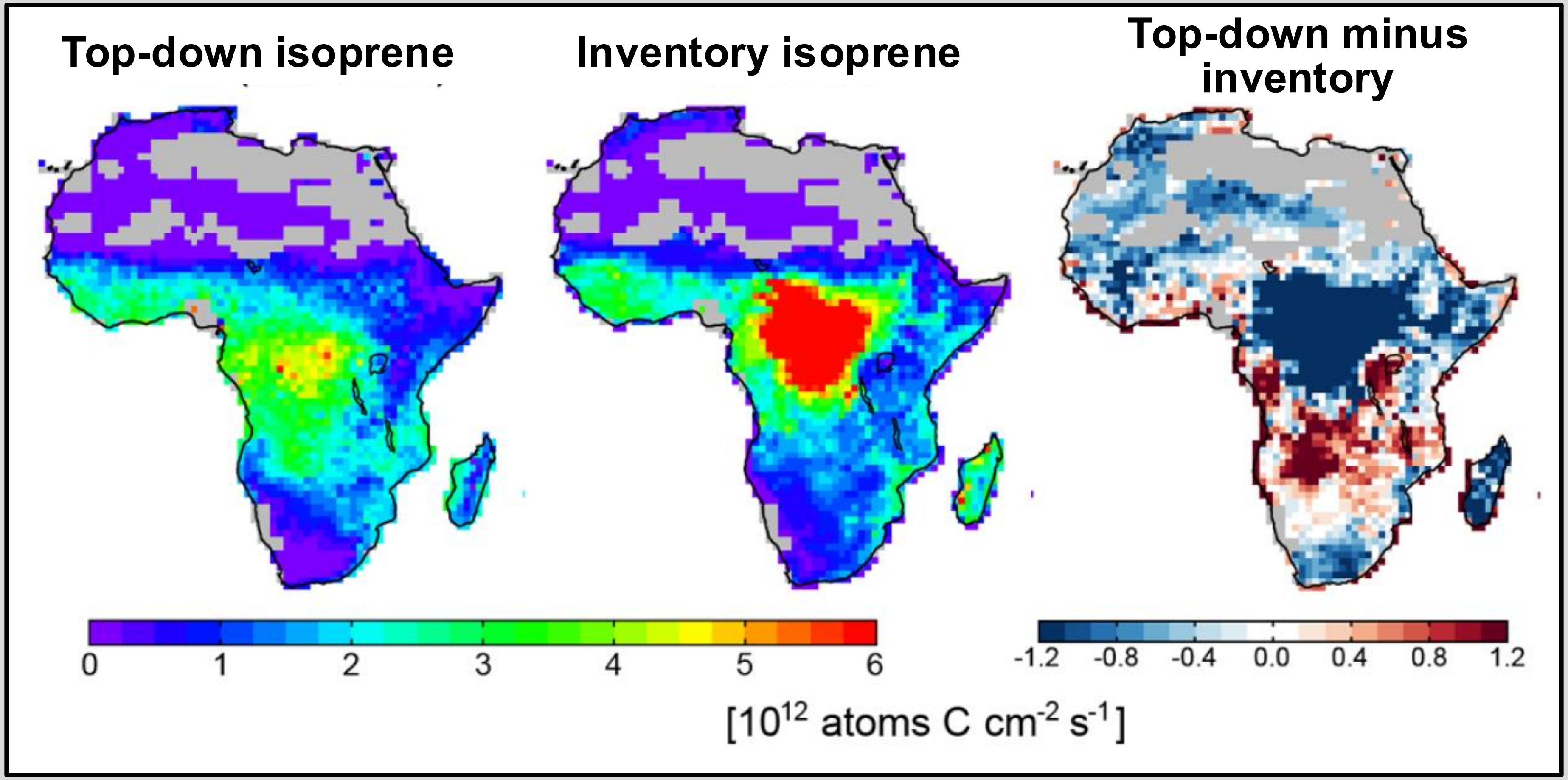
Utility of satellite observations for calculating emissions of air pollutant precursors



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Eloise Marais

https://maraisresearchgroup.co.uk/

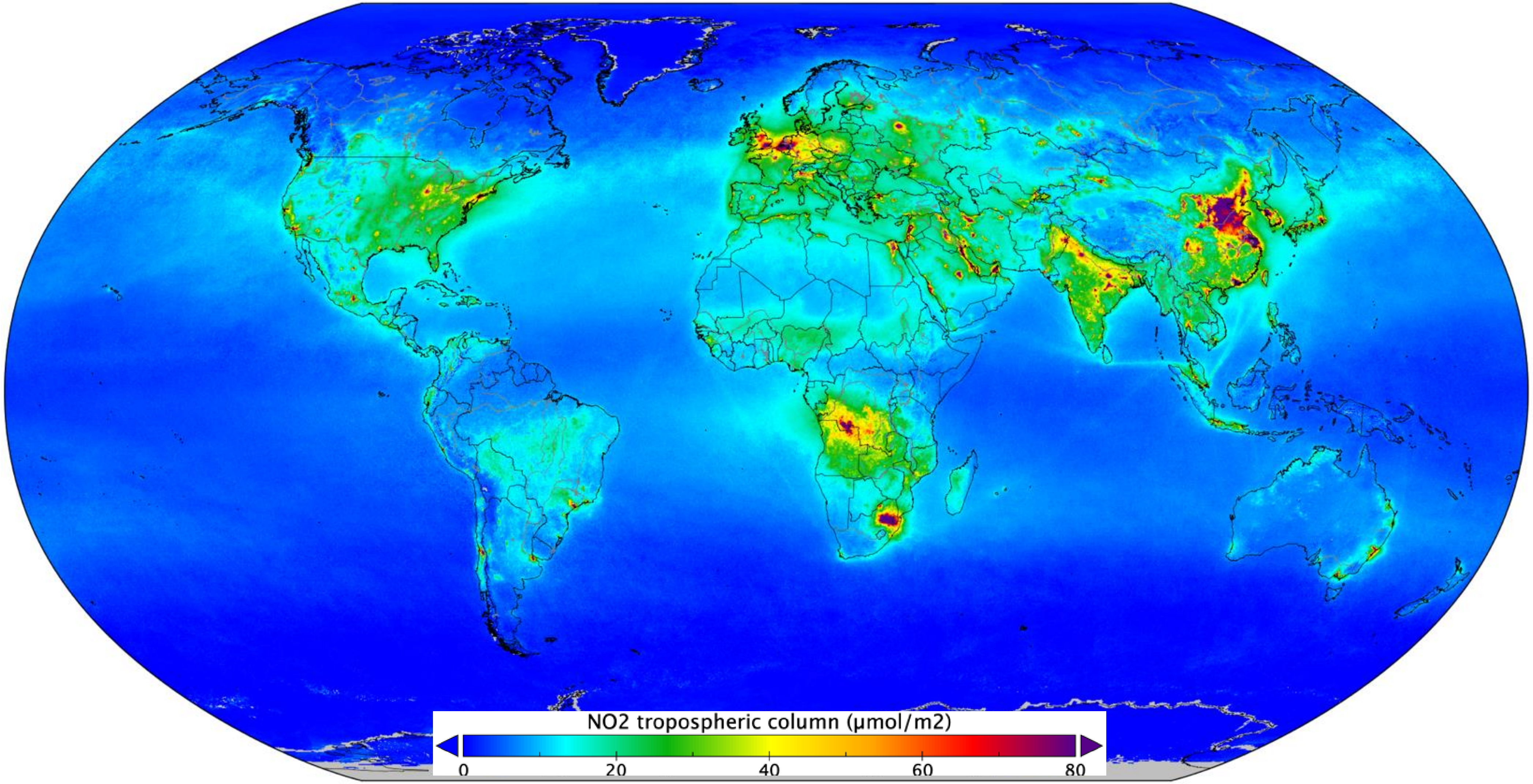
21 October 2025

University College London

UCL

Collocation of pollution abundances and and sources

TROPOspheric Monitoring Instrument (TROPOMI) nitrogen dioxide (NO_2)

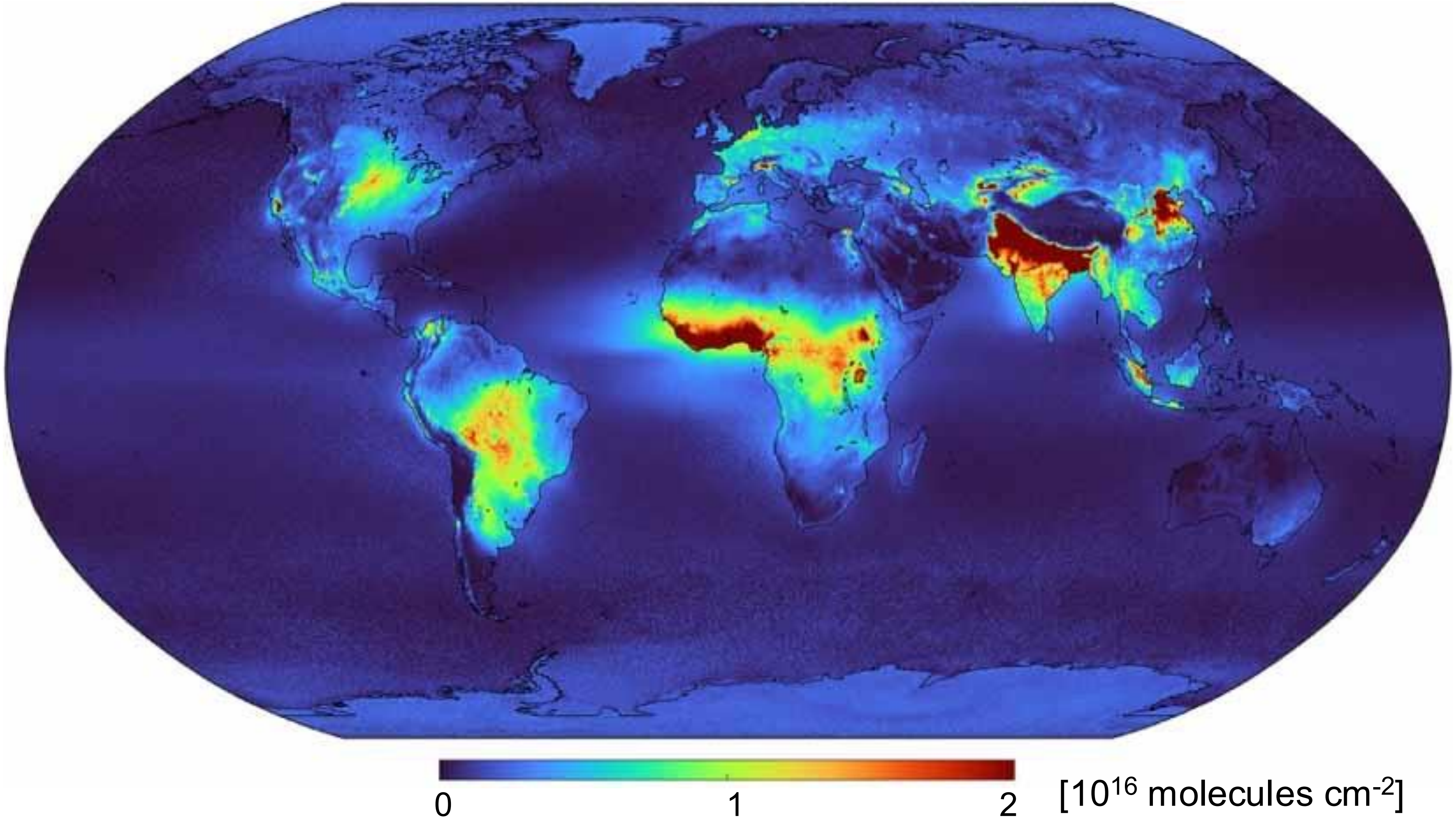


[Source: https://www.esa.int/Applications/Observing_the_Earth/Copernicus/Sentinel-5P/Nitrogen_dioxide_pollution_mapped]

Criteria pollutant, short-lived, indicator of combustion, but satellite sees the whole atmosphere

Collocation of pollution abundances and and sources

Infrared Atmospheric Sounding Interferometer (IASI) ammonia (NH_3)



[Source: Van Damme et al. (2021) https://iopscience.iop.org/article/10.1088/1748-9326/abd5e0]

Short-lived near large sources (industry, agriculture, fires). Toxic to plants. Aerosol precursor.

