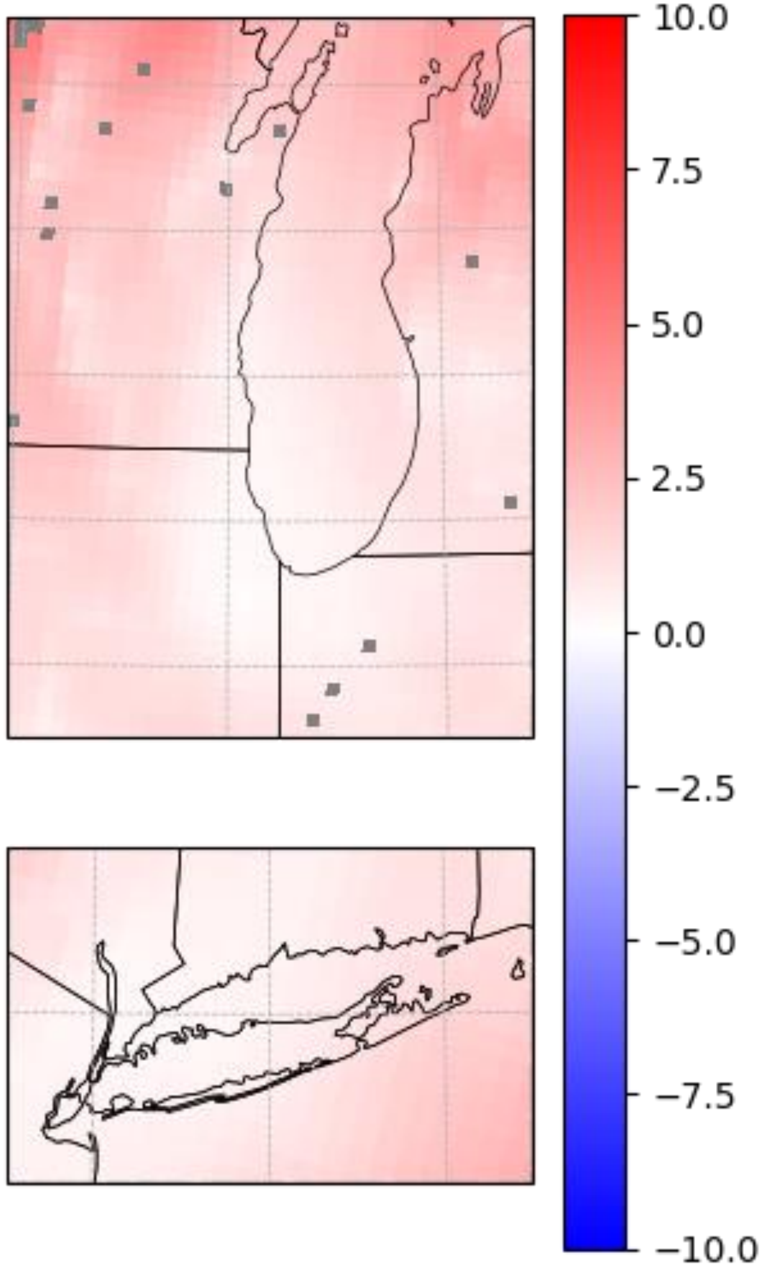
Inferred emissions change $\left(\frac{\Delta E}{E}\right)$

