New insights on NO_x sources from the divergence of the mean NO_2 flux

Steffen Beirle, Christian Borger, Steffen Dörner, Adrian Jost, Thomas Wagner

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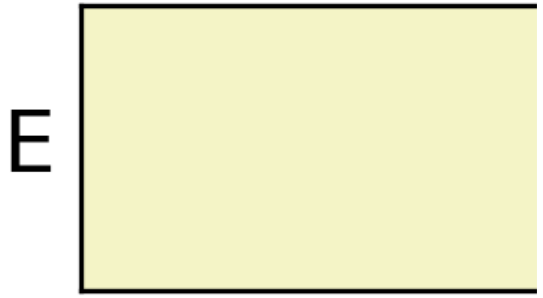
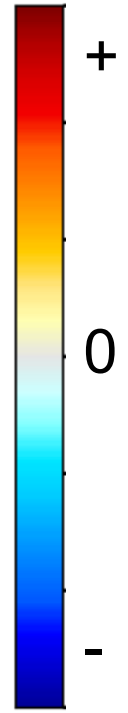
Synthetic data for illustration:

E: Emissions



Created by Symbolon
from Noun Project



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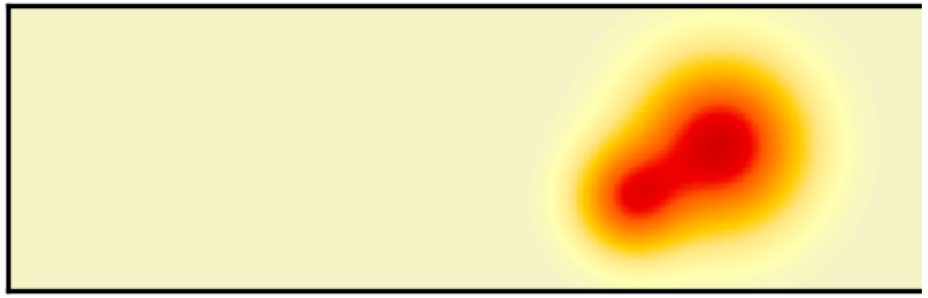

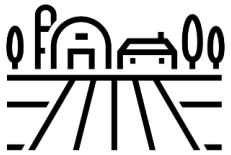

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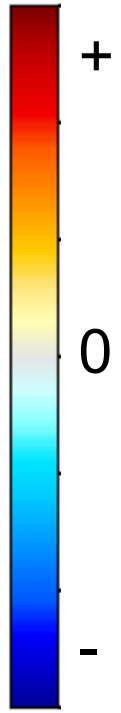

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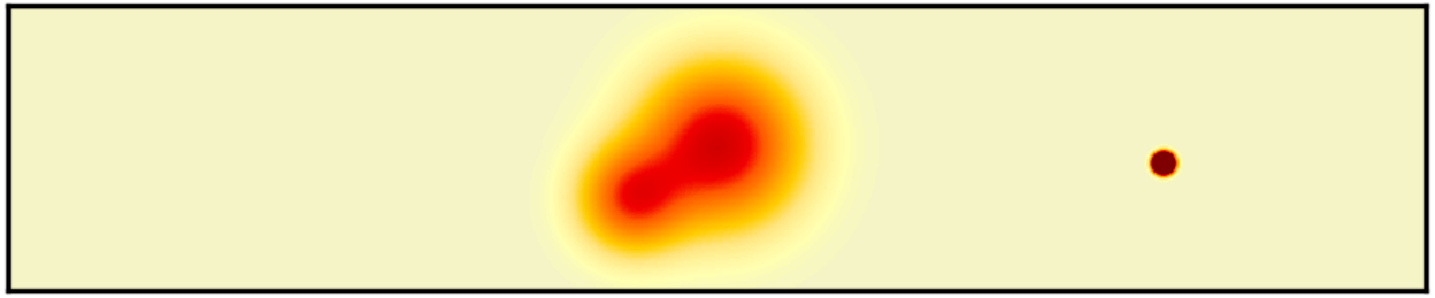