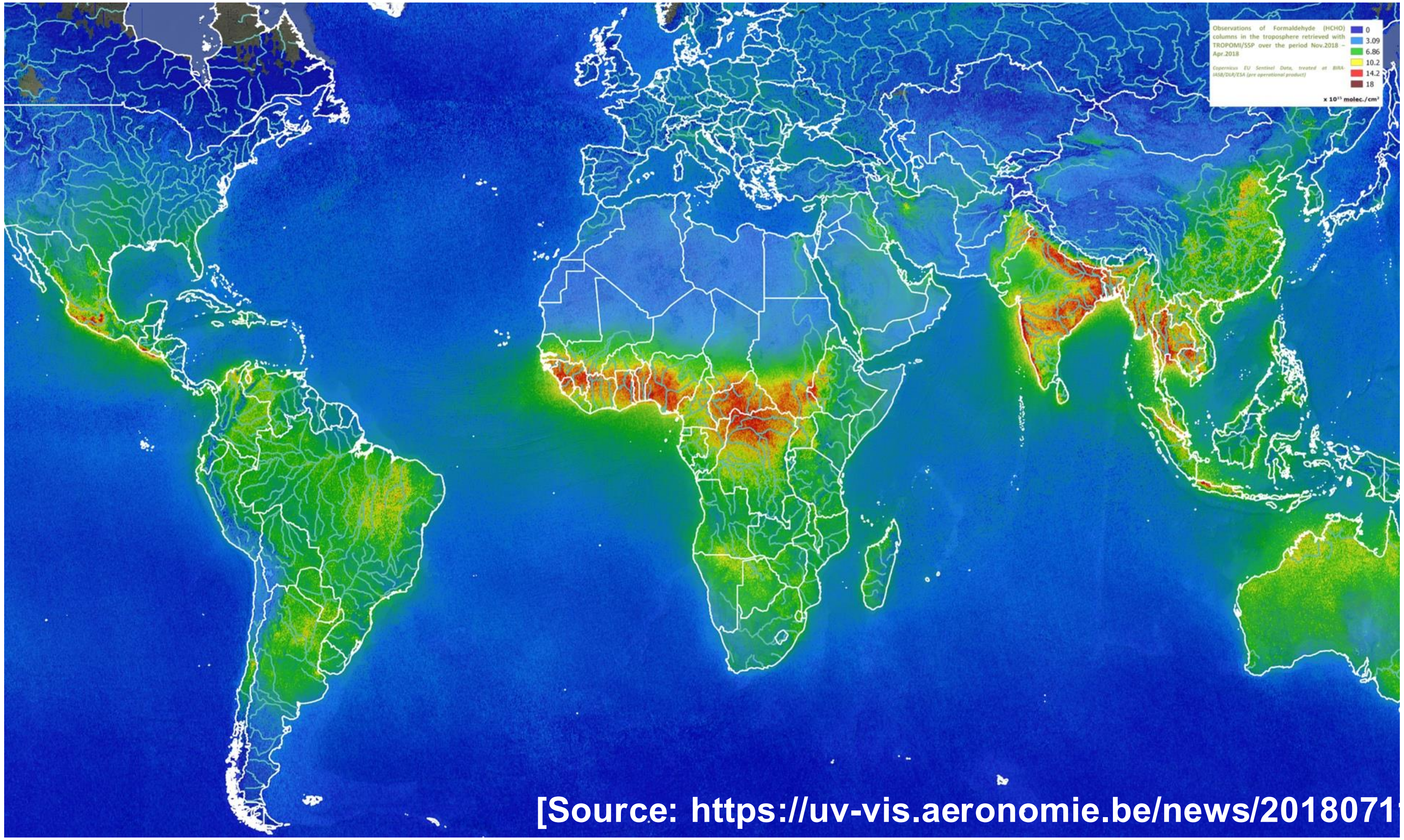
Collocation of pollution abundances and and sources

TROPOMI formaldehyde (HCHO)

VOCs

$\downarrow$ OH

HCHO



Scale:
0-18
[10^{15} molecules cm^{-2}]

Mostly prompt, high-yield, near- ubiquitous oxidation product of volatile organic compounds. Some also directly emitted.

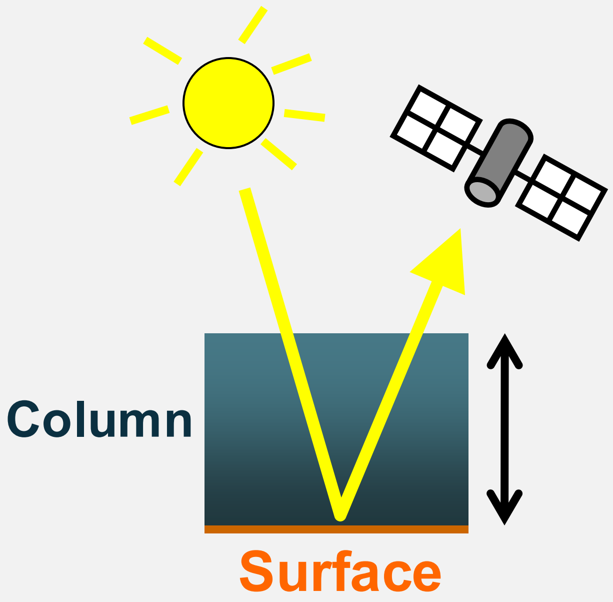
From VOCs that are precursors of ozone pollution and aerosols and that affect atmospheric oxidation.

Approach to Convert Satellite Data into Emissions

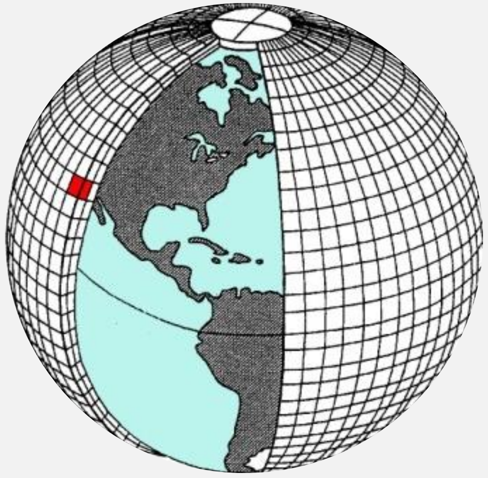
<u>Simple Mass Balance</u>: NO_2 to NO_x and NH_3 concentrations to NH_3 emissions

COLUMNS → **Conversion Factor** → **EMISSIONS**

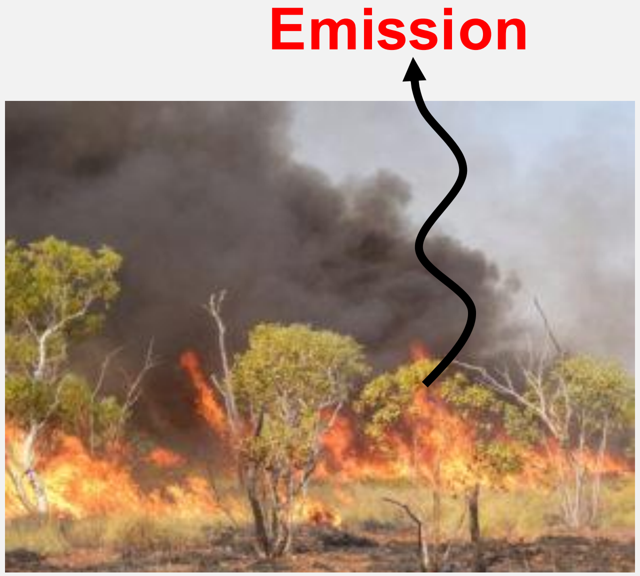
Satellite columns



Column-to-Emission ratio (model)



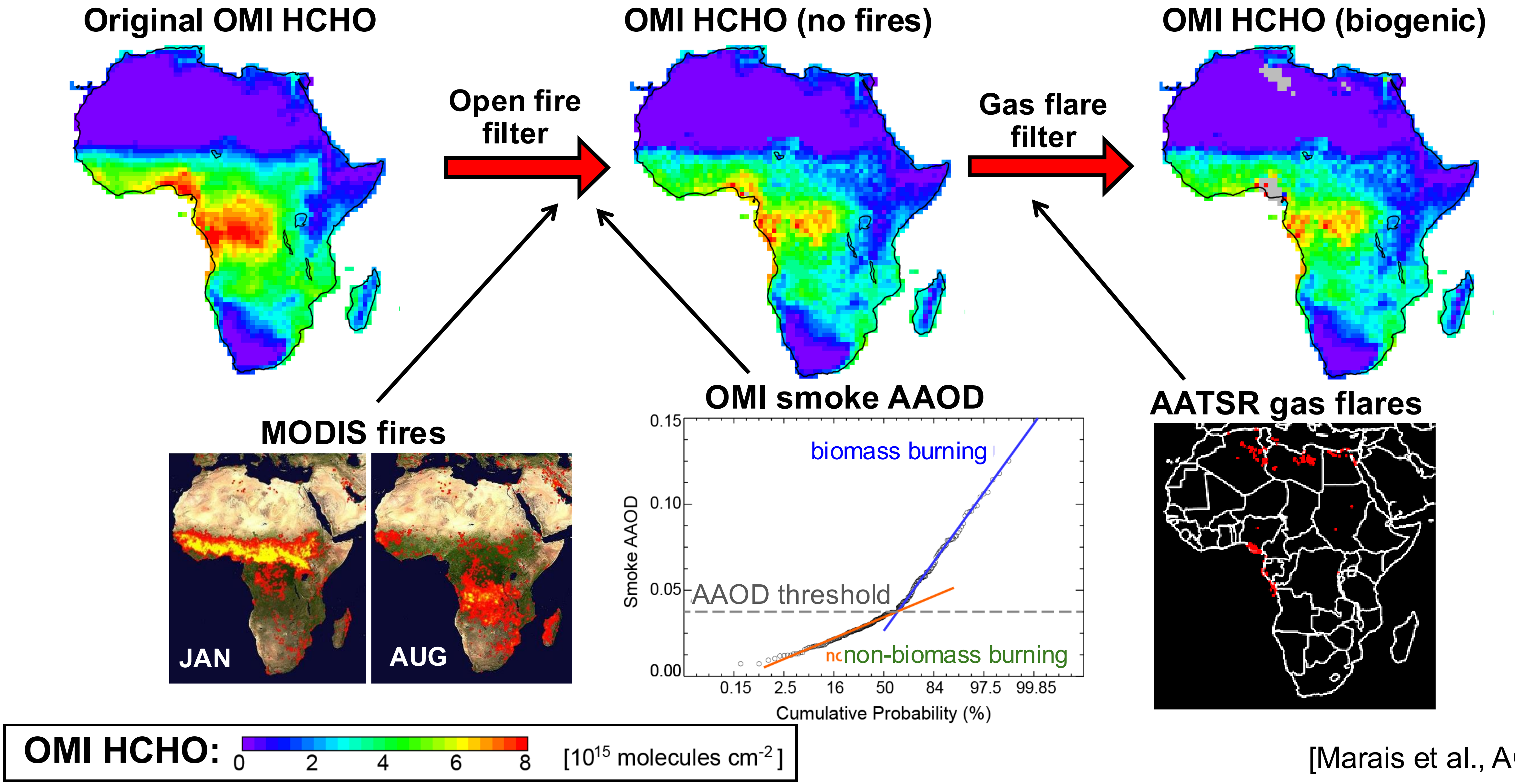
Satellite-derived surface emissions



Simple mass balance approach: short-lived air pollutant and often for Africa it's a first order problem (very uncertain/underconstrained emissions)

