Enhanced representation of inter-continental pollutant transport by assimilating satellite NO_2 and performing NO_x emissions inversions

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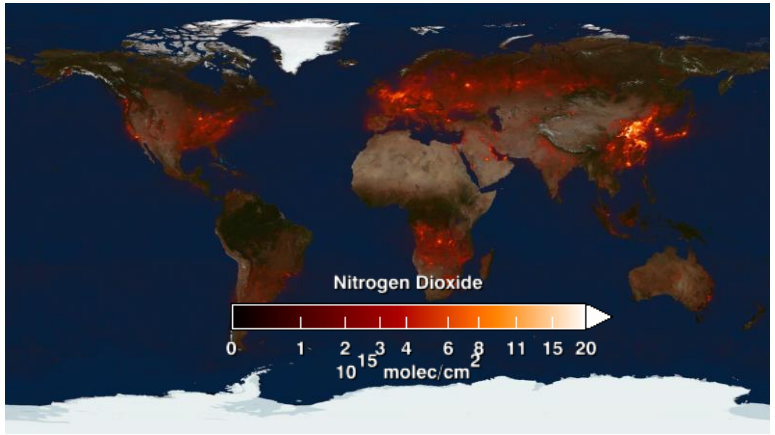
Why estimate emissions by assimilating satellite data?

- Short lifetime of NO_2 along with rich dataset of NO_2 observed from space provides opportunities to estimate NO_x emissions using NO_2 satellite data alongside chemical transport models
- Approaches
  - Finite-difference mass-balance method in Lamsal et al. 2011: Quickly update NO_x emissions with satellite NO_2
  - Recent approaches use 4DVAR/adjoint, but this is less accessible
- Secondary products of NO_x emitted elsewhere can impact US air quality
  - Accurate global emissions inventories are critical for representing this impact, but are challenging to develop and update
  - Satellites, providing data in real time, offer an opportunity to bridge this data gap



Video: Nitrogen Dioxide from Aura/OMI 2013-2014, NASA/Goddard Space Flight Center

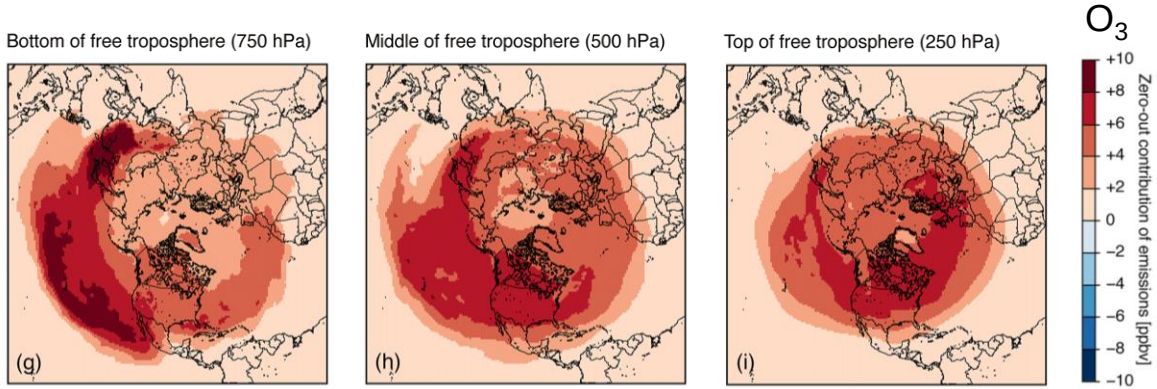


Figure: **Itahashi et al. 2020, ACP.** (Figure 6), Modeling stratospheric intrusion and trans-Pacific transport on tropospheric ozone using hemispheric CMAQ during April 2010 – Part 2: Examination of emission impacts based on the higher-order decoupled direct method