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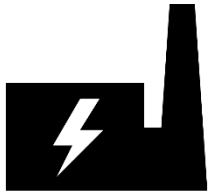

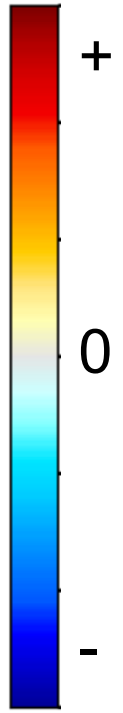

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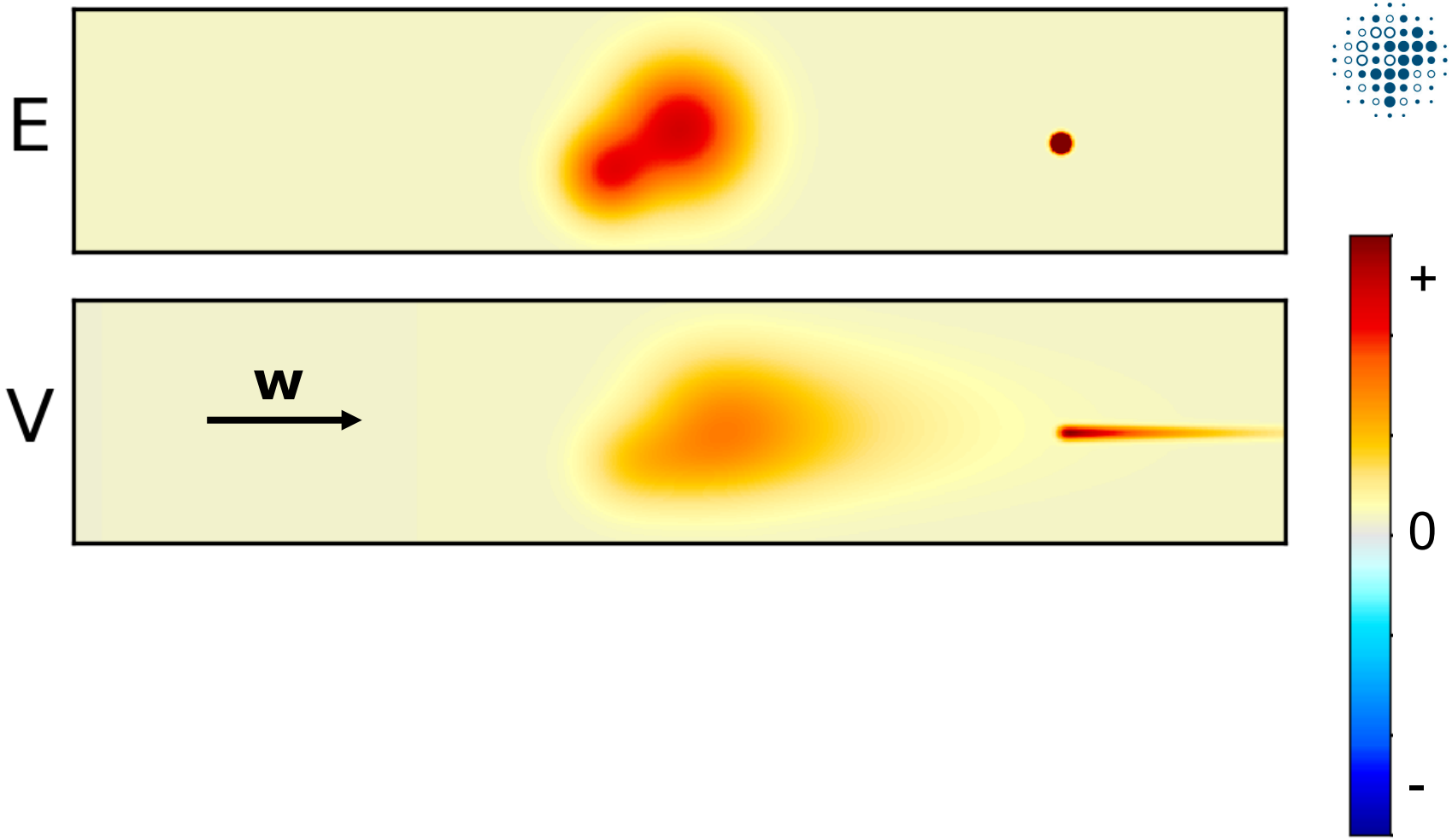