Not as Easy for isoprene emissions from HCHO

HCHO to calculate isoprene emissions, need to isolate the biogenic signal



[Marais et al., ACP, 2012]

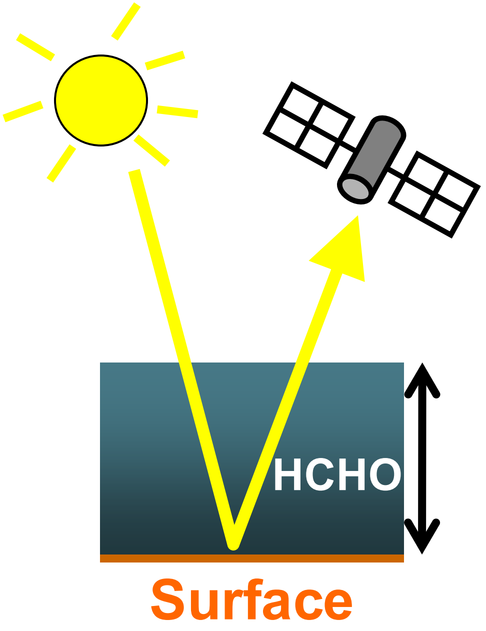
Need to Account for Isoprene Oxidation Yields of HCHO

$\text{Isoprene} \xrightarrow{OH} \textbf{HCHO} \xrightarrow[OH]{h\nu} CO, HO_2$

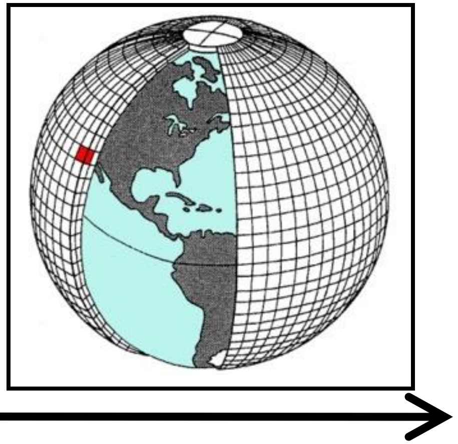
APPROACH:

DATA ⇨ Conversion Factor ⇨ RESULT

Biogenic Component of Satellite HCHO



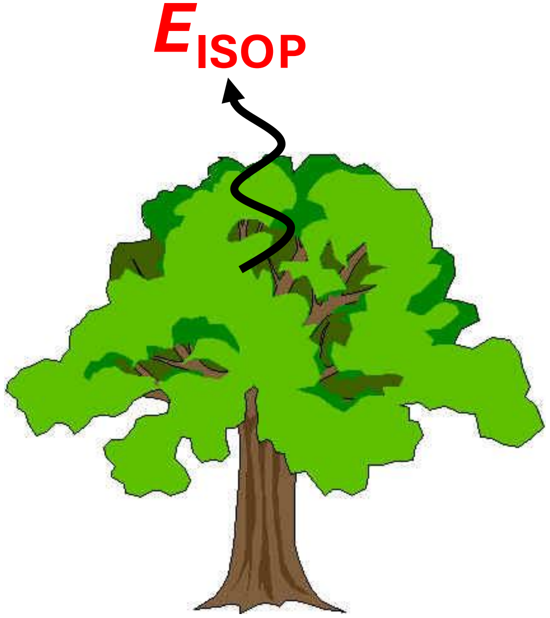
GEOS-Chem



HCHO effective yields:

$$\frac{k_{HCHO}}{Y_{Isop \rightarrow HCHO}}$$

Satellite-derived Isoprene Emissions

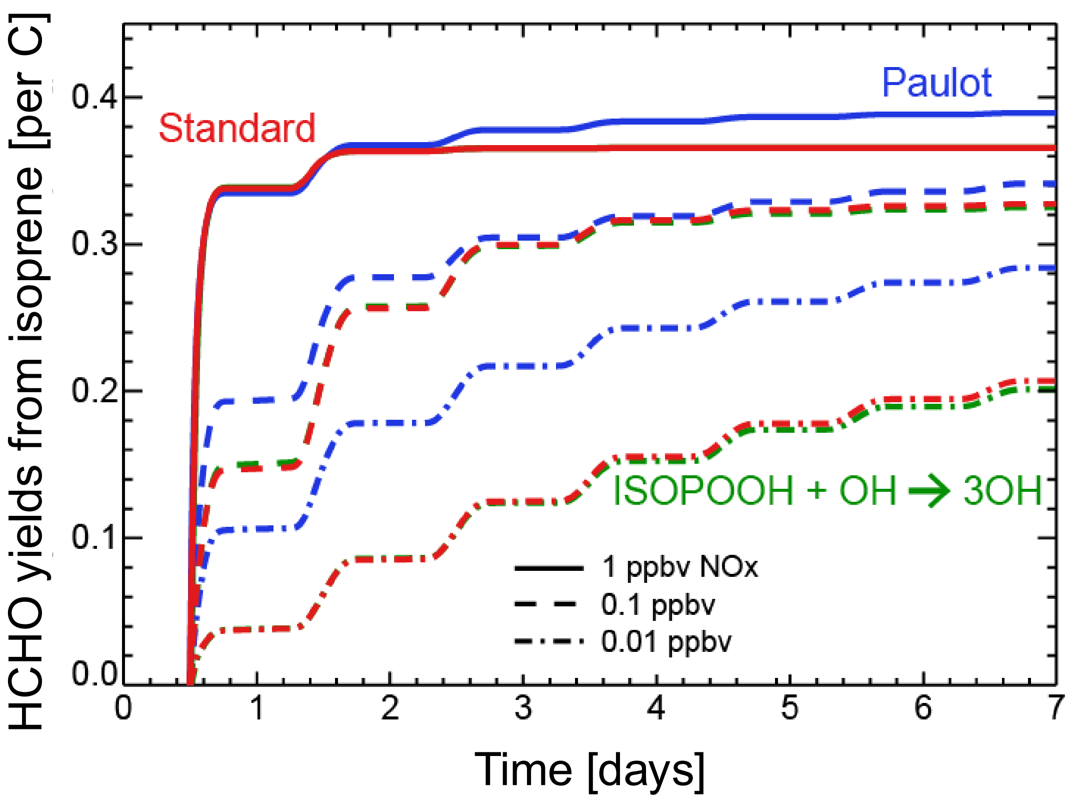


[Palmer et al., 2003; Millet et al., 2008]

HCHO Yields Depend on Ambient Nitrogen Oxides (NO_x)

HCHO yields from isoprene are not uniform in Africa

Time-dependent HCHO yields

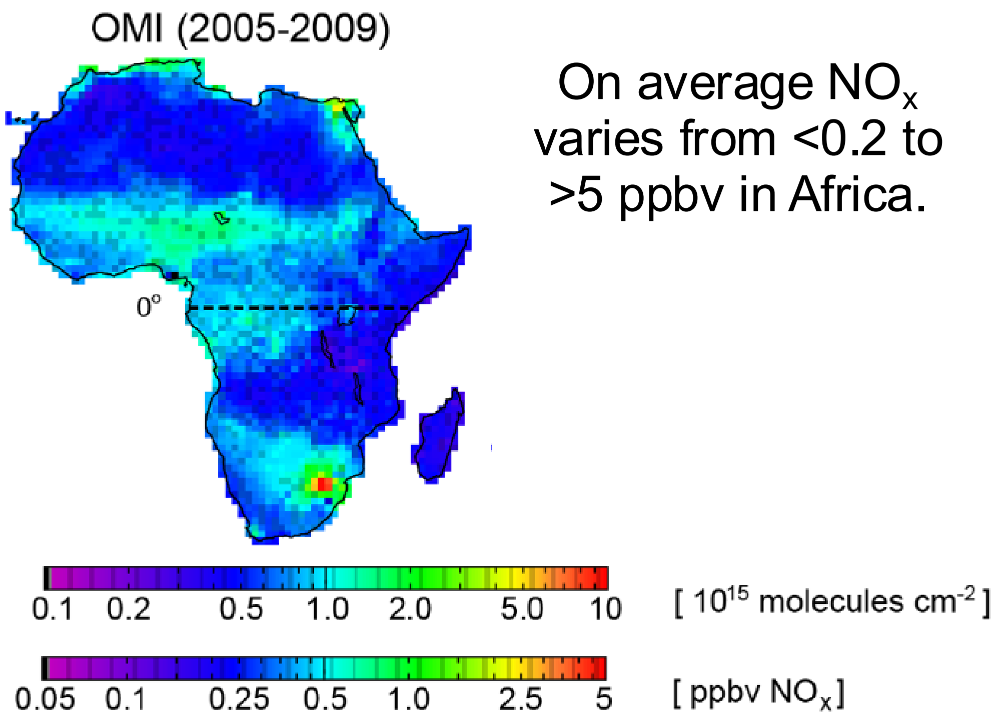


HCHO yields increase with increasing NO_x.

"Standard" chemistry scheme

Scheme updated with new chemistry

Africa tropospheric NO_2 columns



On average NO_x varies from <0.2 to >5 ppbv in Africa.

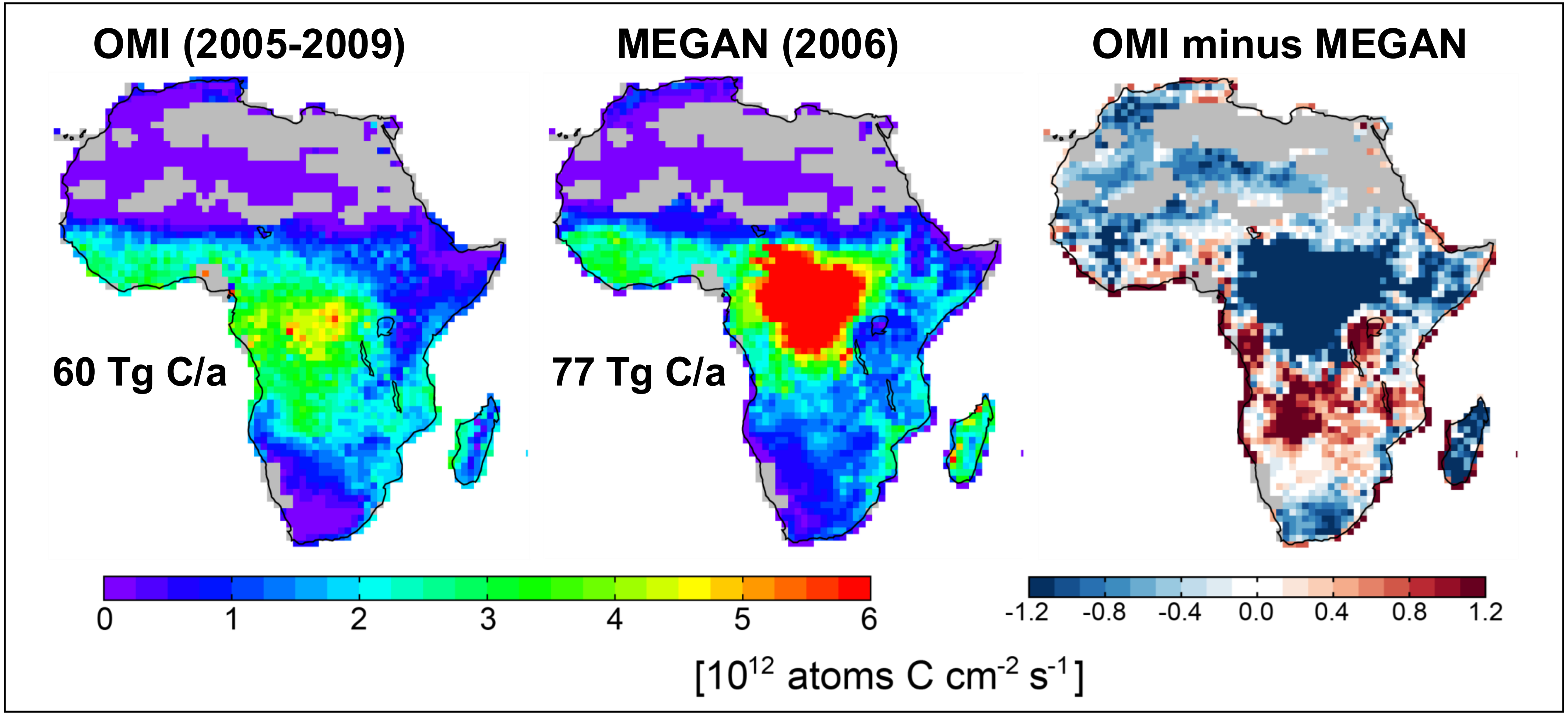
Variable levels of NO_x in Africa will result in non-uniform yields of HCHO