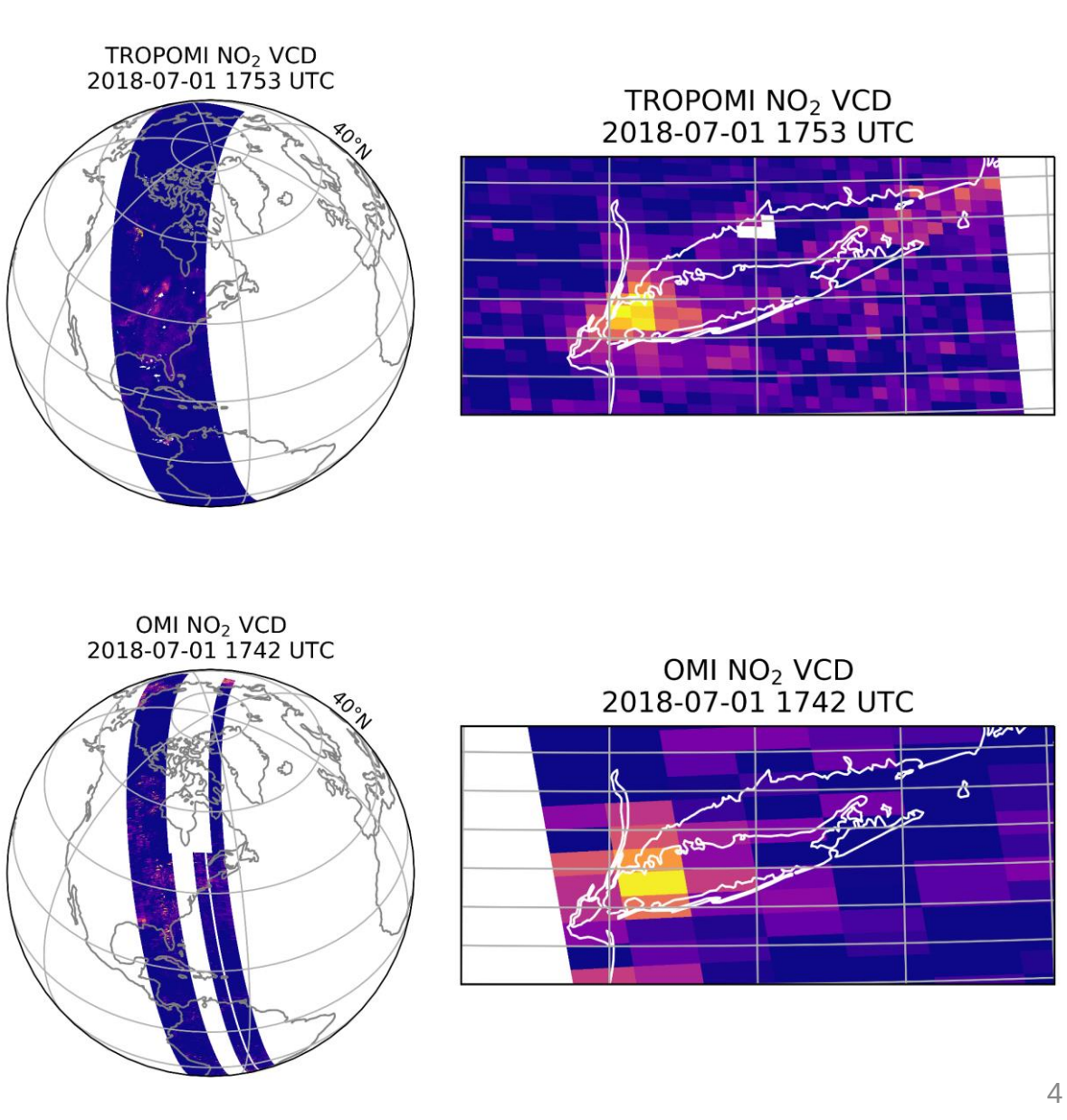
Data assimilation in CMAQ

- Satellite assimilation in CMAQ provides capability to:
  - Constrain international emissions
  - Improve boundary conditions for US air quality simulations
  - Fast first-pass estimates of NOx emissions in response to unexpected changes (e.g. COVID-19)
  - Estimate NOx emissions from some sources with uncertainty, such as soil NOx
- This presentation will share results of applying the data assimilation system to:
  - Infer northern hemisphere NO_x emissions for 2019
  - Explore impact on long range O_3
- This project originated as a HAQAST Tiger Team led by Brad Pierce and Daniel Tong

NO_2 Satellite data

- TROPOMI satellite instrument
  - Was launched in 2018 aboard the Sentinel-5P satellite
  - 1:30pm equatorial overpass time
  - Daily global coverage
  - 3.5km x 5.5km data resolution

- OMI satellite instrument
  - Launched 2004 aboard Aura satellite
  - 1:45pm equitorial overpass time
  - Global coverage in 2 days
  - 13km x 24km data resolution
  - Row anomaly since 2007 causes missing data



Inversion system

A Priori Emissions

Global: HTAPv2 or

Regional: EPA platform

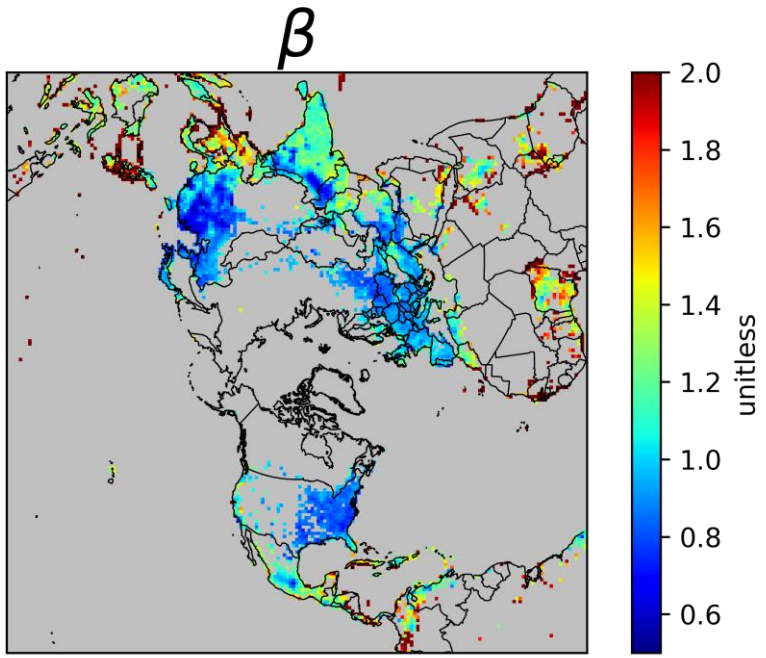
85 %

100 %

Sensitivity

$$\beta = \frac{\Delta E}{E} \frac{\Omega_{V,Q}}{\Omega_{V,Q85} - \Omega_{V,Q}}$$

Monthly



Legend

Vertical Column: Ω_v

Slant Column: Ω_s

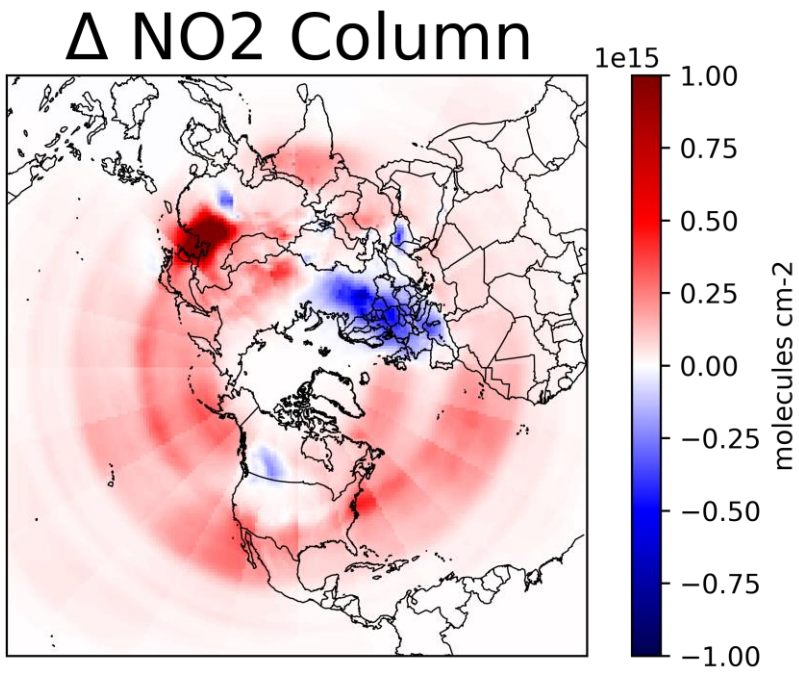
*Only grid cells with substantial anthropogenic emissions are adjusted

Inversion system

A Priori Emissions

Global: HTAPv2 or

Regional: EPA platform



RAW CMAQ Prediction

$\Omega_{V,Q}$

Assimilation CMAQ/GSI

CMAQ Prediction = F(E, Met)