$$\frac{\Delta E}{E} = \beta \frac{\Delta \Omega}{\Omega_{CMAQ}}$$

satellite derived emissions update



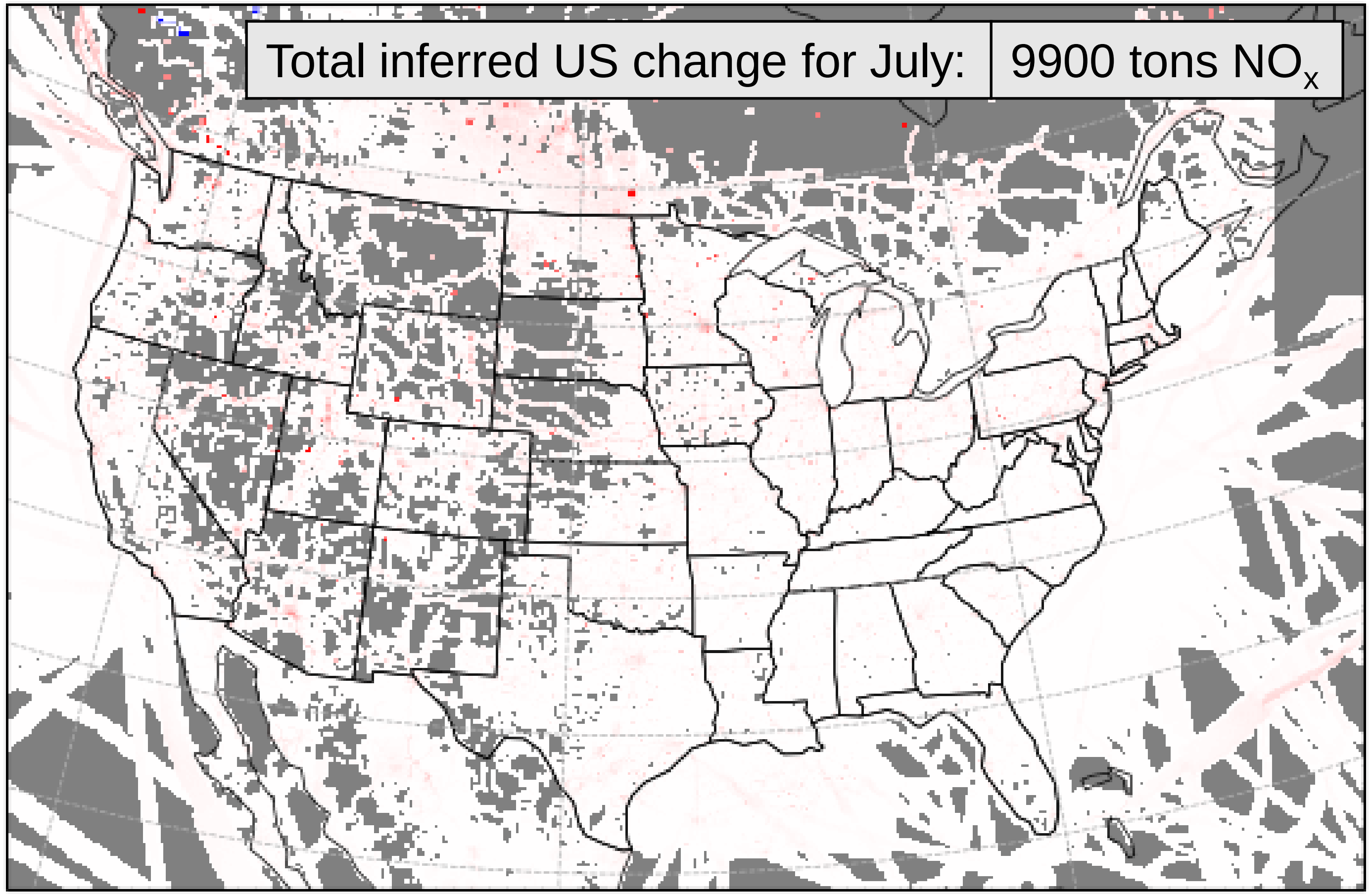


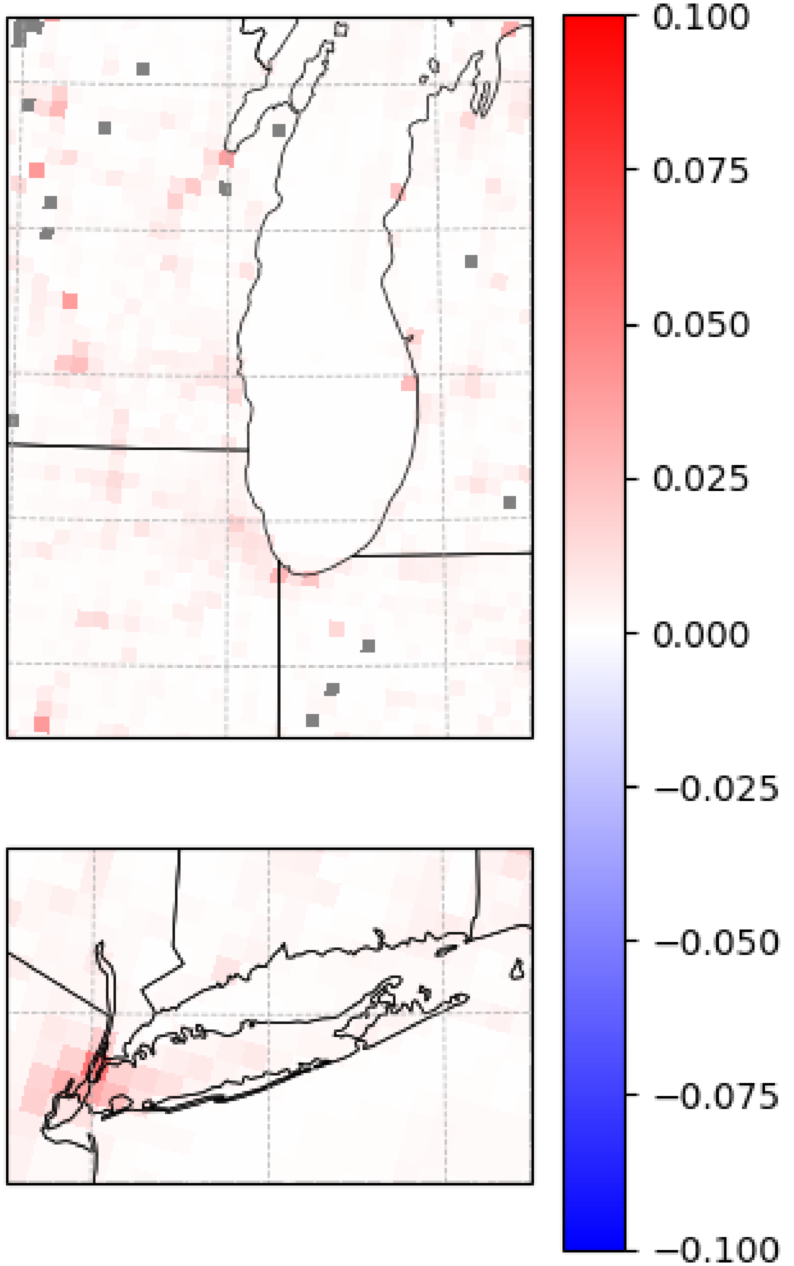
Inferred emissions change(ΔE)

$$\frac{\Delta E}{E} = \beta \frac{\Delta \Omega}{\Omega_{CMAQ}}$$