Satellite-derived Isoprene Emissions

Evaluate state-of-science, widely used bottom-up inventory (**MEGAN**)

Maps: **Midday (12-15 LT) mean isoprene emissions**

Values Inset: **Total (24 hour) isoprene emissions**

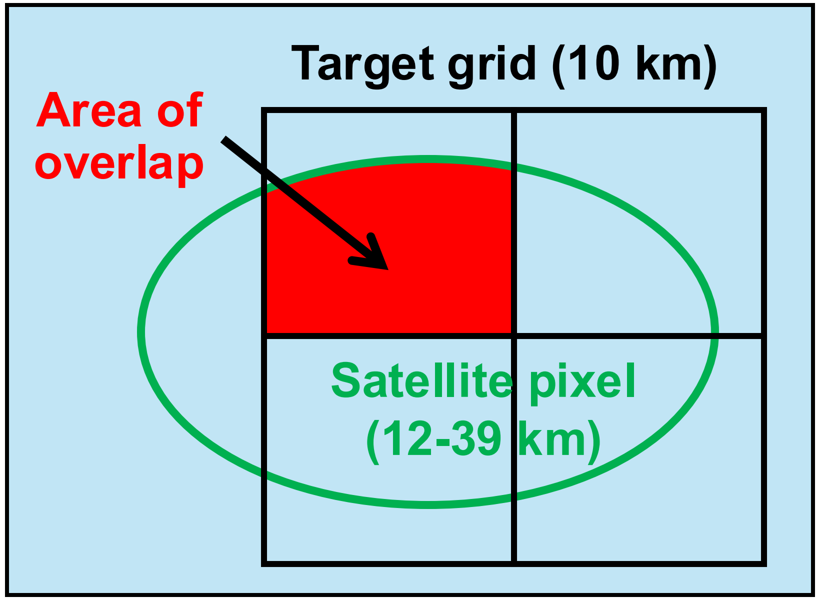


Large regional discrepancies between OMI-derived and state-of-the-science emission inventory

Agricultural Emissions of Ammonia in the UK

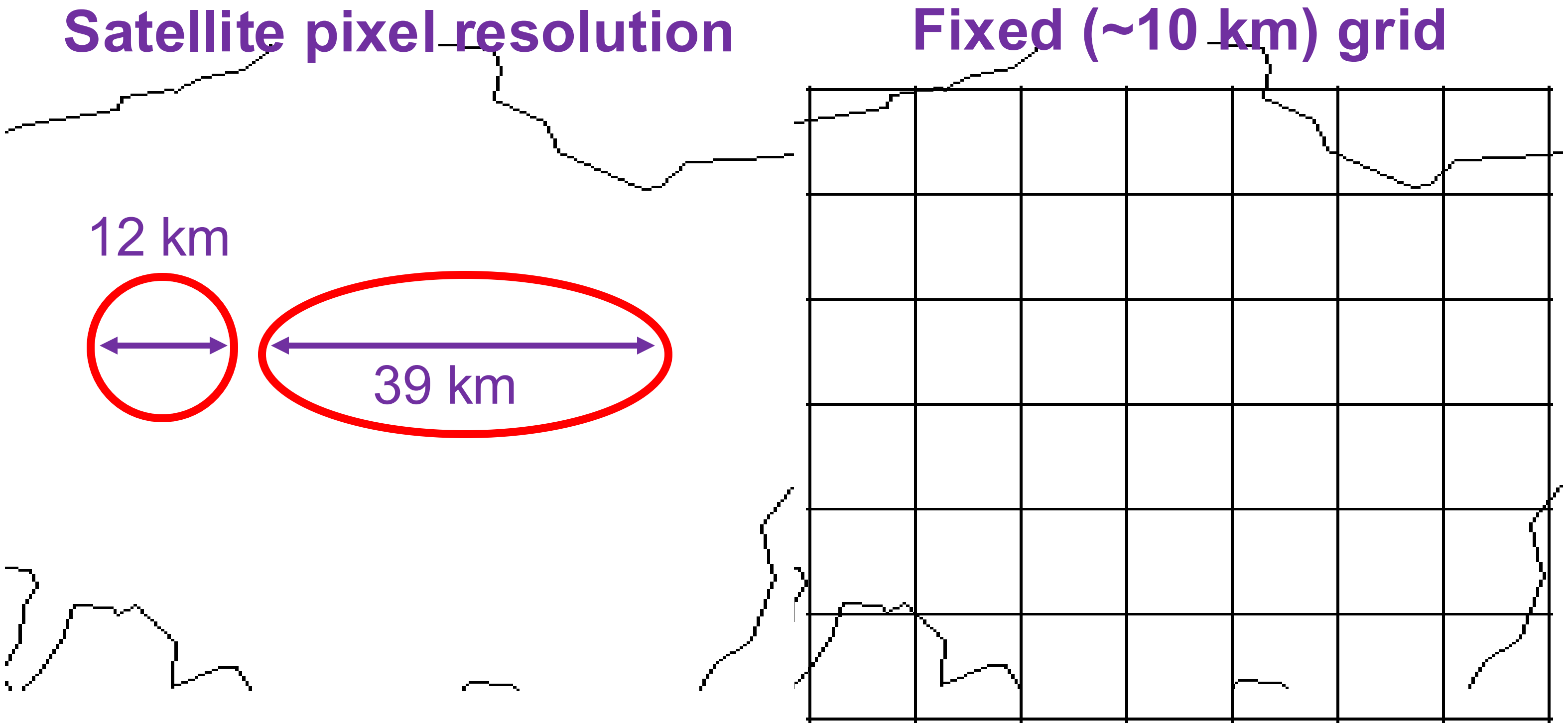
Start by gridding satellite data to finder spatial resolution than the native resolution of instrument

Oversampling Technique



Weights pixel by area of overlap

Oversampling technique over London

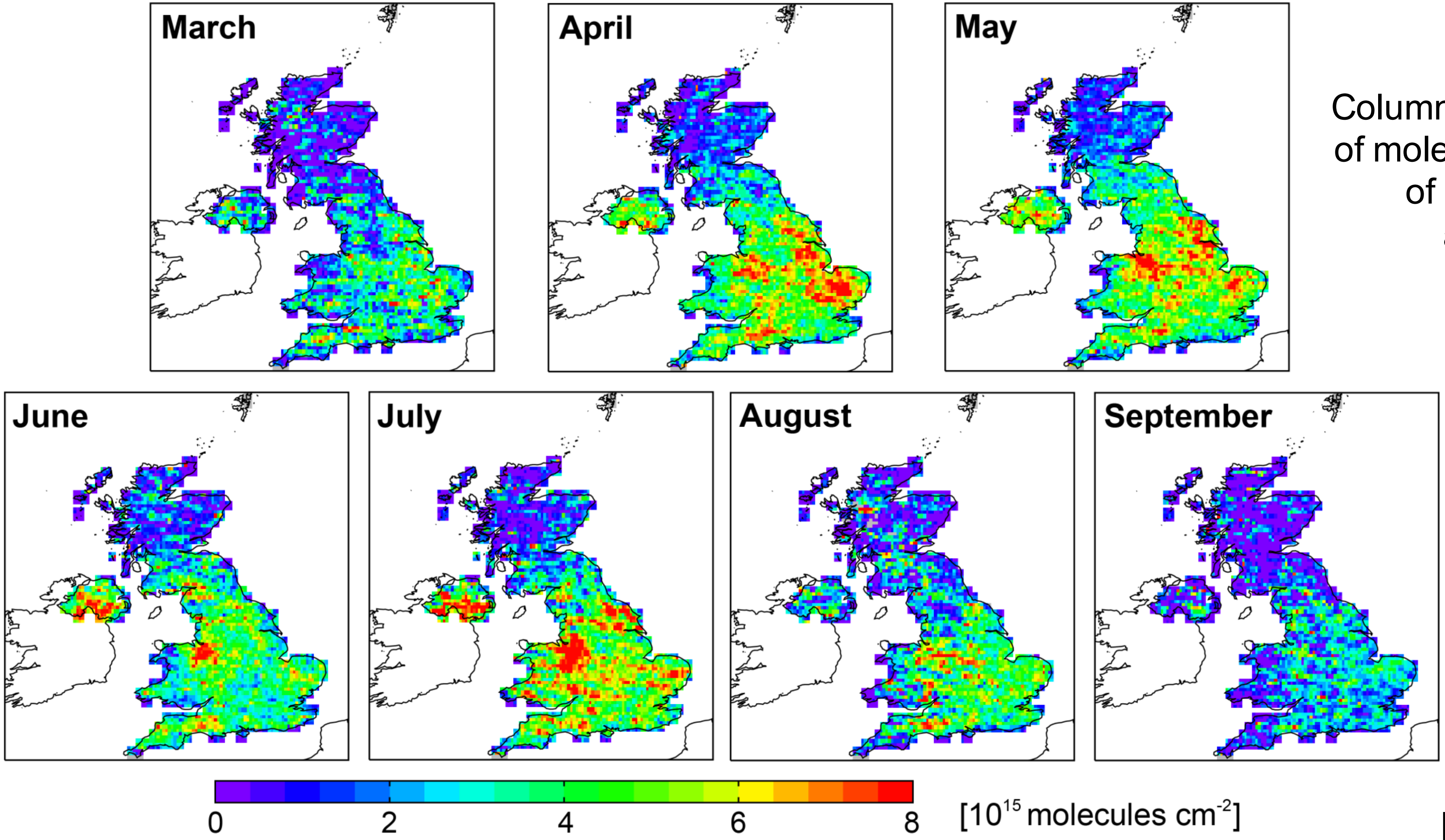


Lose time (temporal) resolution; gain spatial resolution

Improve resolution from 12-40 km to 10 km for an instrument observing ammonia (NH_3)