$\Omega'_{V,Q} = M^{-1}_{w,air} \sum \rho_z \chi_z h_z$

Hourly

GSI Assimilation

$3DVAR(\Omega'_{V,Q} \times AMF_Q, \Omega_{S,Sat})$

Legend

Vertical Column: Ω_v

Slant Column: Ω_s

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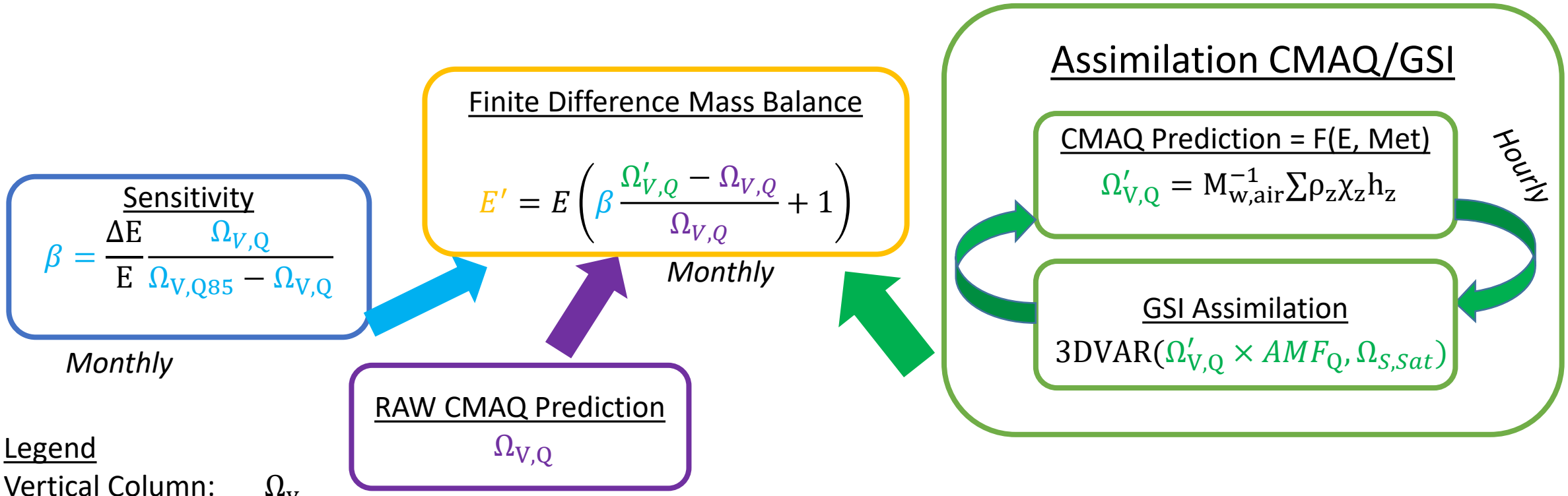
Inversion system



Legend
Vertical Column: Ω_v
Slant Column: Ω_s

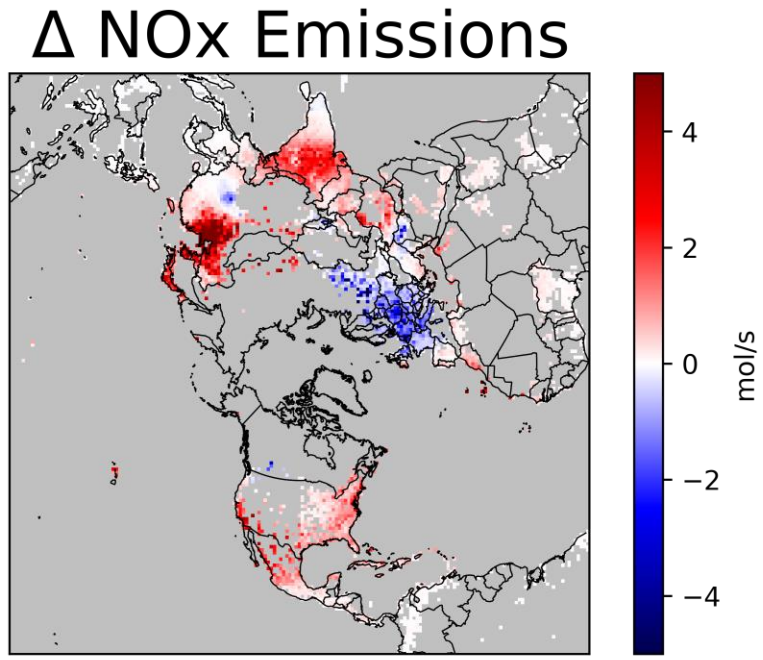
*Only grid cells with substantial anthropogenic emissions are adjusted

Inversion system

Finite Difference Mass Balance

$$E' = E\left(\beta\frac{\Omega'_{V,Q} - \Omega_{V,Q}}{\Omega_{V,Q}} + 1\right)$$

Monthly



Legend

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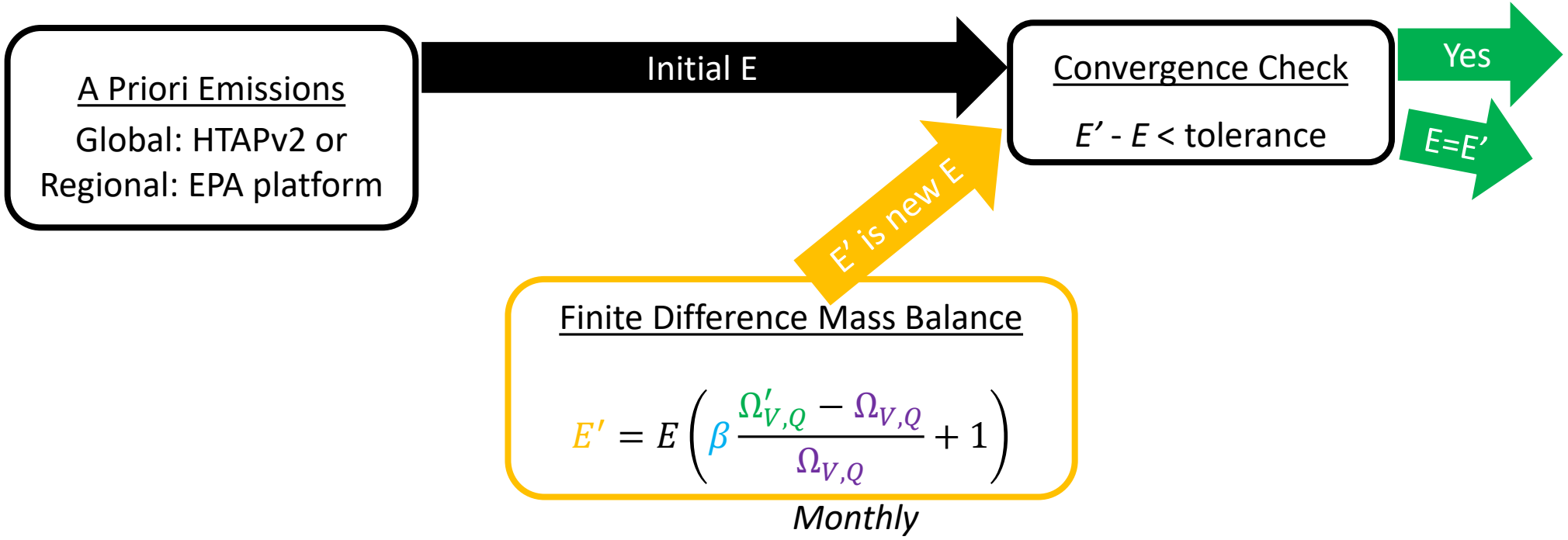
Inversion system