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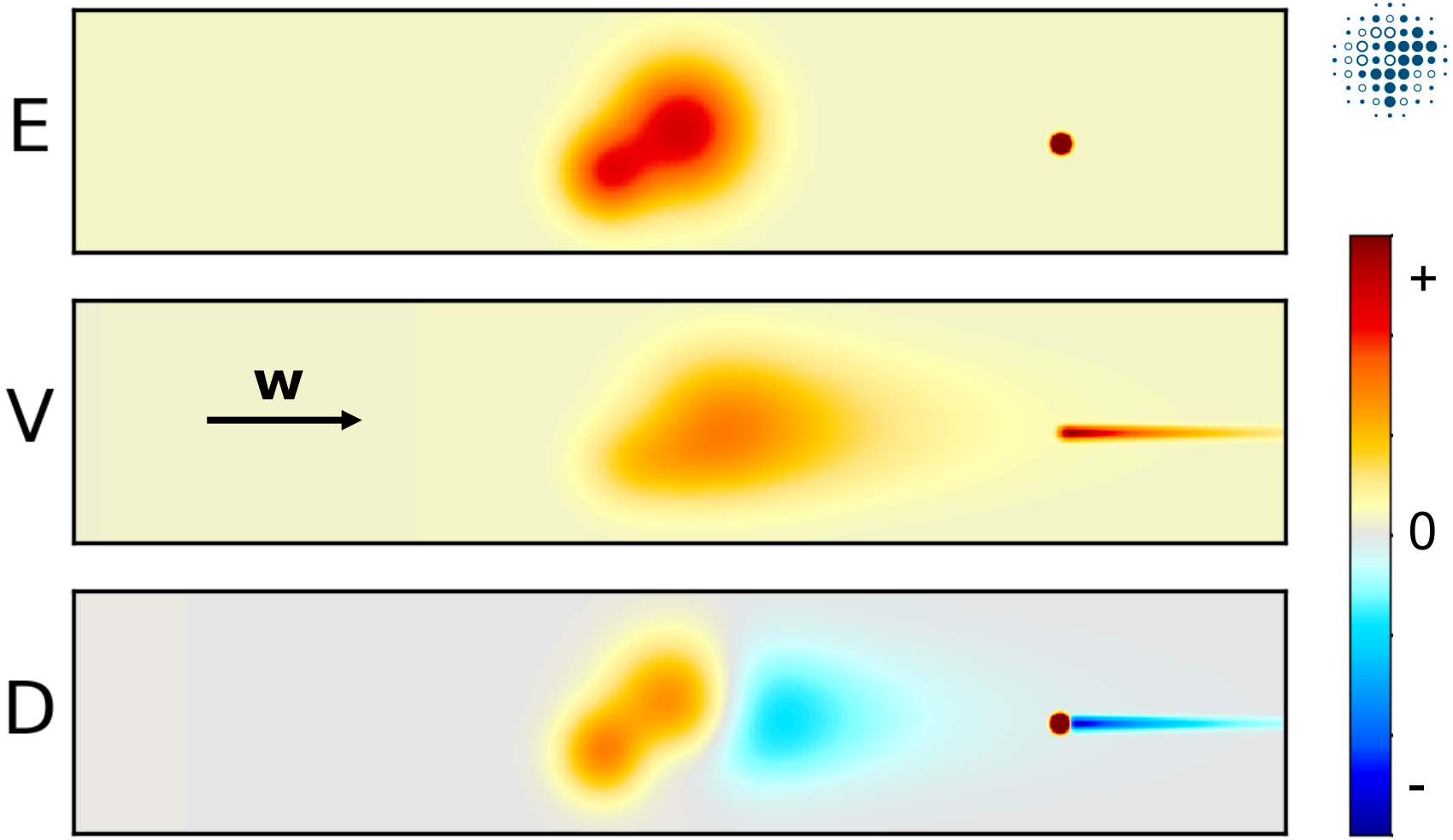
Divergence