Multiyear means from the IASI instrument

Multiyear (2008-2018) monthly means for warmer months of the year



Column densities: number of molecules from surface of Earth to top of atmosphere

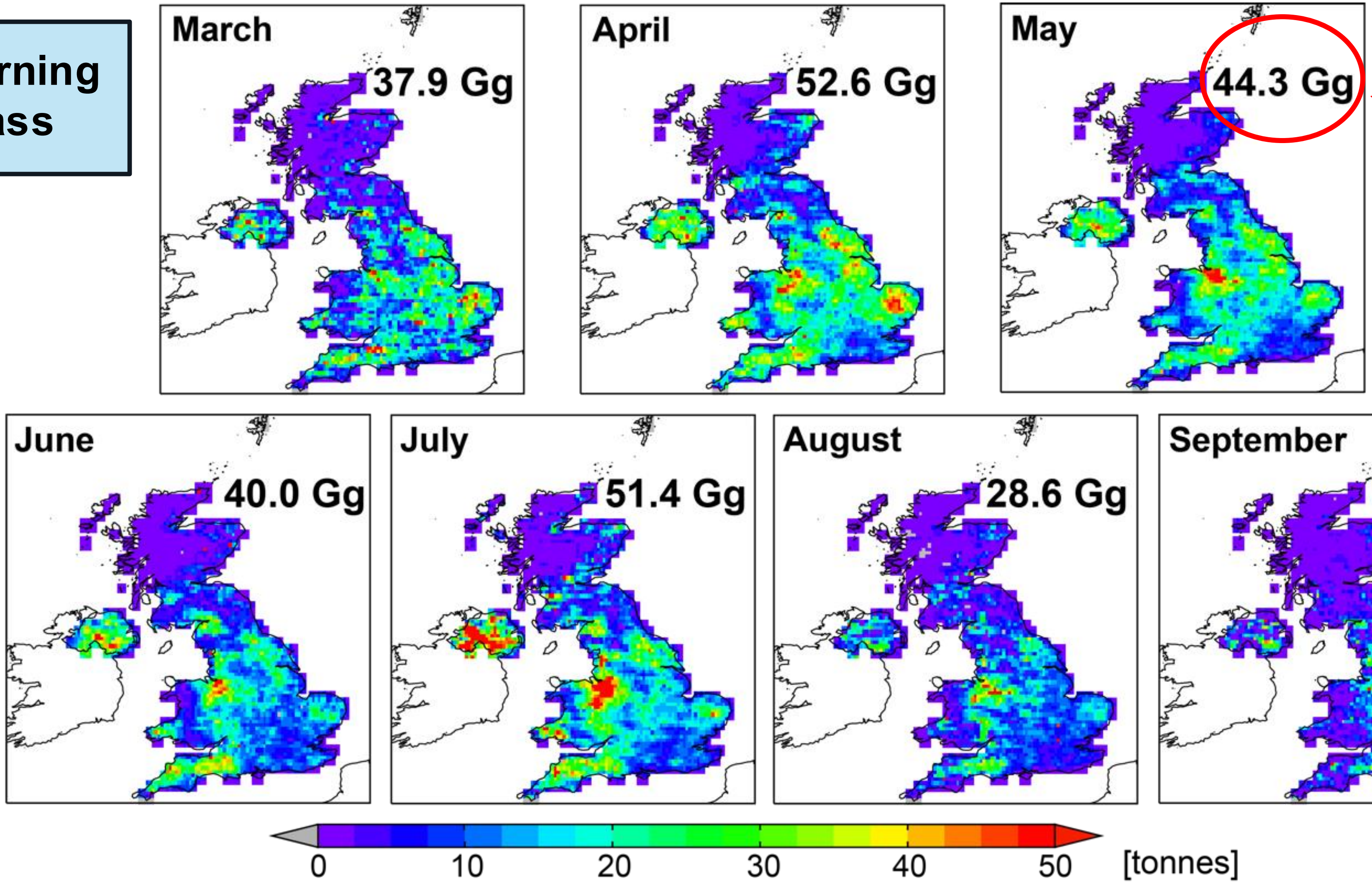
[Marais et al., 2021]

Climatological mean to be consistent with bottom-up ammonia emissions

Top-down multiyear (2008-2018) monthly NH_3 emissions

Focus on **Mar-Sep** when warm temperatures and clearer conditions increase sensitivity to surface NH_3

IASI: morning overpass



Total monthly emissions

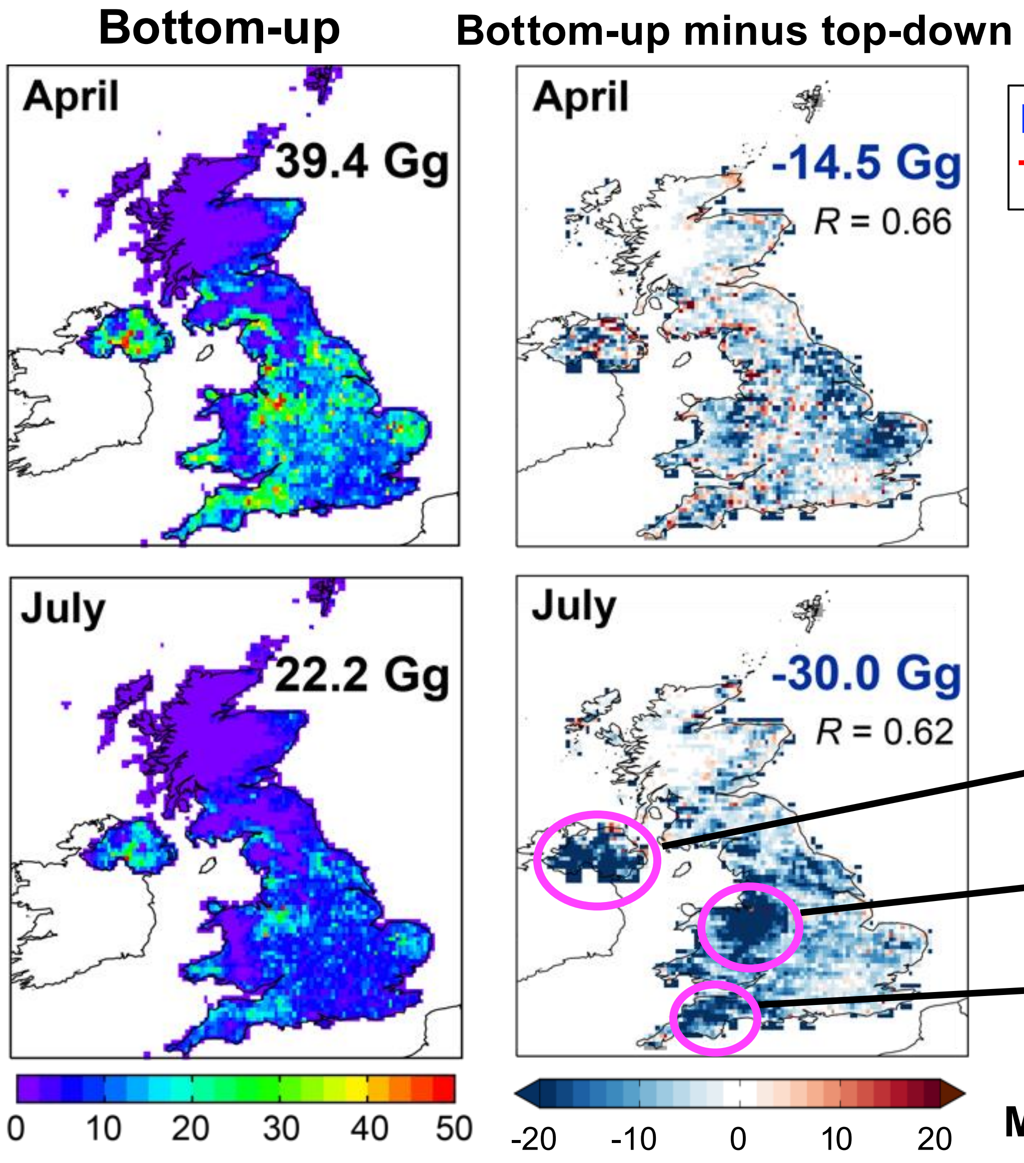
1 Gg = 1 kilotonne

[Marais et al., 2021]

Monthly emissions for March-September from **IASI**-derived estimates sum to **271.5 Gg**

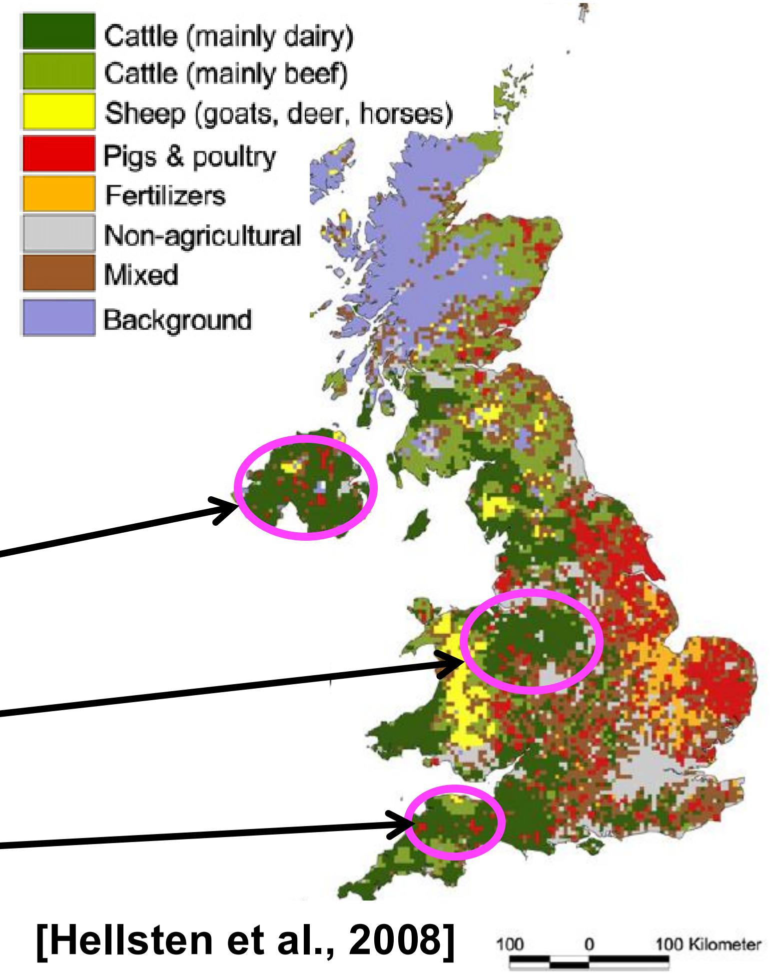
Satellite versus inventory NH_3 emissions

Comparison of months with peak emissions according to IASI (April and July)



Bottom-up < top-down
Top-down > bottom-up

Marais et al., JGR, 2021

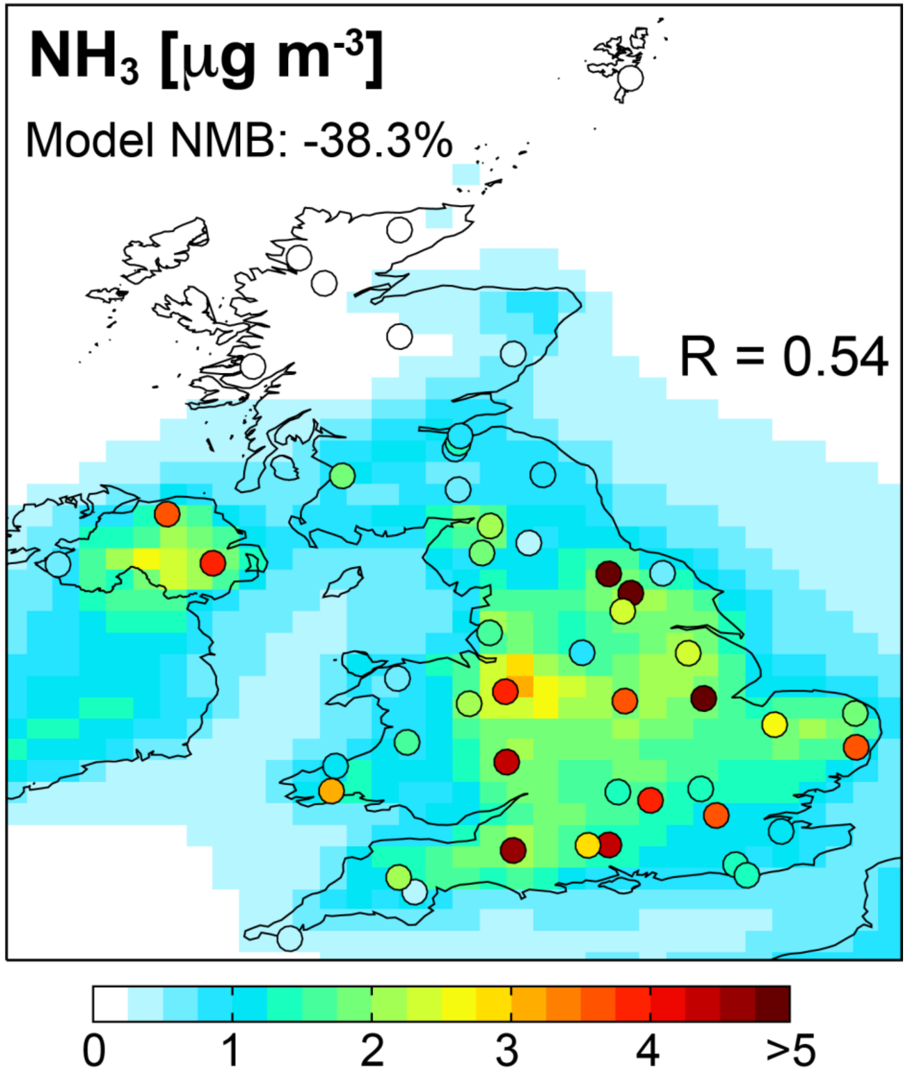


[Hellsten et al., 2008]

Large July difference over locations dominated by dairy cattle. Inventory is 27-49% less than the satellite values.