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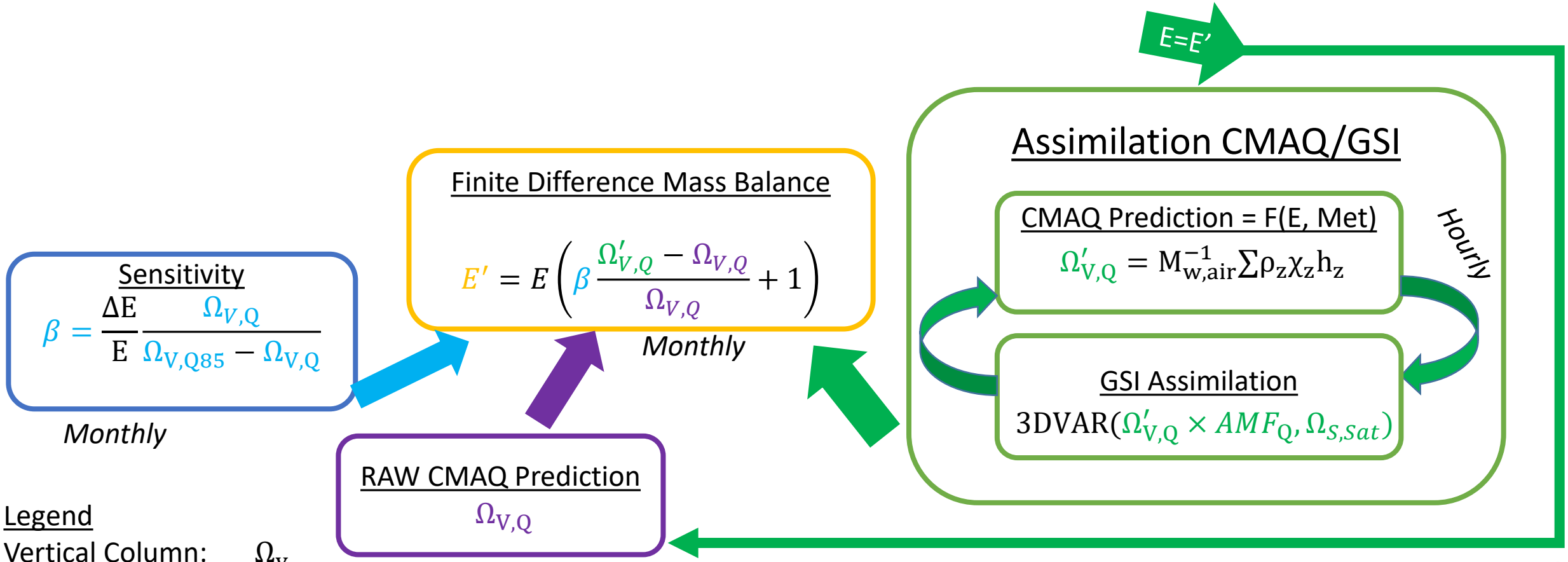
Inversion system



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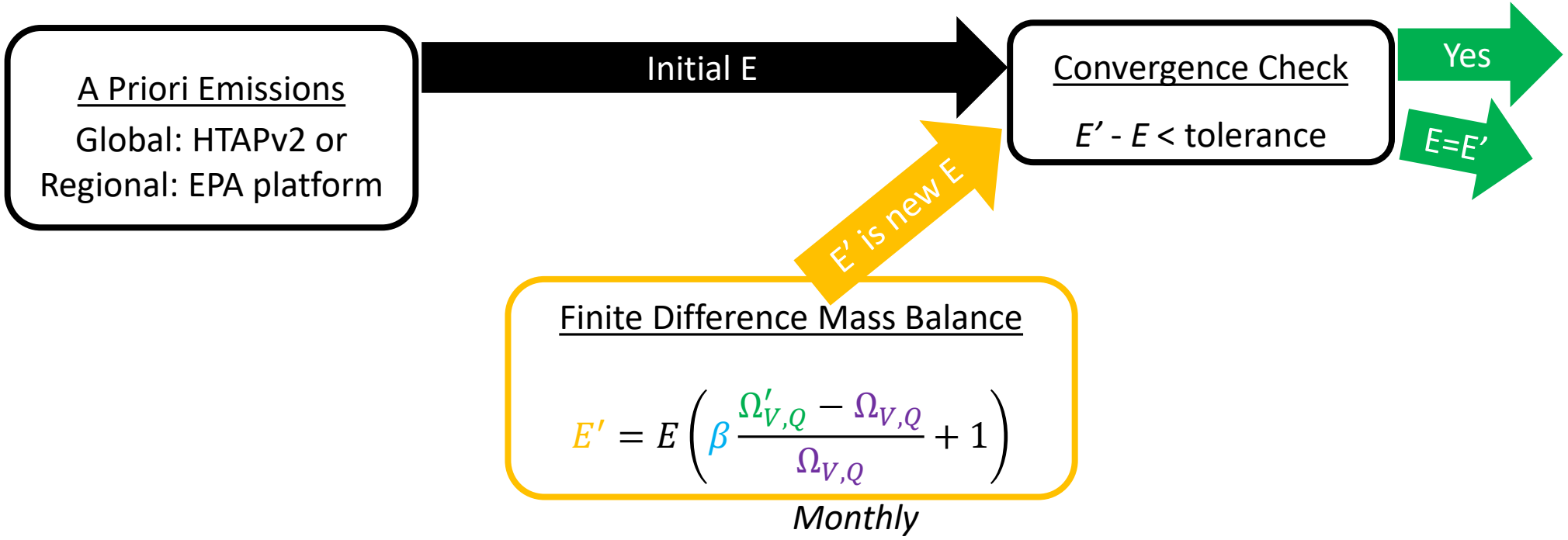
Inversion system