satellite derived emissions update

Inferred absolute NO_x emissions change





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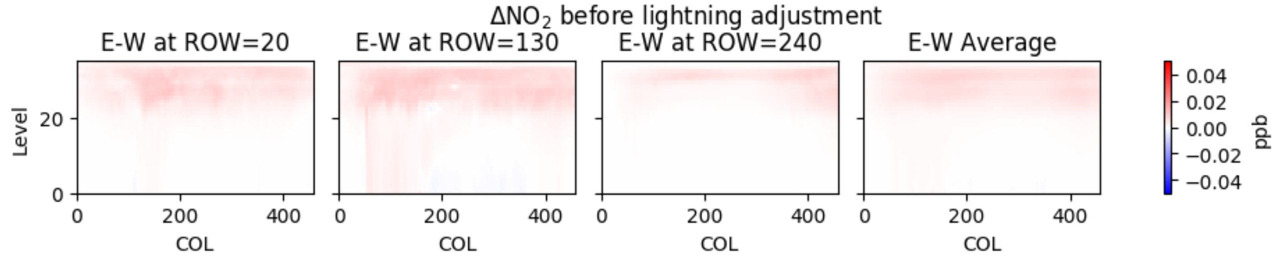
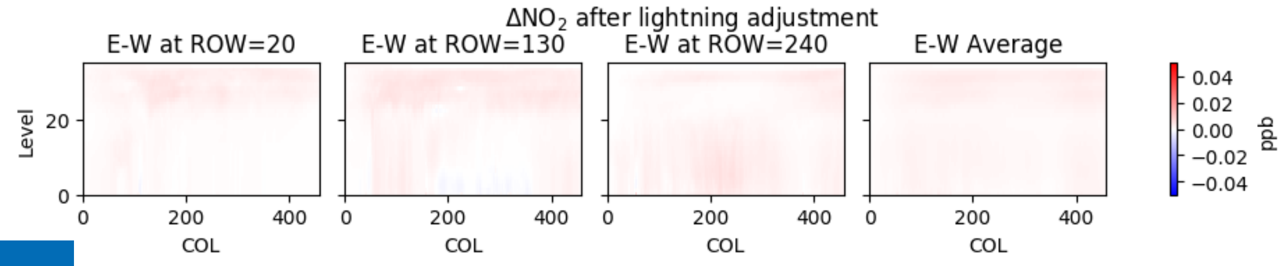
Actually a two-stage process