Ground-truthing Requires Independent Observations

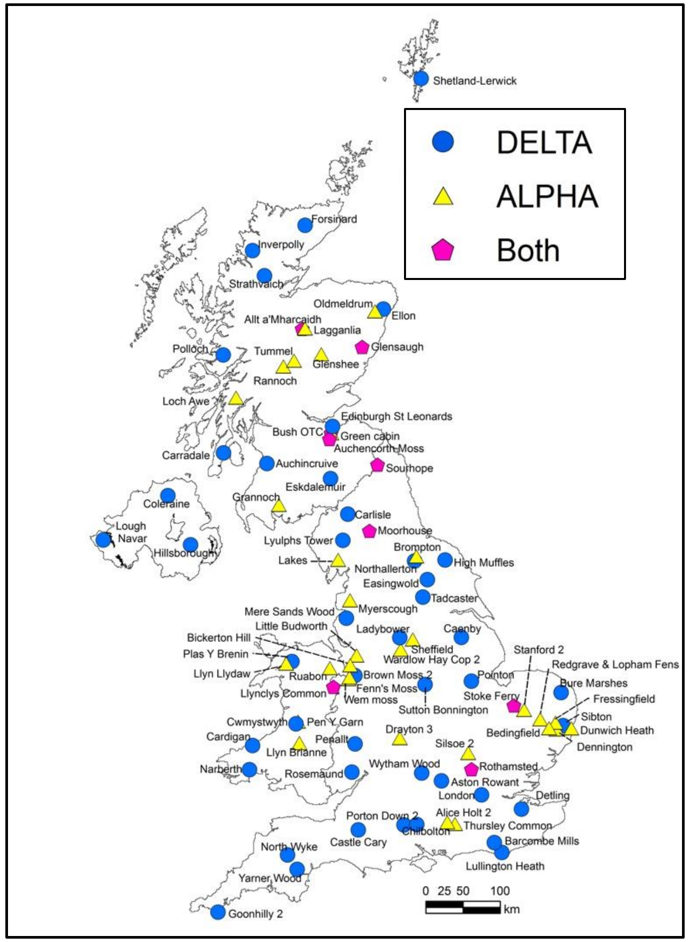
Network (points) and model (background) surface NH_3 in Mar-Sep



Points are for DELTA instruments (blue circles)

DELTA instruments support model underestimate (**NMB = -38%**)

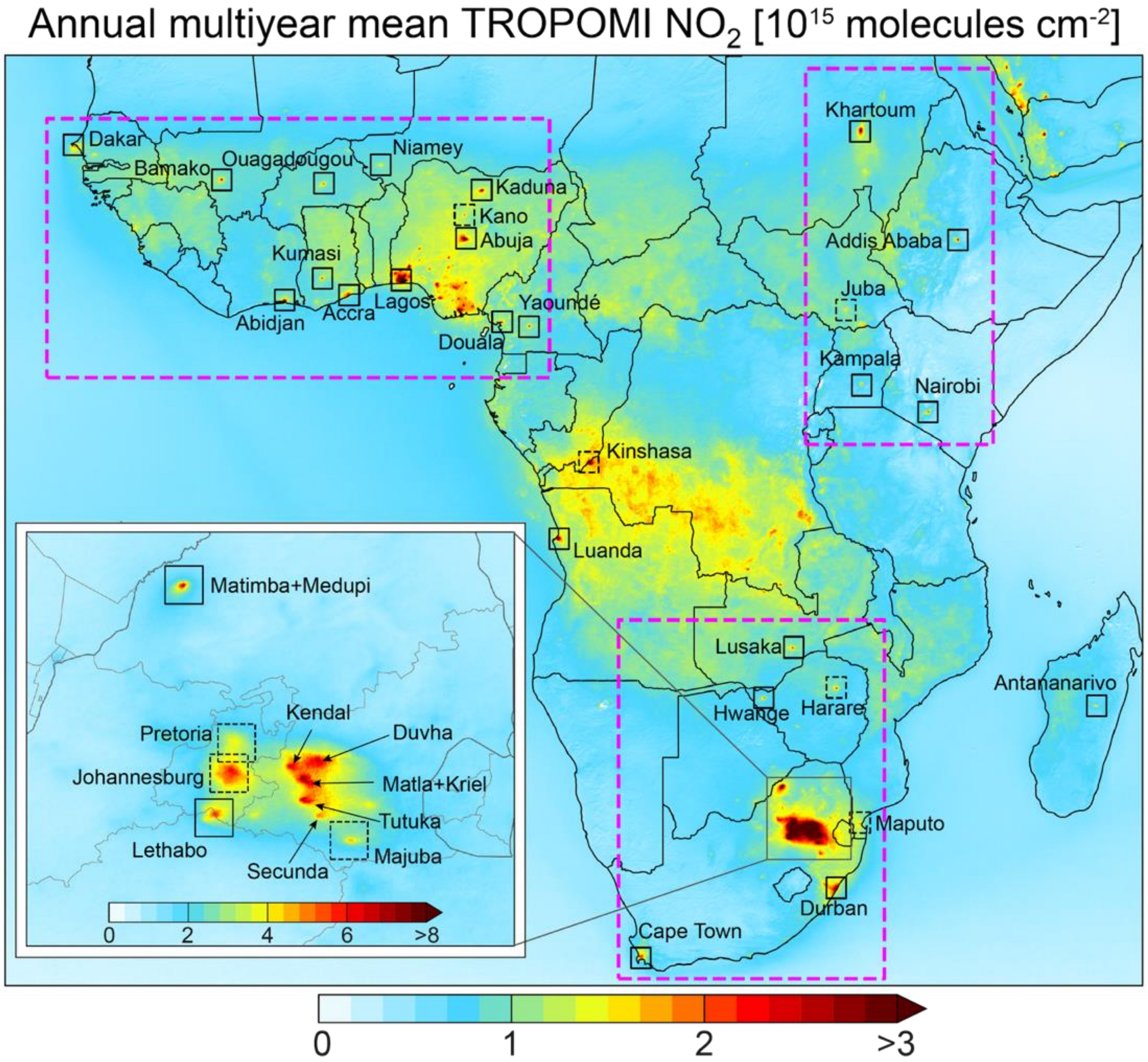
So do passive low-cost ALPHA instruments (yellow triangles) (**NMB = -41.5%**)



GEOS-Chem underestimate in surface NH_3 driven with the NAEI corroborates results from IASI

Leads to reluctance to uptake by inventory developers and integration in policy decisions

Urban and Point Sources of NO_x Resolved with TROPOMI



Oversample 4 years of TROPOMI data to finer scale (~2 km) than nadir resolution

Identify 32 isolated hotspots: most urban, 4 power plants

Boxes: dashed if attempt to calculate emissions fails; solid if succeeds

Hotspot NO_x Emissions in Sub-Saharan Africa

The largest anthropogenic point source emissions of NO_x are in Sub-Saharan Africa (South Africa)

Rank	Lat [° N]	Long [° E]	Emissions [kg s^{-1}]	Error [kg s^{-1}]	Power plants (GPPD)[1]	Cities (WCD)[1]	Comment[2]
1	−26.2875	29.1625	2.76	0.47	Matla; Kriel		
2	−26.5625	29.1625	2.47	0.39			Secunda CTL[3]
3	−23.6875	27.5875	2.47	0.56	Matimba		also Medupi (not listed in GPPD)
4	−26.7375	27.9875	2.03	0.44	Lethabo	Vereeniging	
5	−27.1125	29.7875	2.03	0.31	Majuba		
6	22.3875	82.6875	2.01	0.59	Korba		
7	40.6375	109.7375	1.81	0.57	Baotou	Baotou	
8	21.0125	107.1375	1.80	0.42	Quang Ninh	Ha Long; Cam Pha	
9	−26.0875	28.9875	1.74	0.32	Kendal		
10	−32.4125	151.0125	1.73	0.30	Bayswater; Liddell		

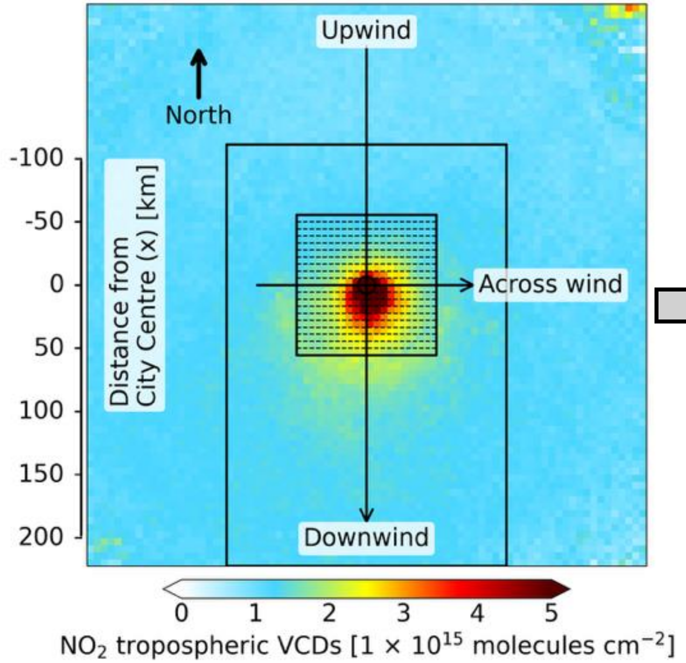
[Beirle et al., 2023]

Unregulated coal-fired power plants (Kriel, Matimba, Lethabo, Majuba, Kendal) and a synthetic fuels plant (Secunda)

Top-down Estimate of Hotspot NO_x Emissions

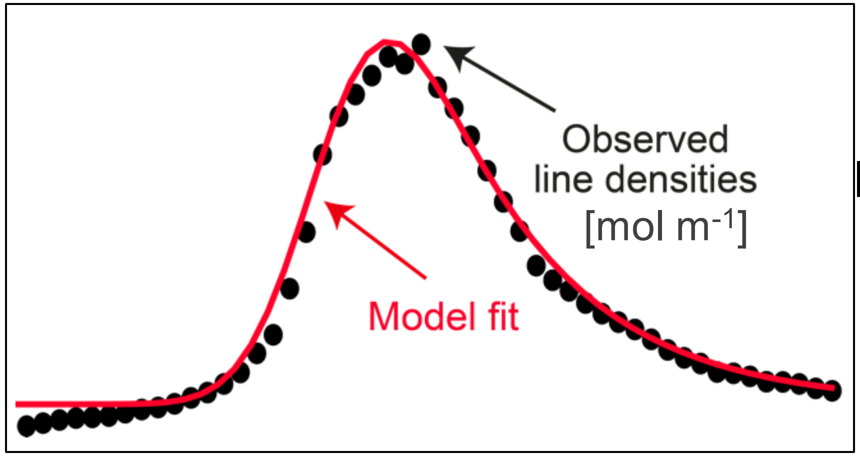
Derive NO_x emissions of isolated hotspots viewed by UV-visible space-based sensors