Legend
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Slant Column: Ω_s

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Inversion system

Legend

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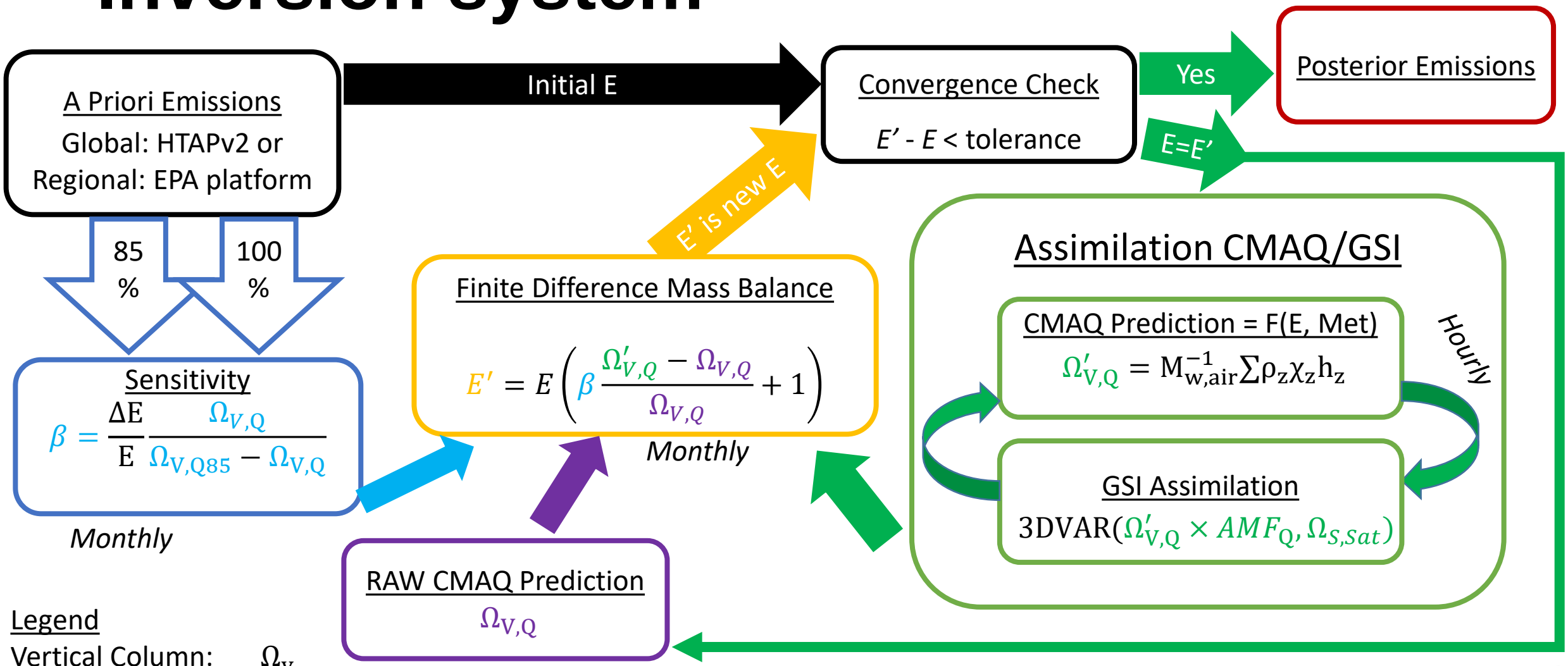


Legend
Vertical Column: Ω_v
Slant Column: Ω_s

*Only grid cells with substantial anthropogenic emissions are adjusted

Study design

Simulations
Base Case with prior emissions*
Assimilation with prior emissions
Posterior emissions run

×

Seasons
January 2019
July 2019

×

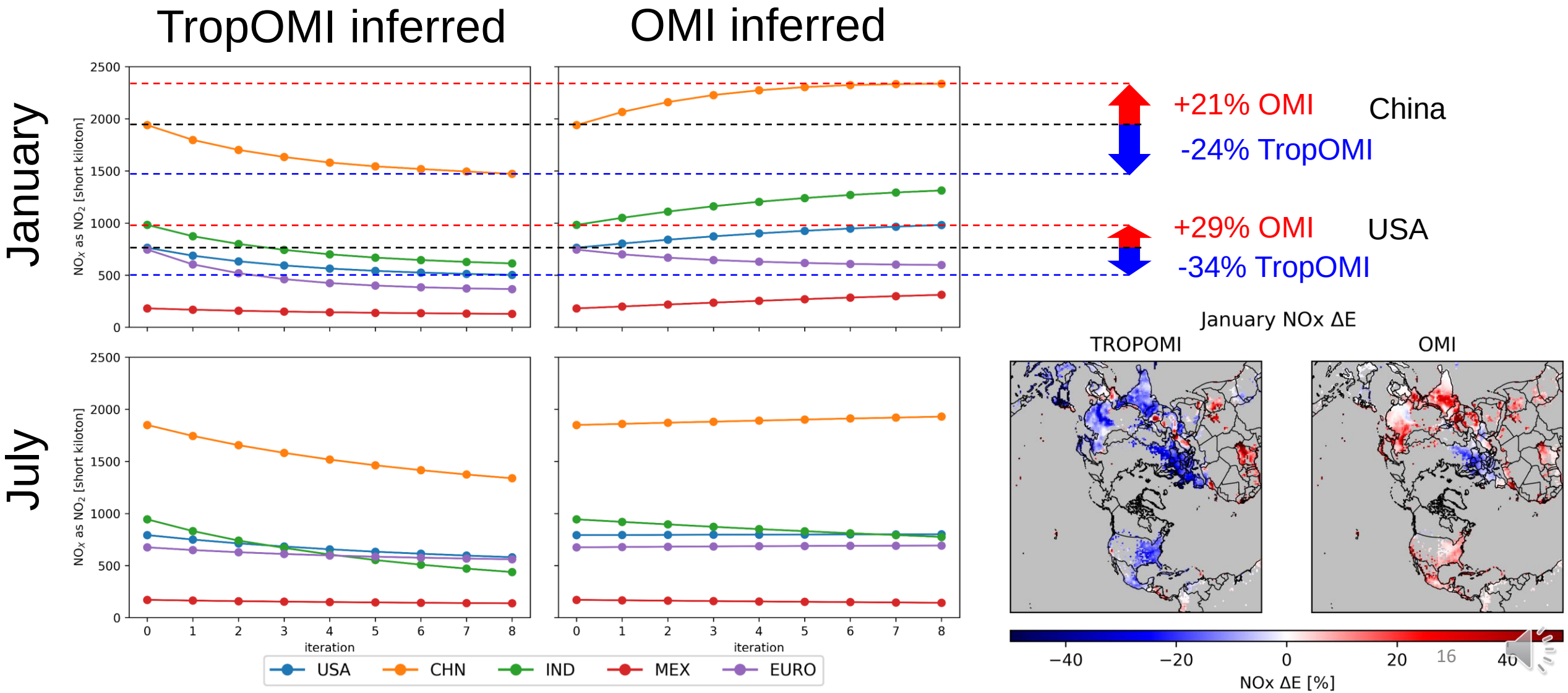
Satellites
OMI NO_2
TropOMI NO_2

Simulation inputs	
Emissions (North America & rest of hemisphere)	**2017** EPA platform
Emissions (China)	**2015** Tsinghua University
Meteorology	**2019** WRF
Satellite Observation year	**2019**