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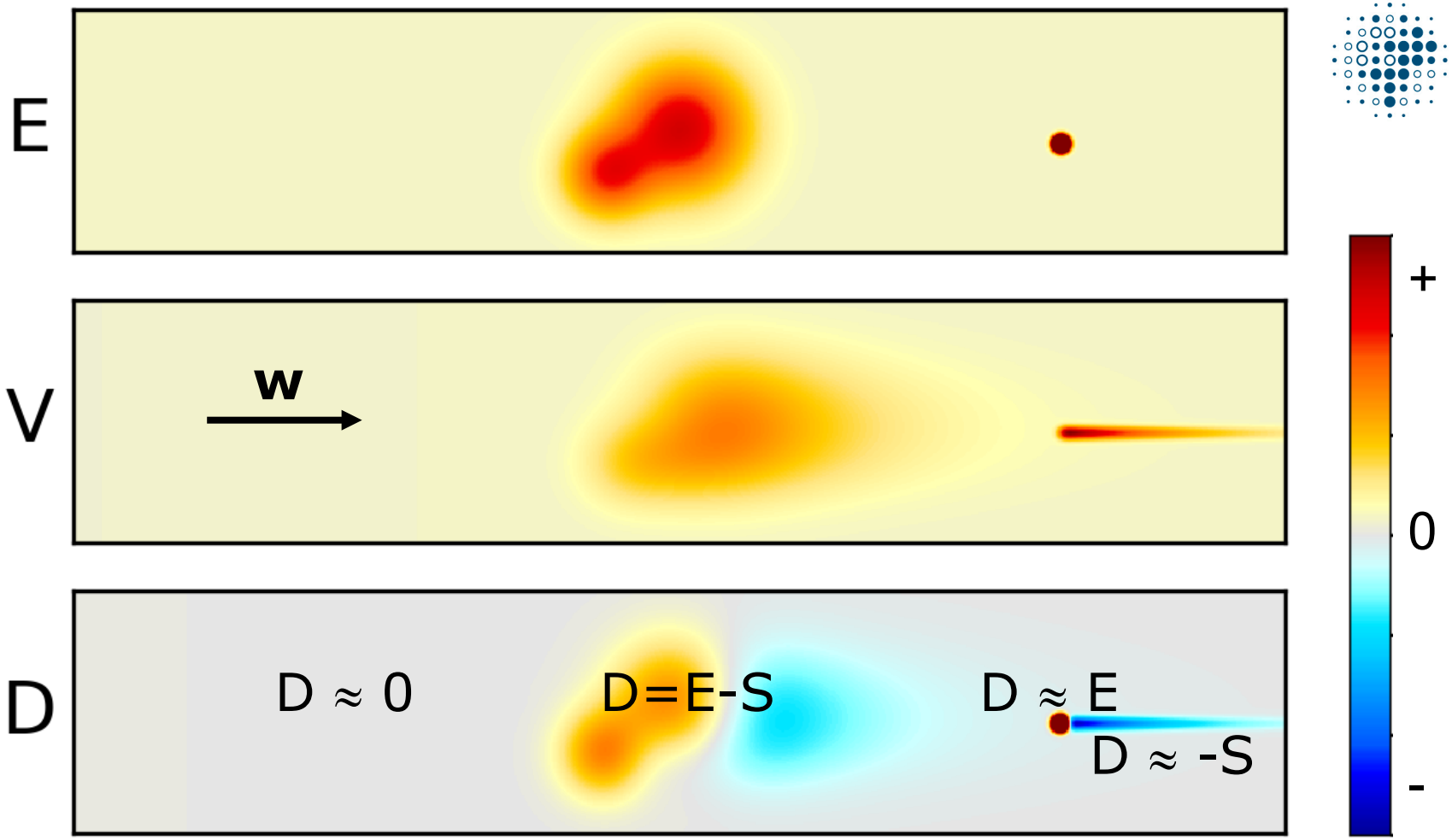