Wind rotated TROPOMI NO_2 over Lagos



Model fit to line densities to yield best-fit parameters

Across-wind sum of vertical columns



Lagos NO_x emissions and effective lifetime

28 mol NO_x s^{-1}

~3 h

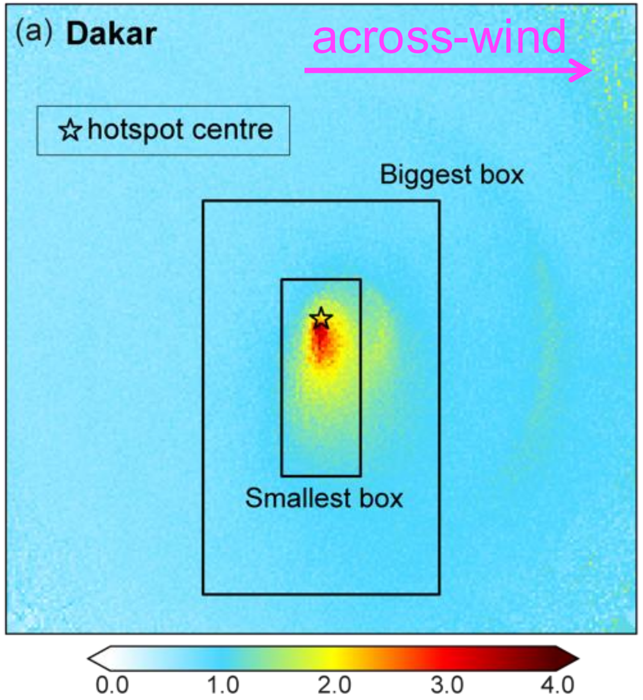
Target hotspots in understudied regions of the world:

Cities in South and Southeast Asia completed [Lu et al., 2025]

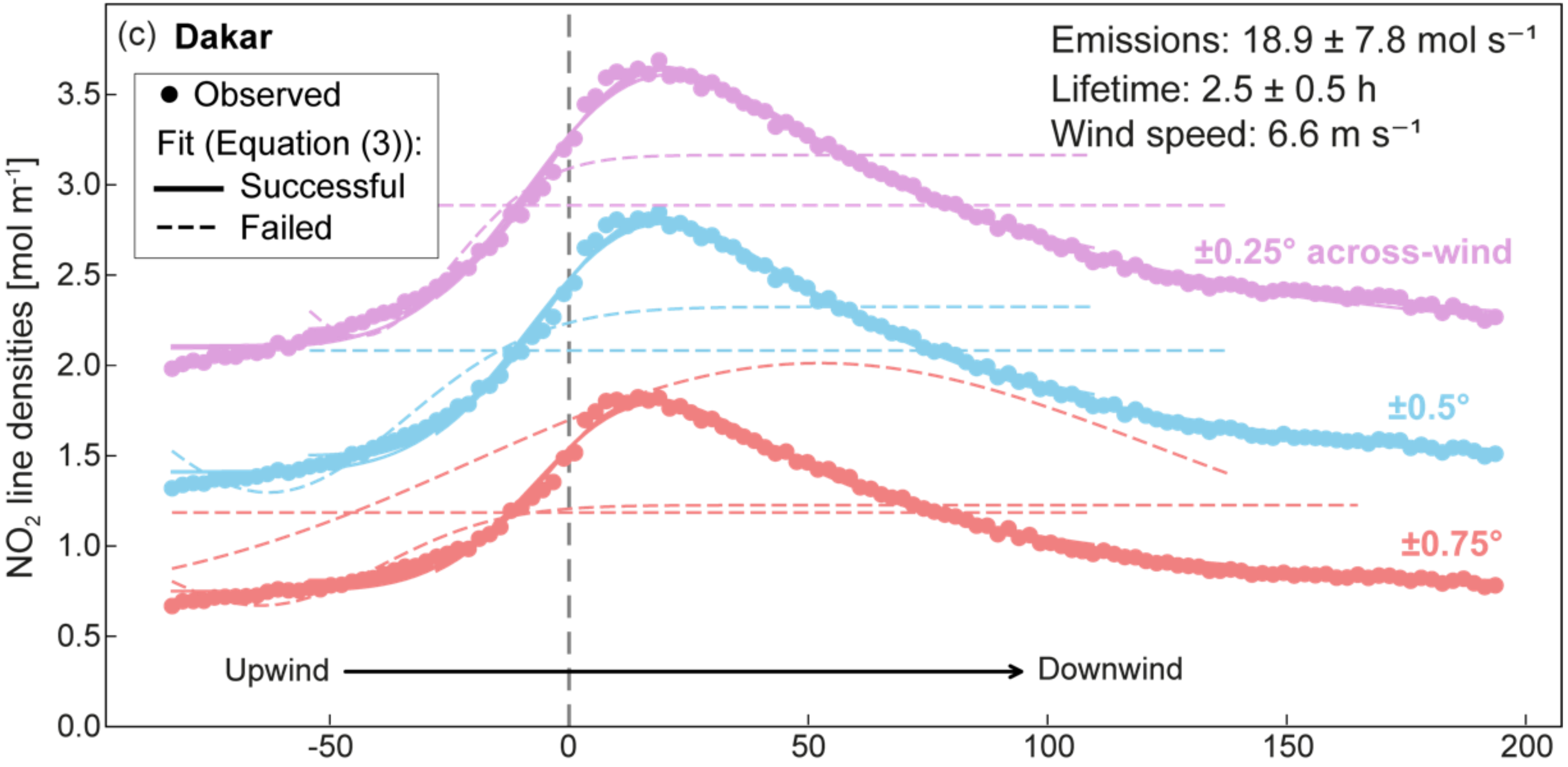
Hotspots in Sub-Saharan Africa in progress [Marais et al., *in prep*]

Hotspot NO_x Emissions Inversion Method

Wind rotate TROPOMI NO_2 about the hotspot centre



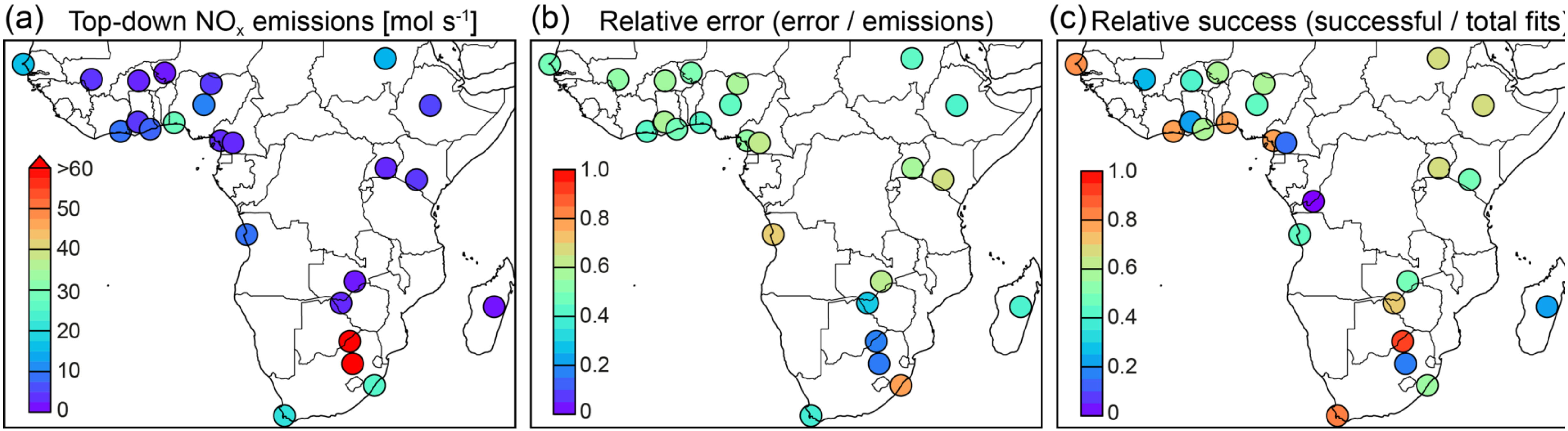
Sum across-wind NO_2 to yield 1D line densities and apply an Exponentially Modified Gaussian (EMG) fit



29 out of 36 successful fits for Dakar (Senegal) yielding the following quantities:

18.9±7.8 mol NO_x emitted s^{-1}, 2.5±0.5 h effective lifetime, 6.6 m s^{-1} wind speed

NO_x Emissions for All Successful Hotspots



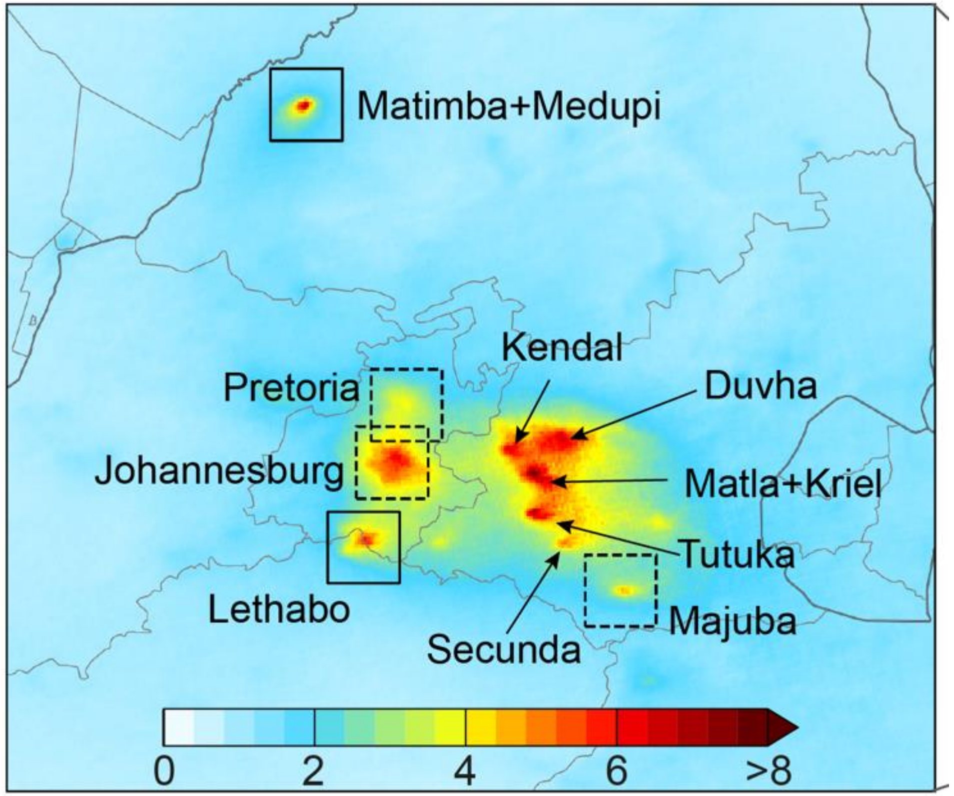
Derived emissions for 24 hotspots compared to at most 5 Sub-Saharan hotspots in past studies

Emissions total 207.3 kilotonnes NO

Most hotspots very small (<10 mol s^{-1}) sources of NO_x compared to urban hotspots in Southeast and Southeast Asia (> 60 mol s^{-1} for Delhi and Dhaka [Lu et al., 2025])

Are Power Plant Hotspot NO_x Emissions Accurate?