Stage 1: Lightning updates

- OMI assimilated with a background error covariance sensitive to *lightning* NO_X
- Calculate ΔE as a scaling factor for lightning NO emissions (7.5%)

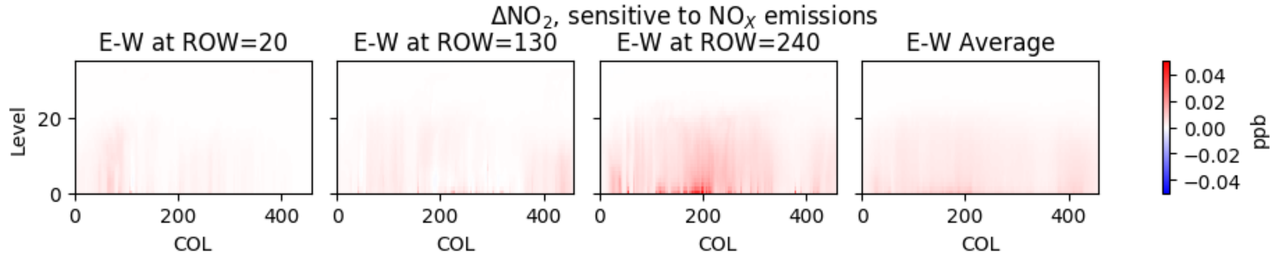


Applying 7.5% lightning scaling factor improves model agreement with OMI in upper troposphere