*LNOx emissions are adjusted before running Base Case

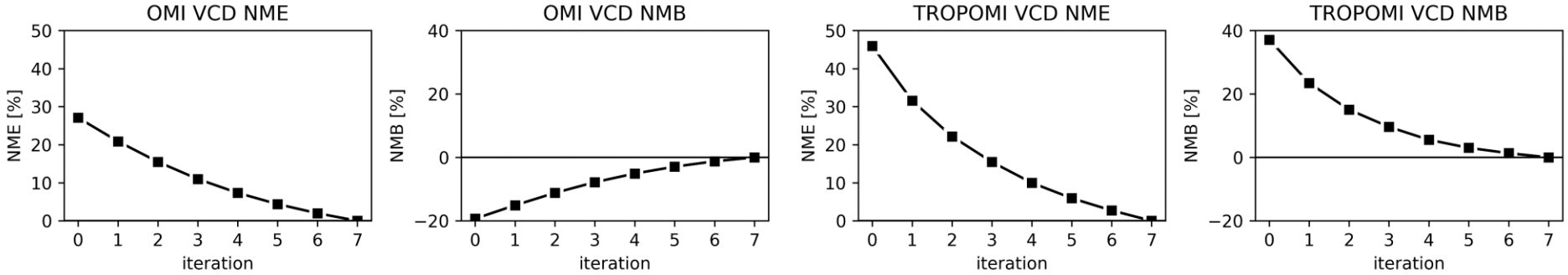
Note: Preliminary data from East et al. *in prep*, please do not distribute

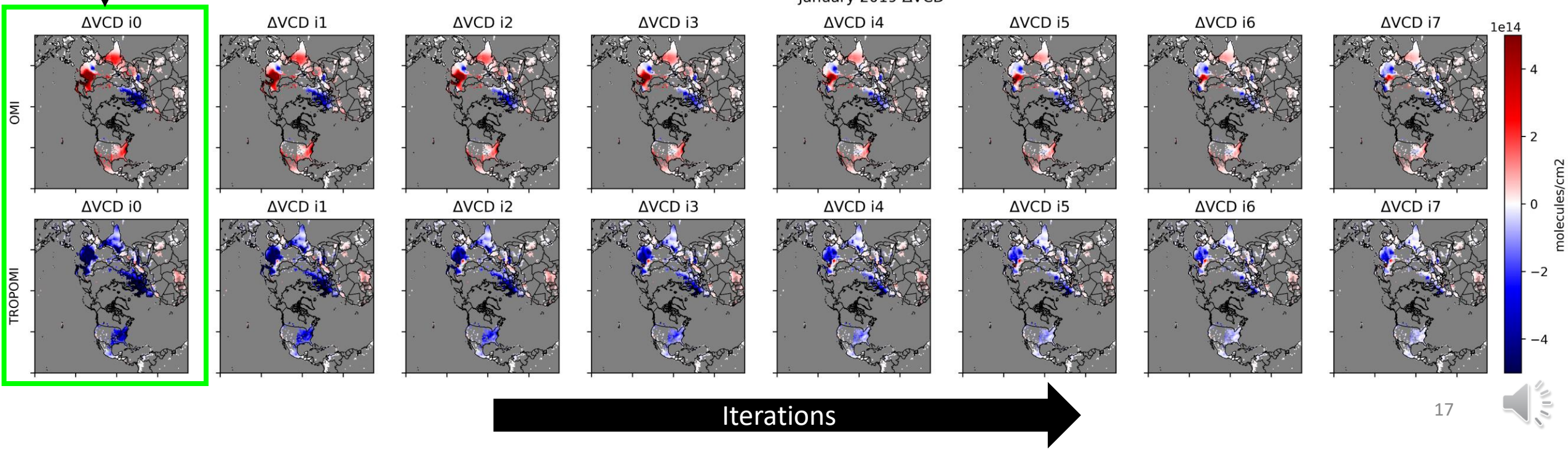
Satellites push CMAQ emissions different directions