Steady state:
D = E - S
S: Sinks
S = V/τ
E = D + S

Synthetic data for illustration:

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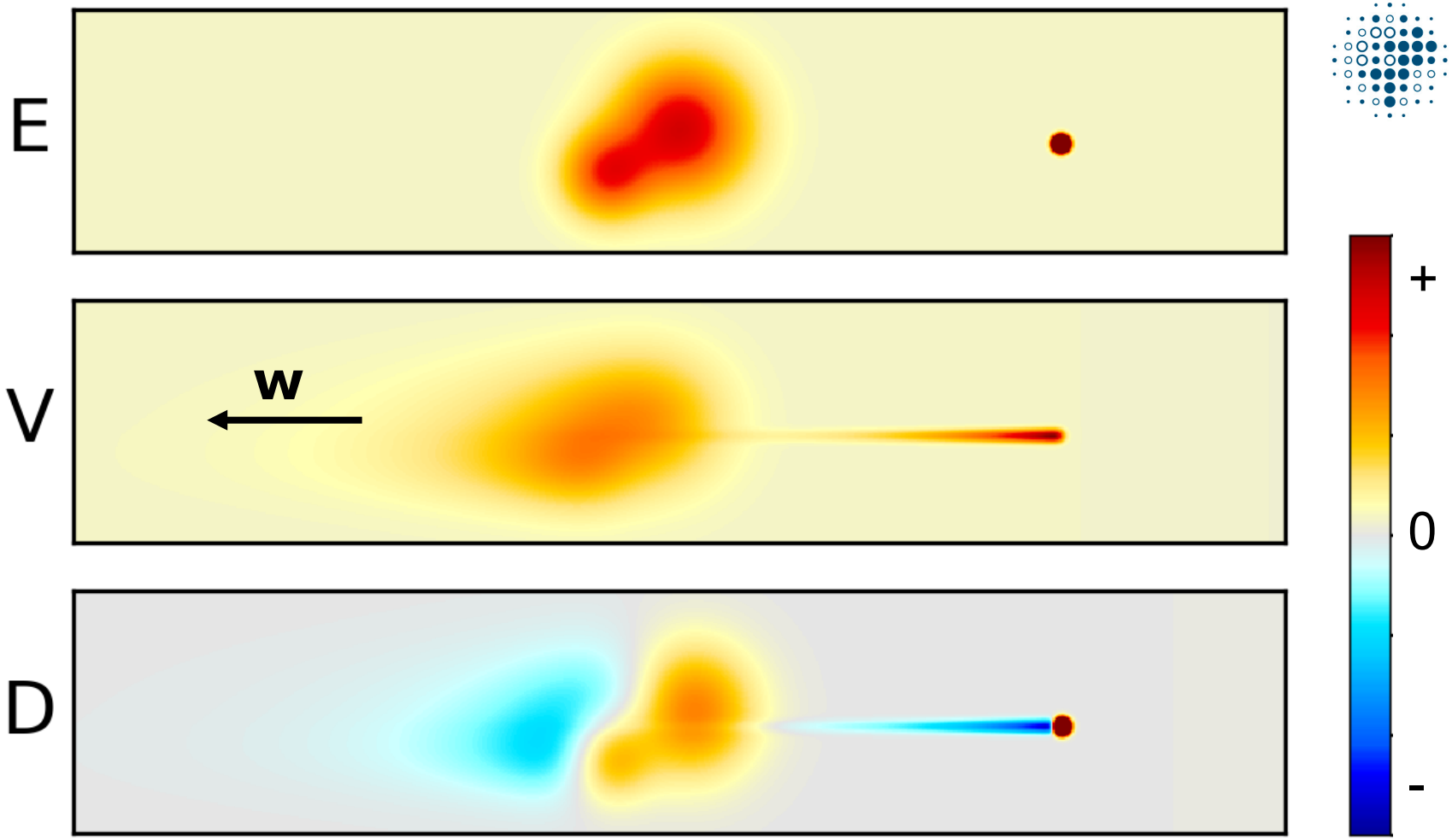