Stage 2: Anthropogenic Updates

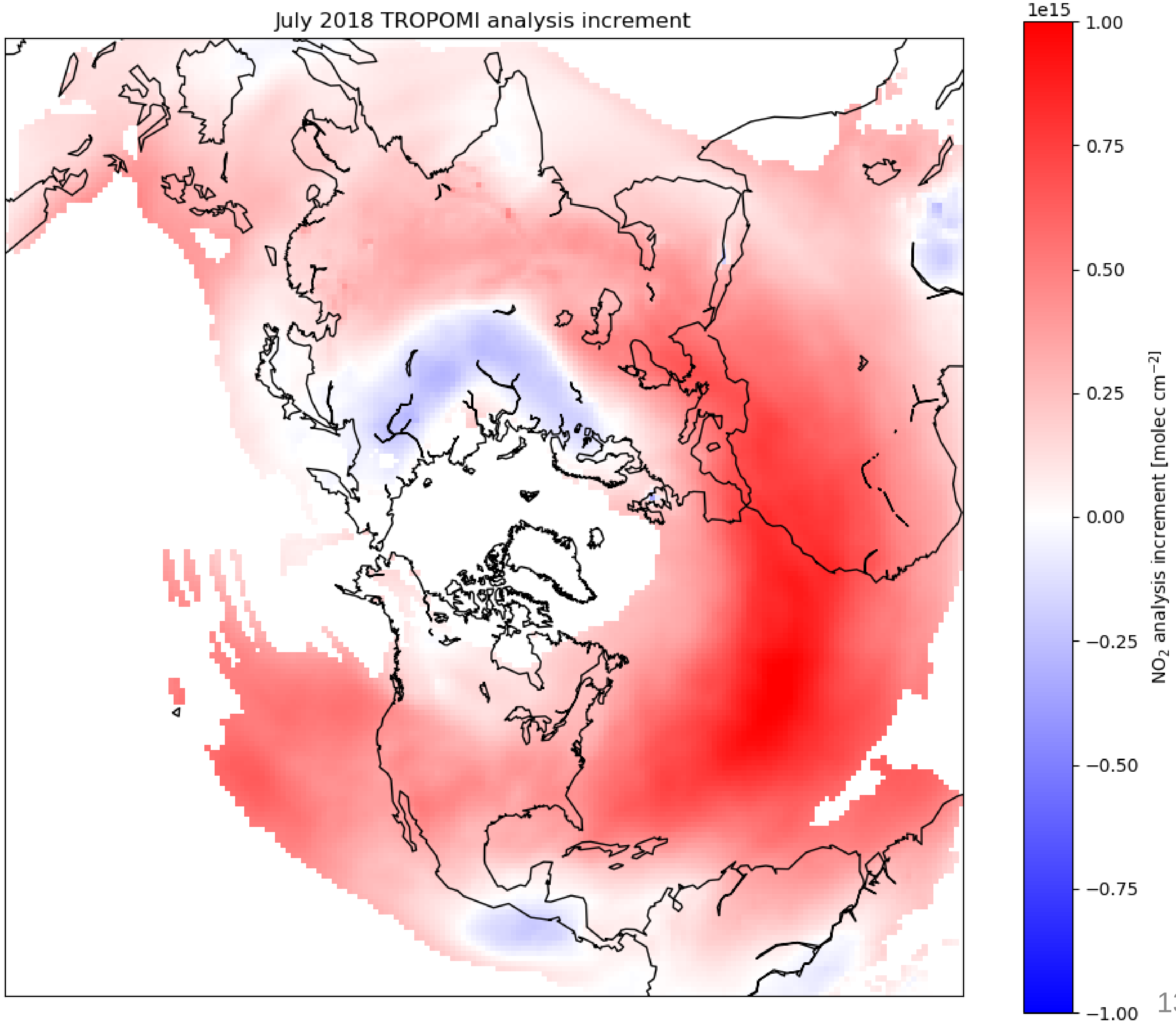
- OMI assimilated with a background error covariance sensitive to *anthropogenic emissions*
- Lightning scaling factor is applied



Preliminary hemispheric TROPOMI results

- Assimilation with TROPOMI NO_2
- Higher resolution, available beginning 2018
- July 2018 with "representative day emissions"
- NO_2 analysis increment