South Africa power plant emissions measured with Continuous Emissions Monitoring Systems (CEMS) (https://www.eskom.co.za/dataportal/emissions/ael/)



Matimba and Medupi:

CEMS: 74.1 mol s^{-1}

Top-down (this work): 69.8 ± 25.7 mol s^{-1}

Top-down (Beirle et al., 2023): 82.3 ± 18.7 mol s^{-1}

Lethabo:

CEMS: 65.2 mol s^{-1}

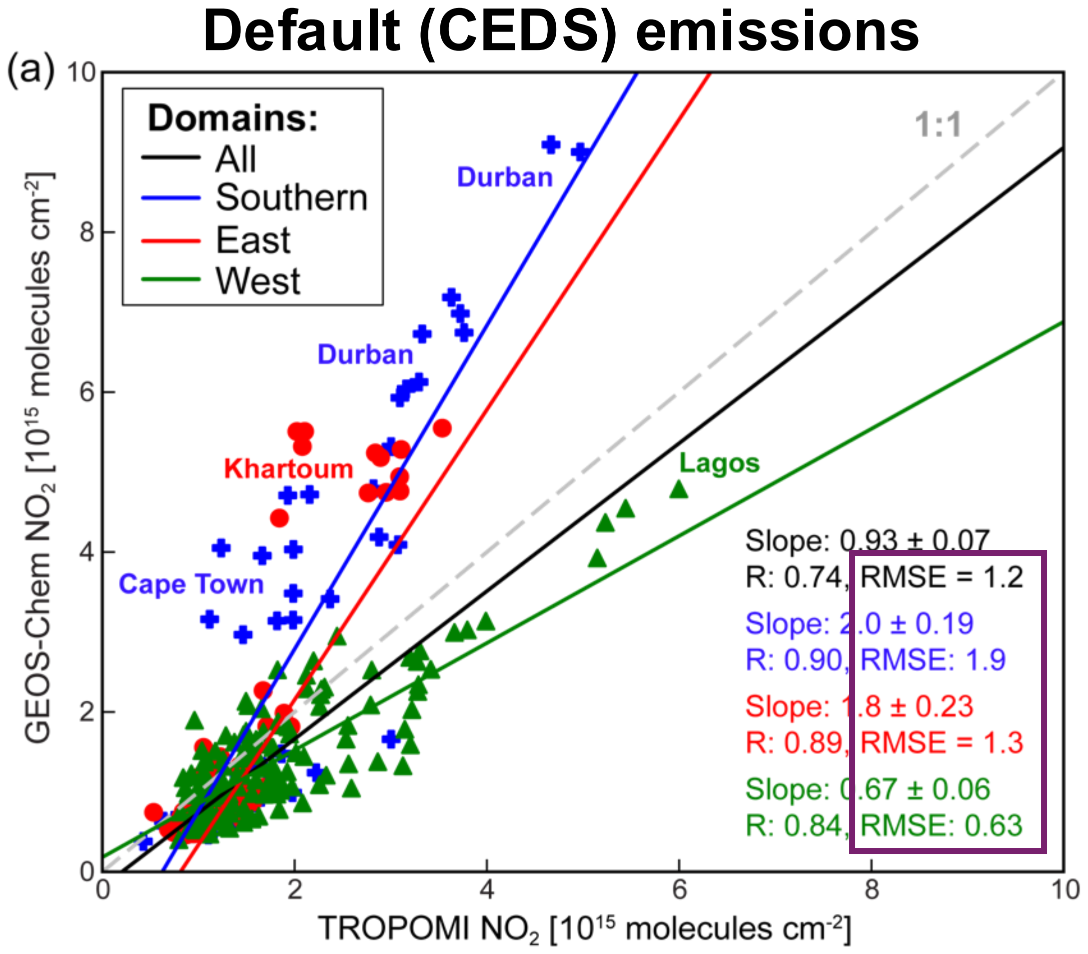
Top-down (this work): 70.4 ± 23.8 mol s^{-1}

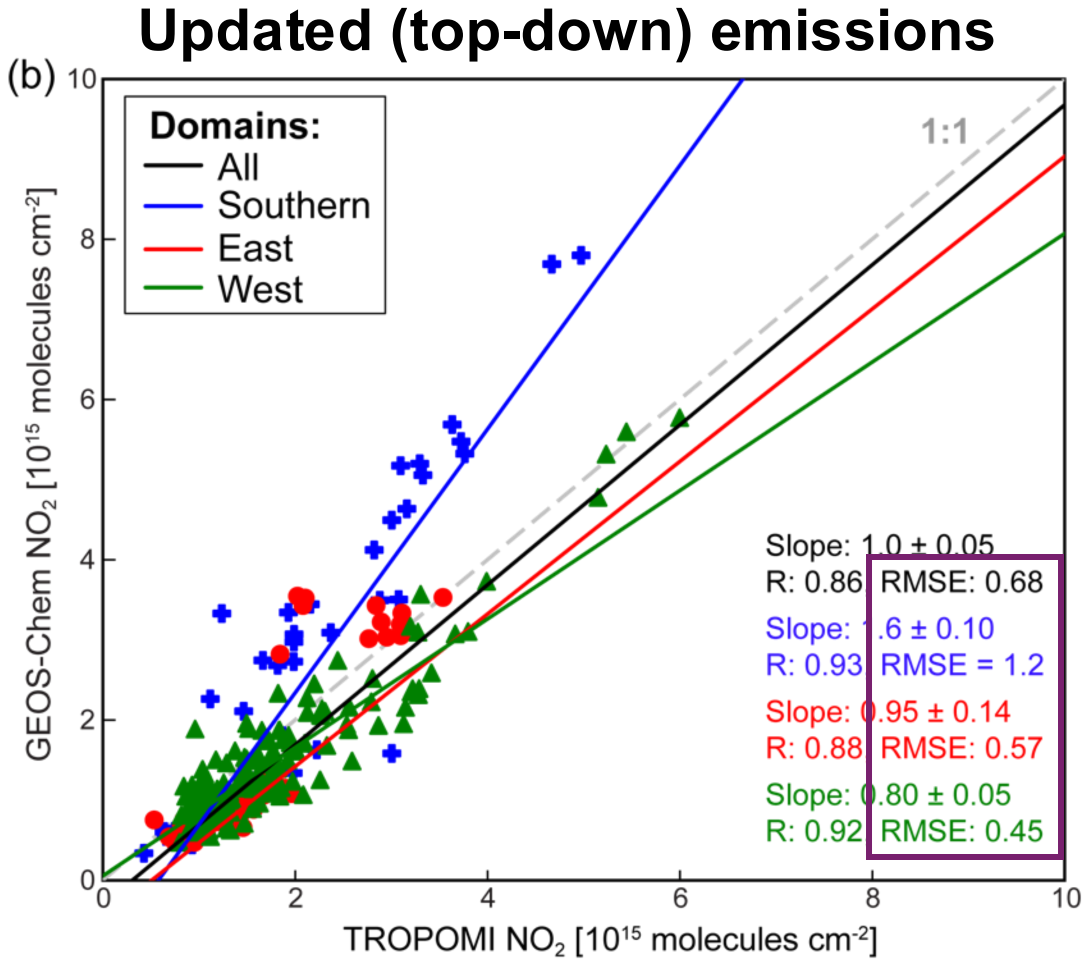
Top-down (Beirle et al., 2023): 67.7 ± 14.7 mol s^{-1}

Our values are within 18-20% of CEMS and within 4-15% of an alternate top-down approach

Are Urban Hotspot NO_x Emissions Accurate?

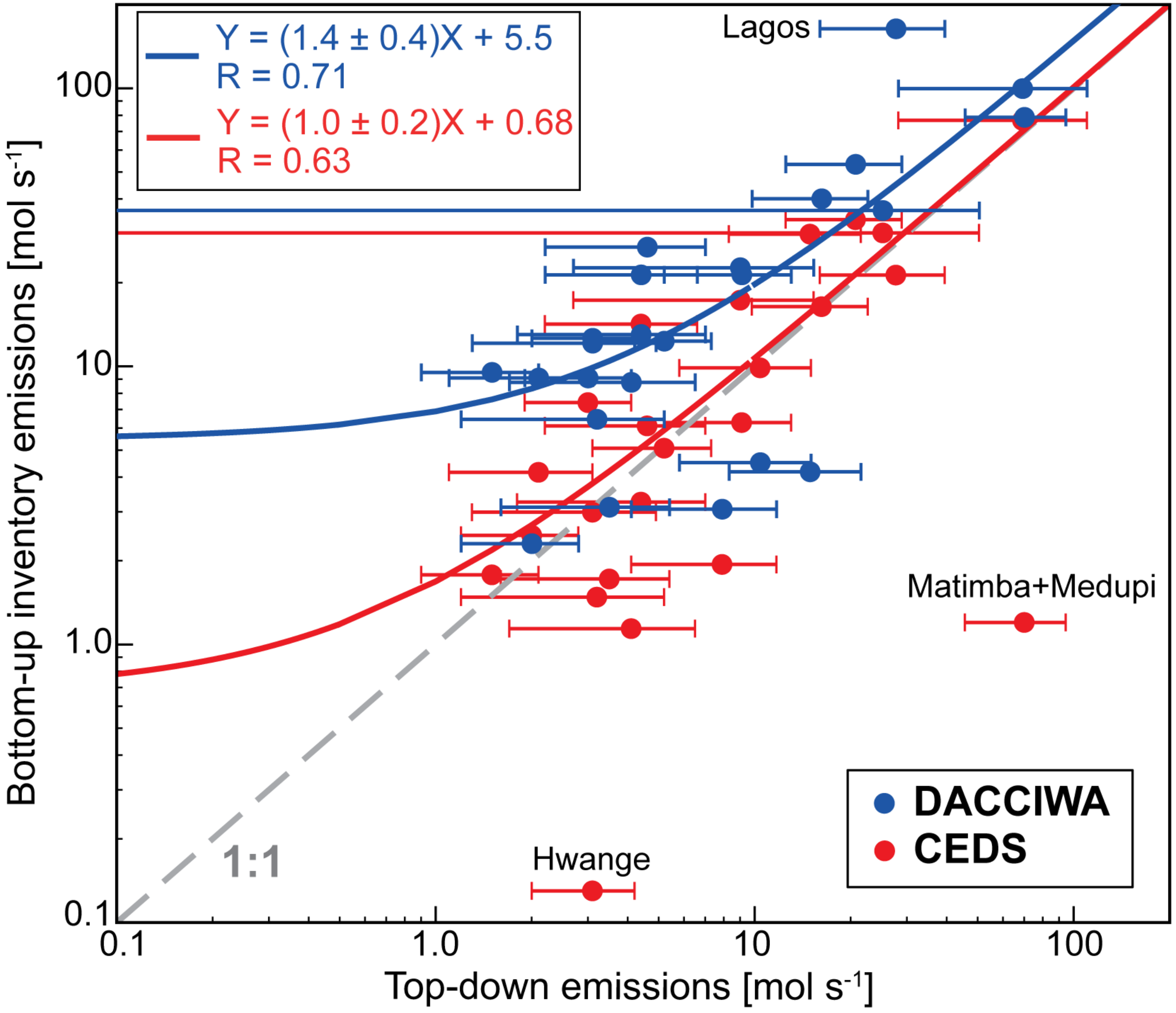
Emissions → GEOS-Chem → NO_2 column densities





Urban CEDS emissions total 159 kilotonnes NO, whereas top-down total 135 kilotonnes NO

Top-down versus inventory Hotspot NO_x Emissions



Comparison on log-log scale

DACCIWA: regional emissions inventory for Africa

CEDS: global emissions inventory widely used in models

<u>CEDS</u> on average consistent (slope = 1.0), but missing Medupi and Matimba power plants and underestimate Hwange power plant

<u>DACCIWA</u> on average 40% more than top-down emissions. Almost factor of 6 more for Lagos!

Closing Remarks / Recommendations

- Satellite-derived emissions are not necessarily truth and bottom-up false
- Top-down and bottom-up comparison can reinforce emissions estimates if consistent and direct future research if disagreements are large
- Use of a reliable, state-of-science chemical transport model is important
- Collaboration with satellite data providers is key for ensuring correct use of the data
- Critical to use independent, reliable observations where available. Where not available, the science community needs to be more accommodating! Otherwise, Africa-focused research will hardly be published!
- Where investment is feasible, ground-based observations for validating satellite observations should be a priority (surface concentrations or total column concentrations)
- Knowledge of hourly variability in emissions is needed to relate single time of day satellite overpass emissions to full day (24-hour) emissions