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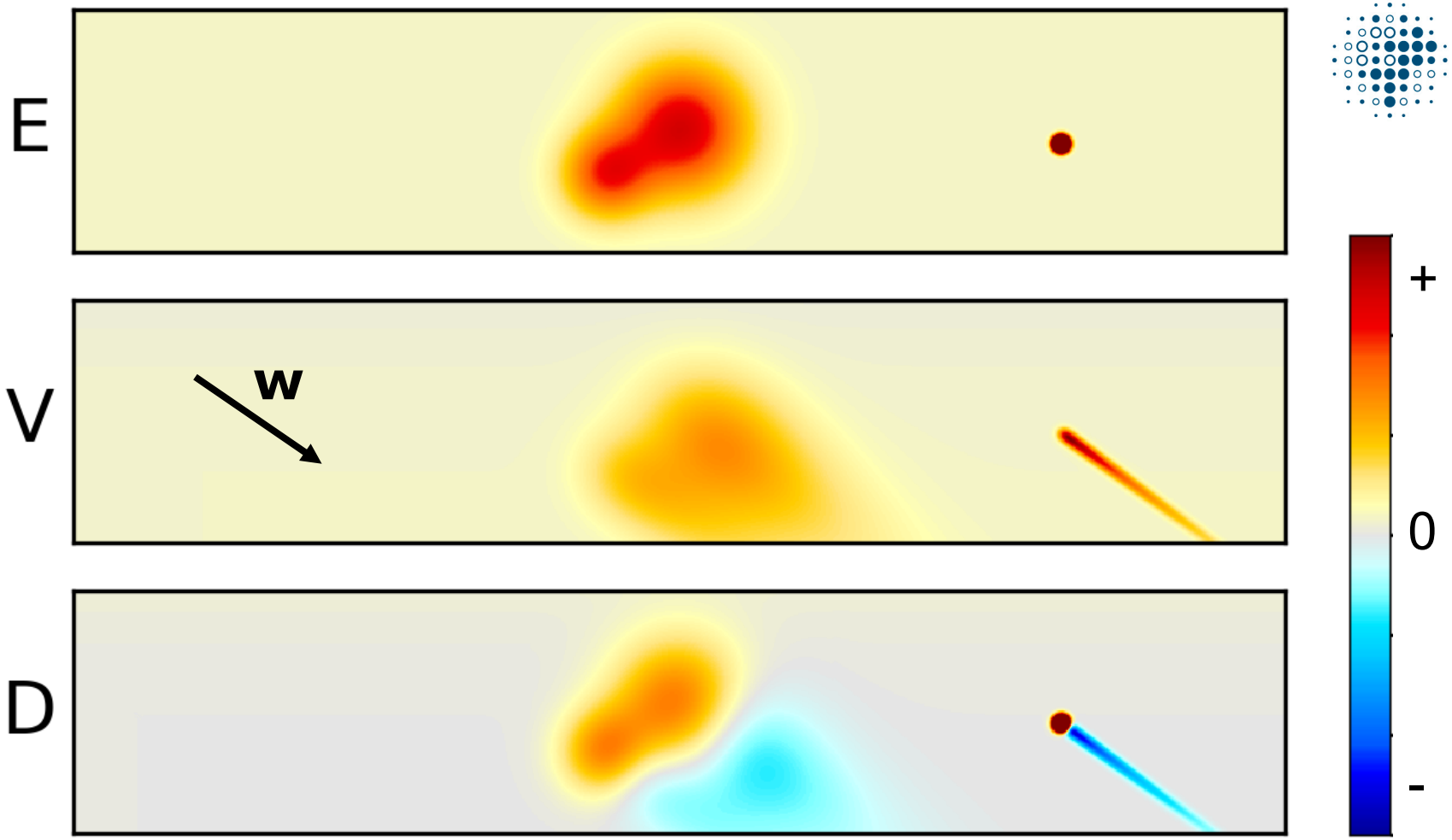