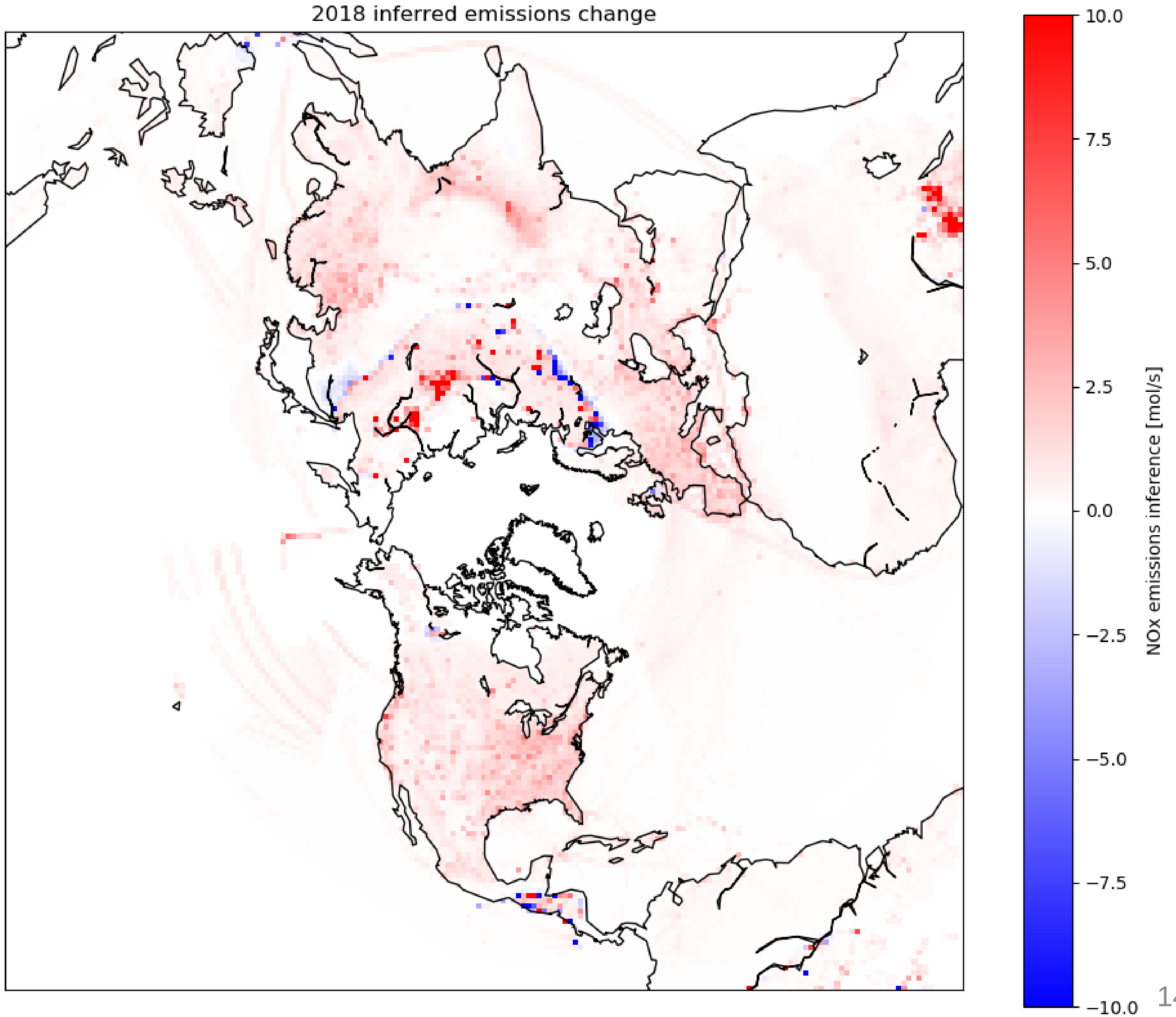
Preliminary – please do not cite or share



Preliminary hemispheric TROPOMI results

- NO_x emissions inference
- Positive emissions inference across the domain
- Many uncertainties remain
- Next step towards identifying emissions biases

Preliminary – please do not cite or share



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Summary

- We implemented a test scenario over CONUS for July 2014 to prepare for an operational system on a hemispheric domain
  - Initial results suggests small NO_x emissions underestimation

This simulation lays the groundwork for an operational system:

- Further refinement of the beta sensitivity parameter will increase precision of emissions estimates
- Can be applied to international emissions to derive improved boundary conditions for US simulations
- Can be quickly applied in situations such as COVID-19 driven emissions changes

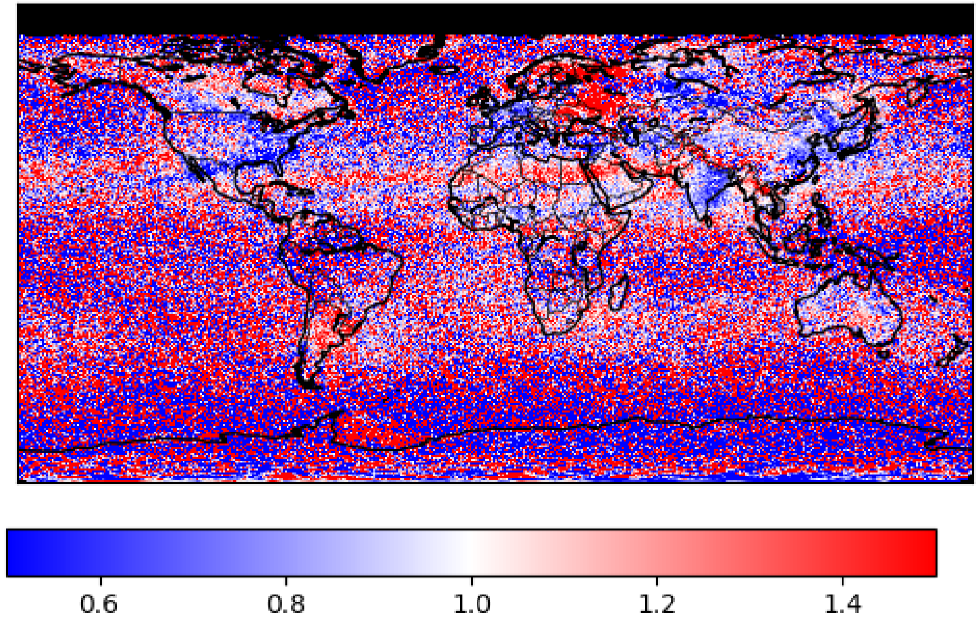
Preliminary results and next steps:

- TROPOMI NO_2 retrievals: higher resolution, available starting 2018
- Hemispheric scale simulations

Future work: COVID-19 emissions changes

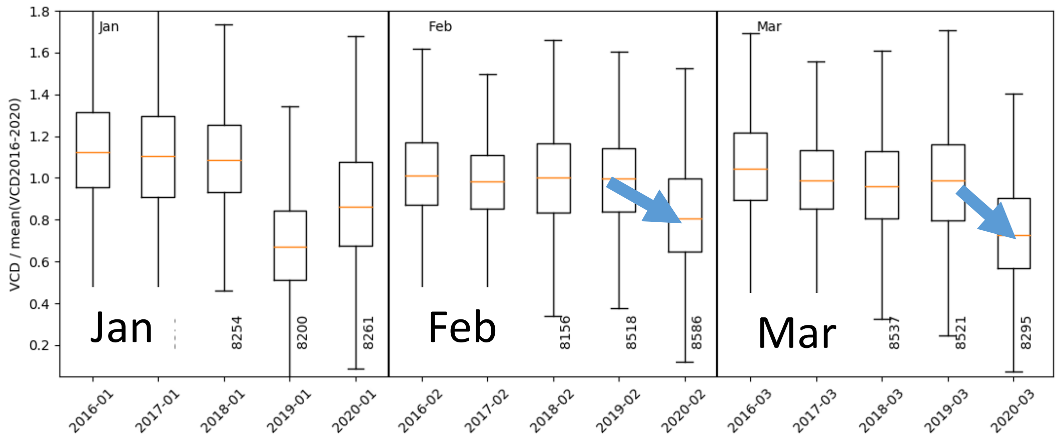
- Satellite data show significant NO_2 decreases in March 2020 compared to previous years
- An operational system would have the capability to provide immediate NO_x emission estimates for these changes

2020-03 / (2016-2019)-03

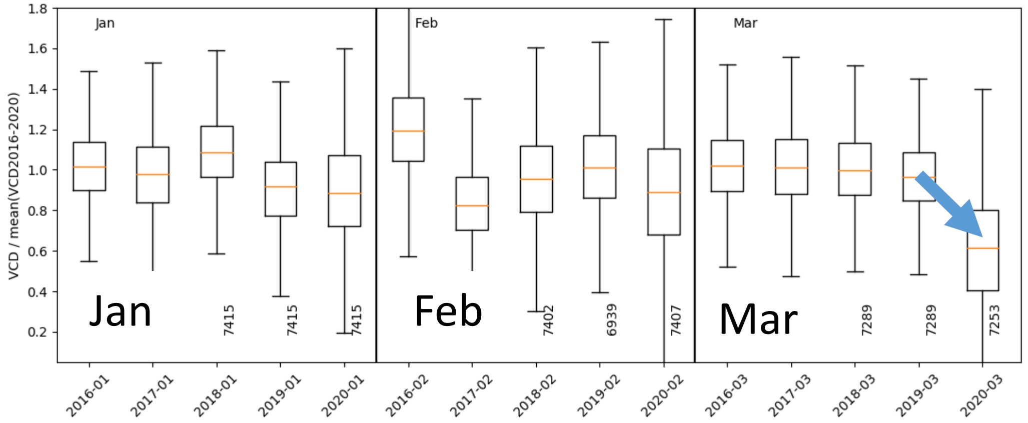


VCD2020:VCD2016-2019

Region: Ohio Valley



Region: Southeast



Thank you!

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