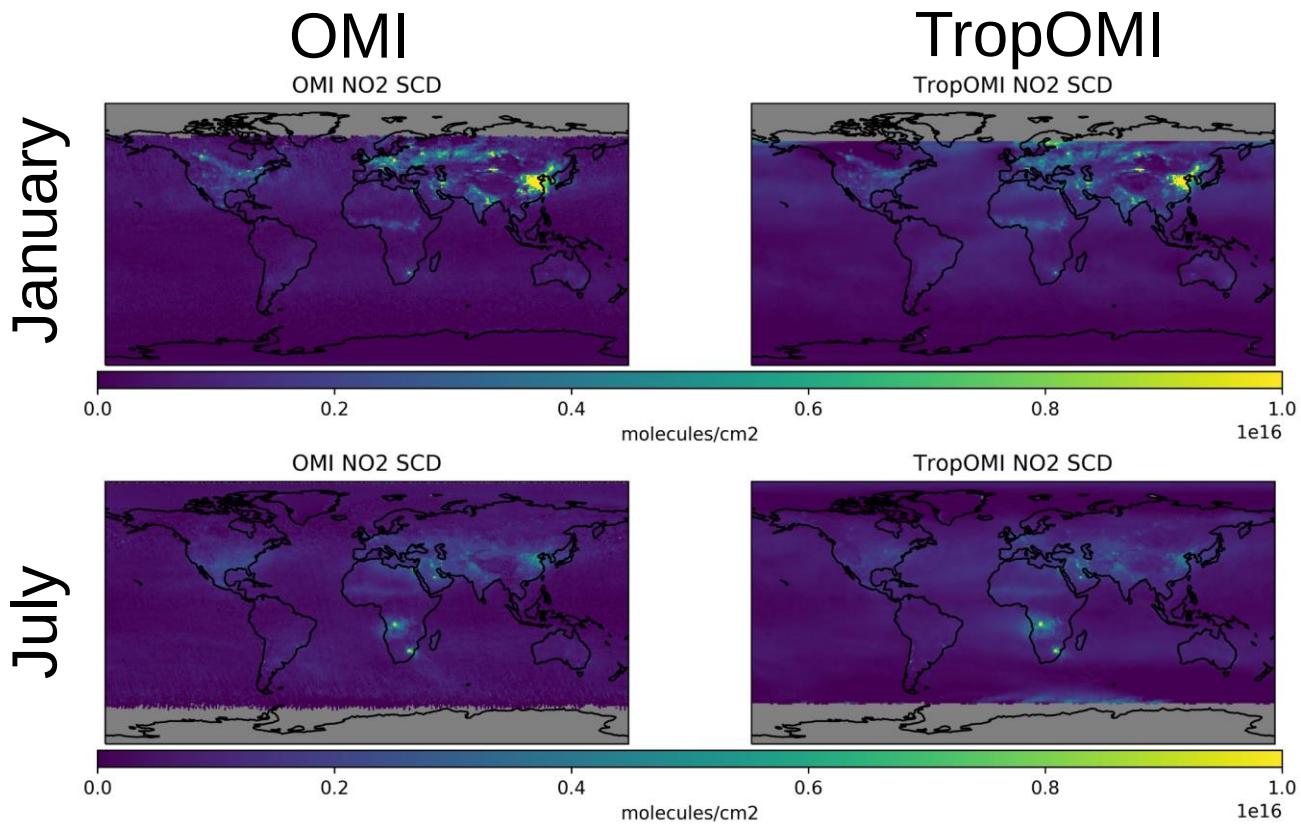
Analysis increment reflects same trend

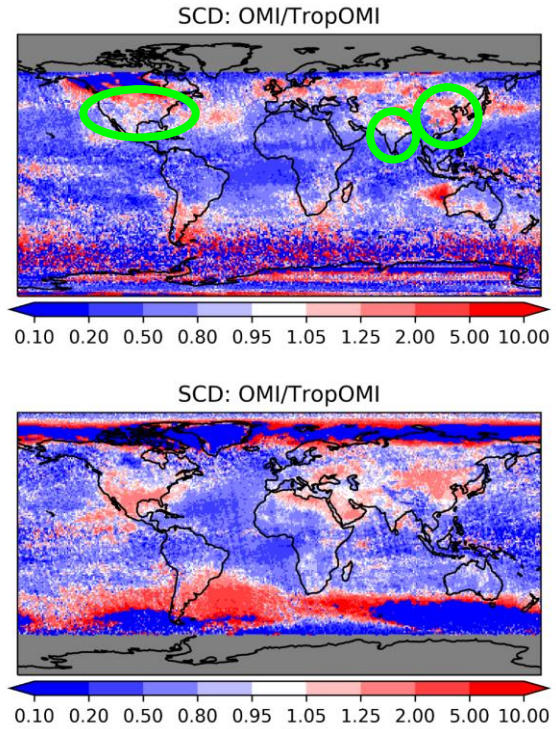
Except for the satellite data assimilated, these two simulations are identical



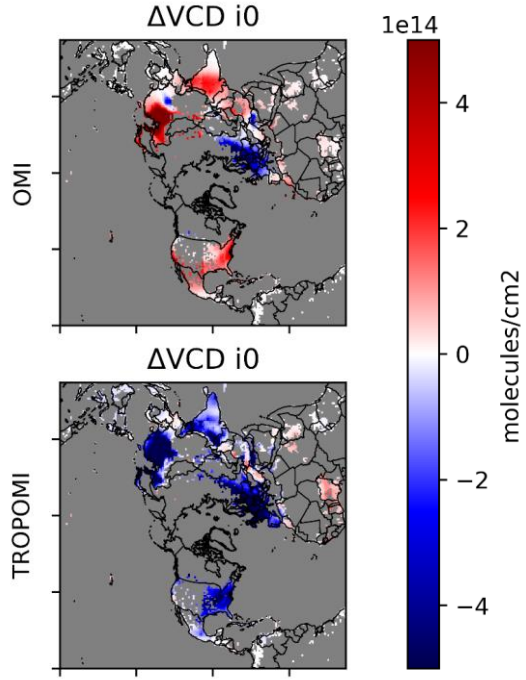


Slant column observations





January analysis increment



OMI filtering:

- 1x1 degree binned
- <30% cloud cover
- Solar zenith angle < 85
- VCD Quality flag = 0

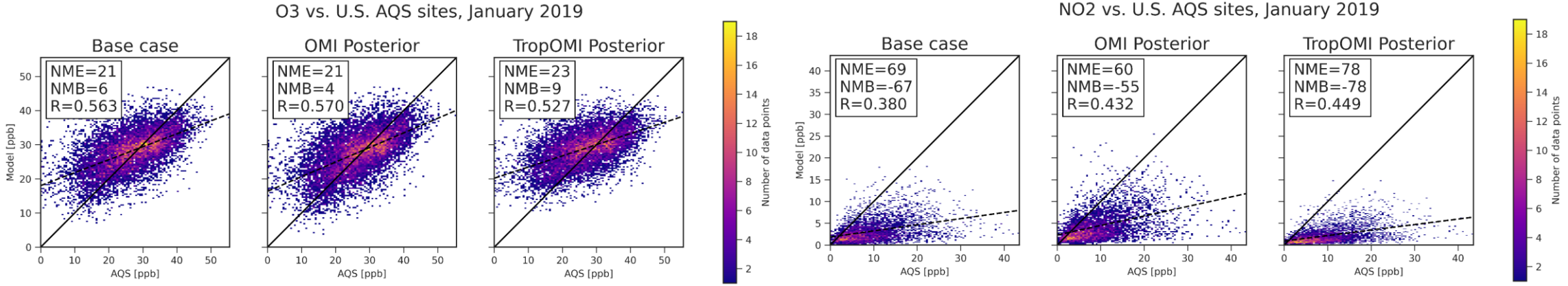
TropOMI filtering:

- 1x1 degree binned
- <30% cloud cover
- Solar zenith angle < 85
- QA Flag >= 0.75

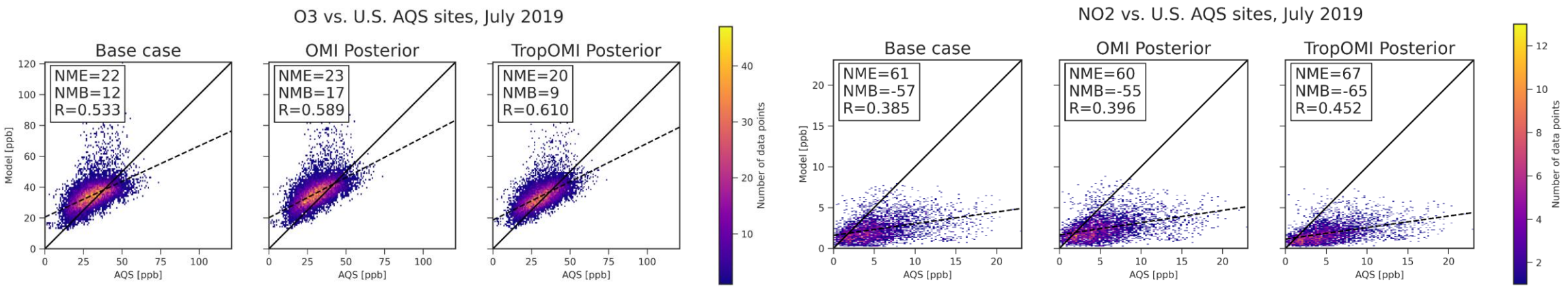
Impact on U.S. AQS O_3 performance depends on season