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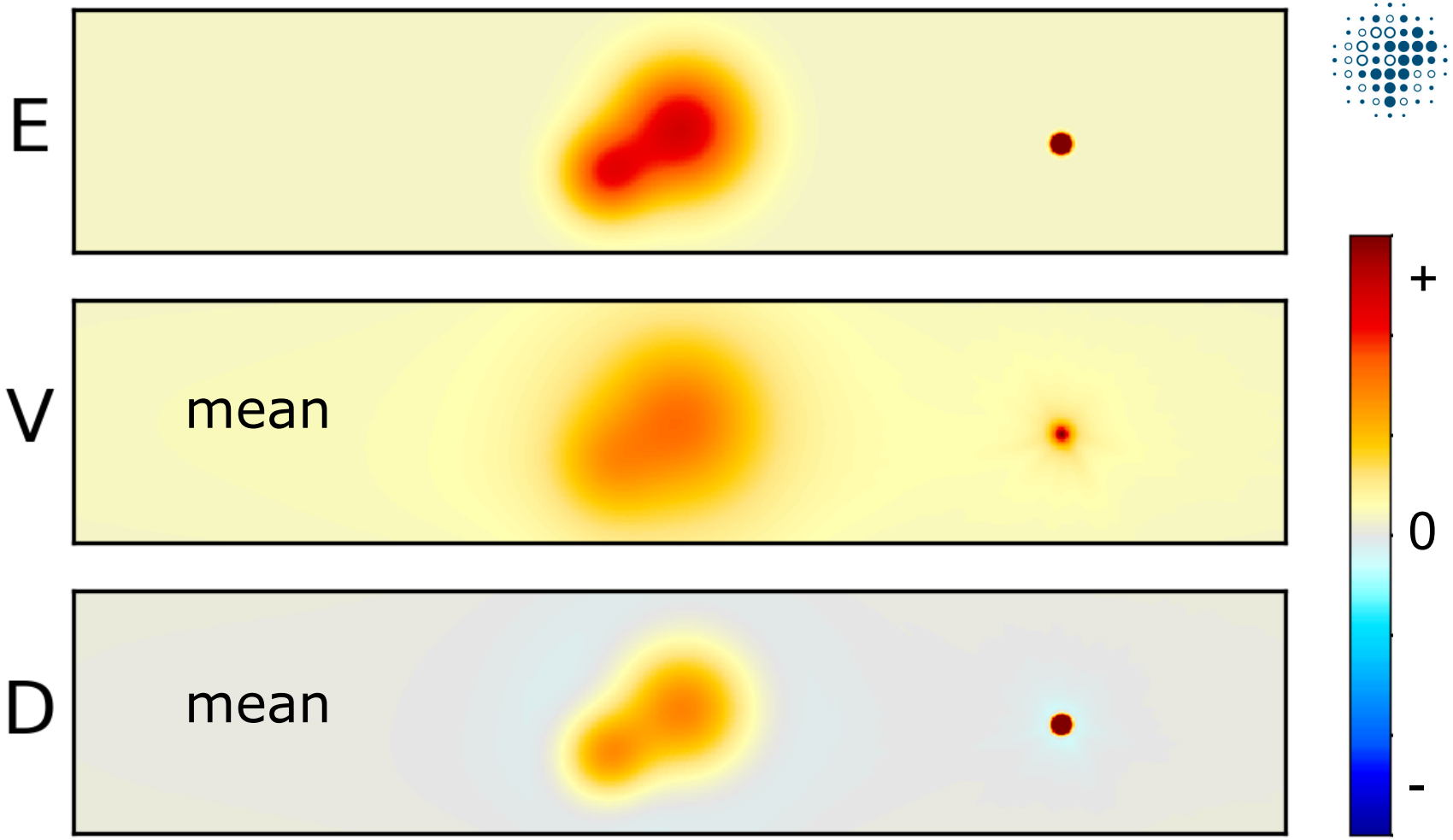

Steady state:
D = E - S
S: Sinks
S = V/τ
E = D + S

Reality is more complex:

- Turbulence & diffusion
- τ might change with downwind distance
- 3rd dimension: **w** and τ change with altitude
- No steady state: **w**, E, τ... change with time

Not critical for point sources!