O_3 NO_2

January



July



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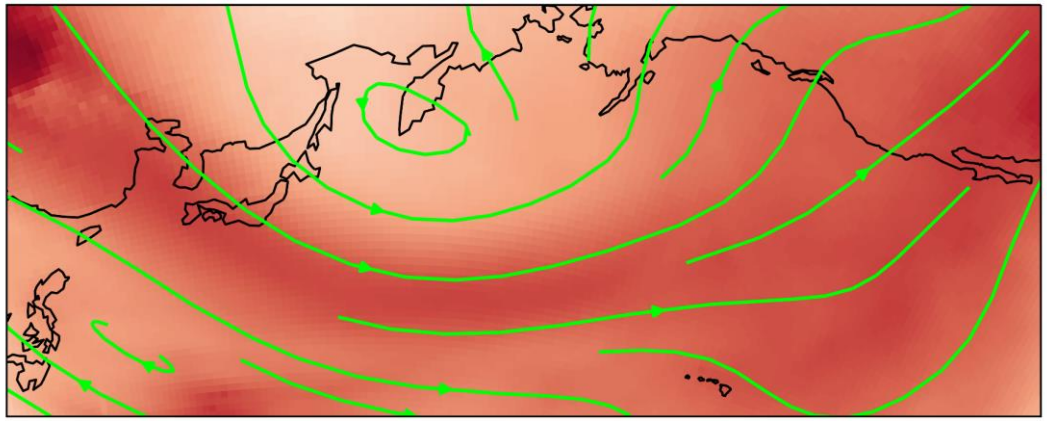
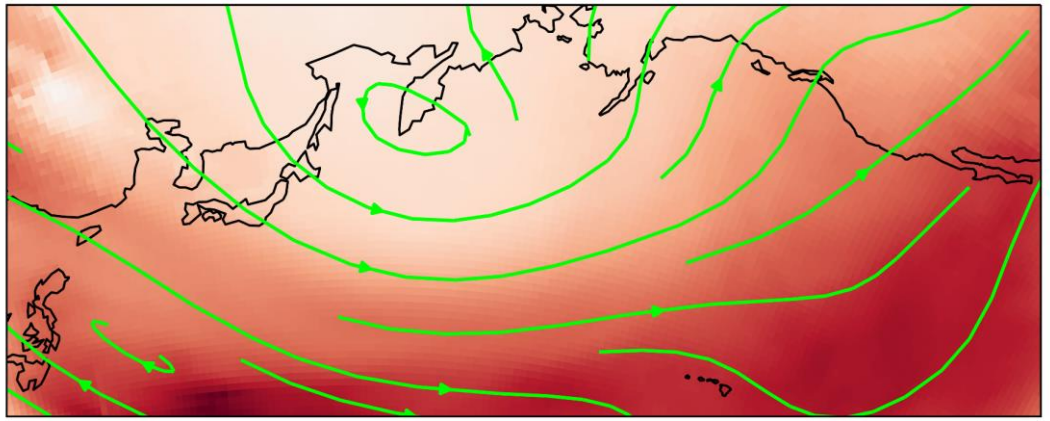
Satellite differences have implications for long range transport

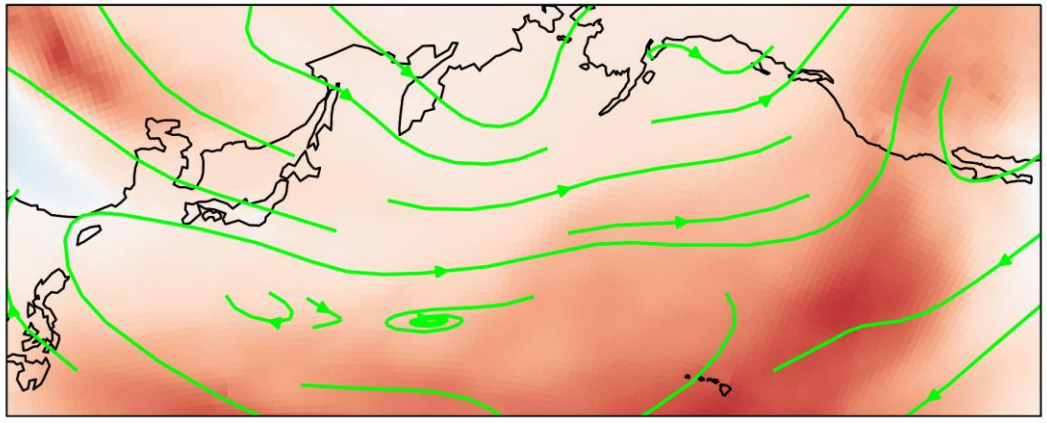
Free troposphere O_3 (750 to 250 hPa) OMI Posterior, January



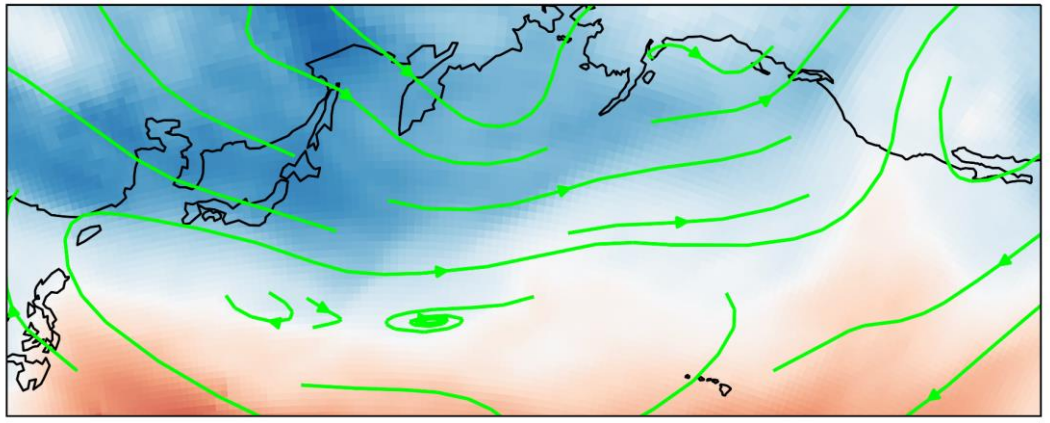
Free troposphere O_3 (750 to 250 hPa) TropOMI Posterior, January



Free troposphere O_3 (750 to 250 hPa) OMI Posterior, July



Free troposphere O_3 (750 to 250 hPa) TropOMI Posterior, July



Conclusions

- Satellite data assimilation in CMAQ enables the capability to adjust NO_2 and to update NO_x emissions based on observations.
- OMI and TropOMI observations push emissions estimates in different directions.
  - NOx emissions differences can reach +/- 30% (U.S.) and +/- 20% (China).
- OMI inferred emissions perform slightly better than TropOMI in the US, except for summertime O_3
- There is an impact on transpacific O_3 of up to 3 ppb difference (winter) in the free troposphere, depending on which satellite is used.
- We continue to investigate the differences between OMI and TropOMI in this data assimilation context.

Thank you!

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Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

Acknowledgement: James East is supported in part by an appointment to the ORISE participant research program supported by an interagency agreement between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Energy (DOE).