SCIENCE ADVANCES | RESEARCH ARTICLE

ATMOSPHERIC SCIENCE

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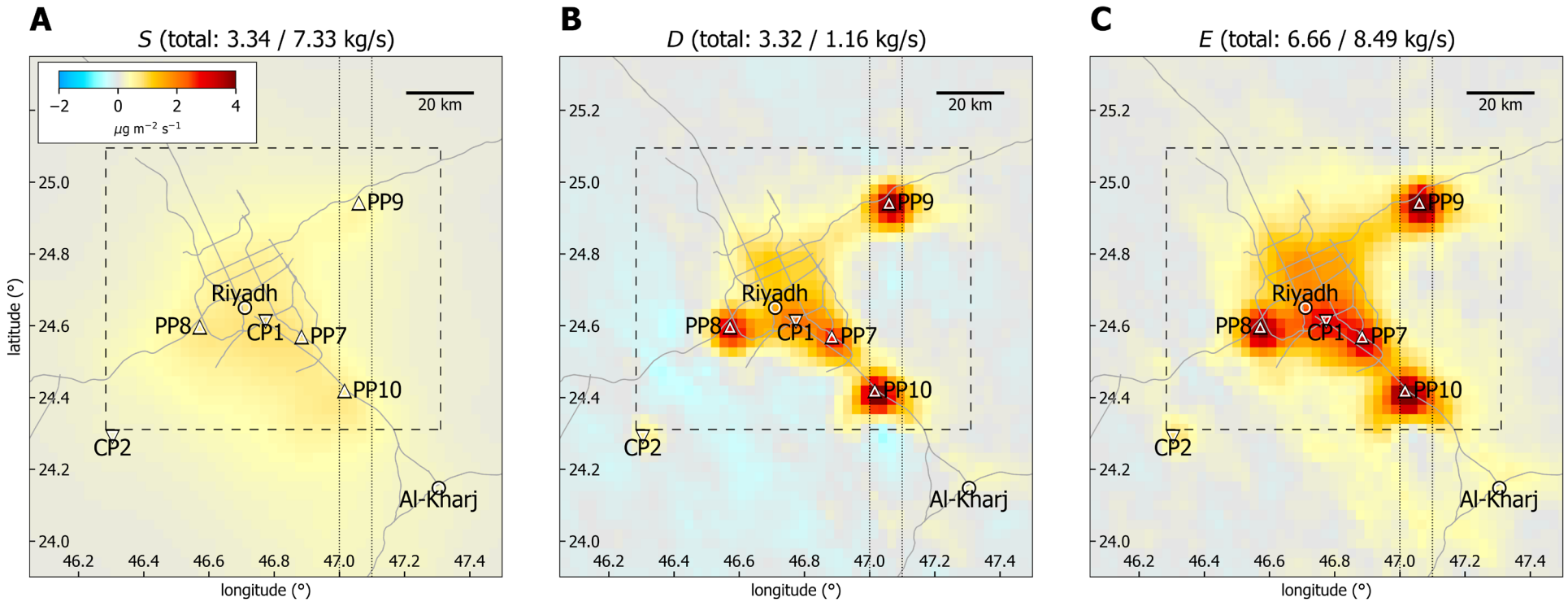
Pinpointing nitrogen oxide emissions from space

Steffen Beirle[1]*, Christian Borger[1], Steffen Dörner[1], Ang Li[2], Zhaokun Hu[2], Fei Liu[3,4], Yang Wang[1], Thomas Wagner[1,5]

Beirle *et al.*, *Sci. Adv.* 2019;**5**:eaax9800 13 November 2019

Riyadh

$S = V/\tau$ $D = \nabla (V\mathbf{w})$ $E = S + D$



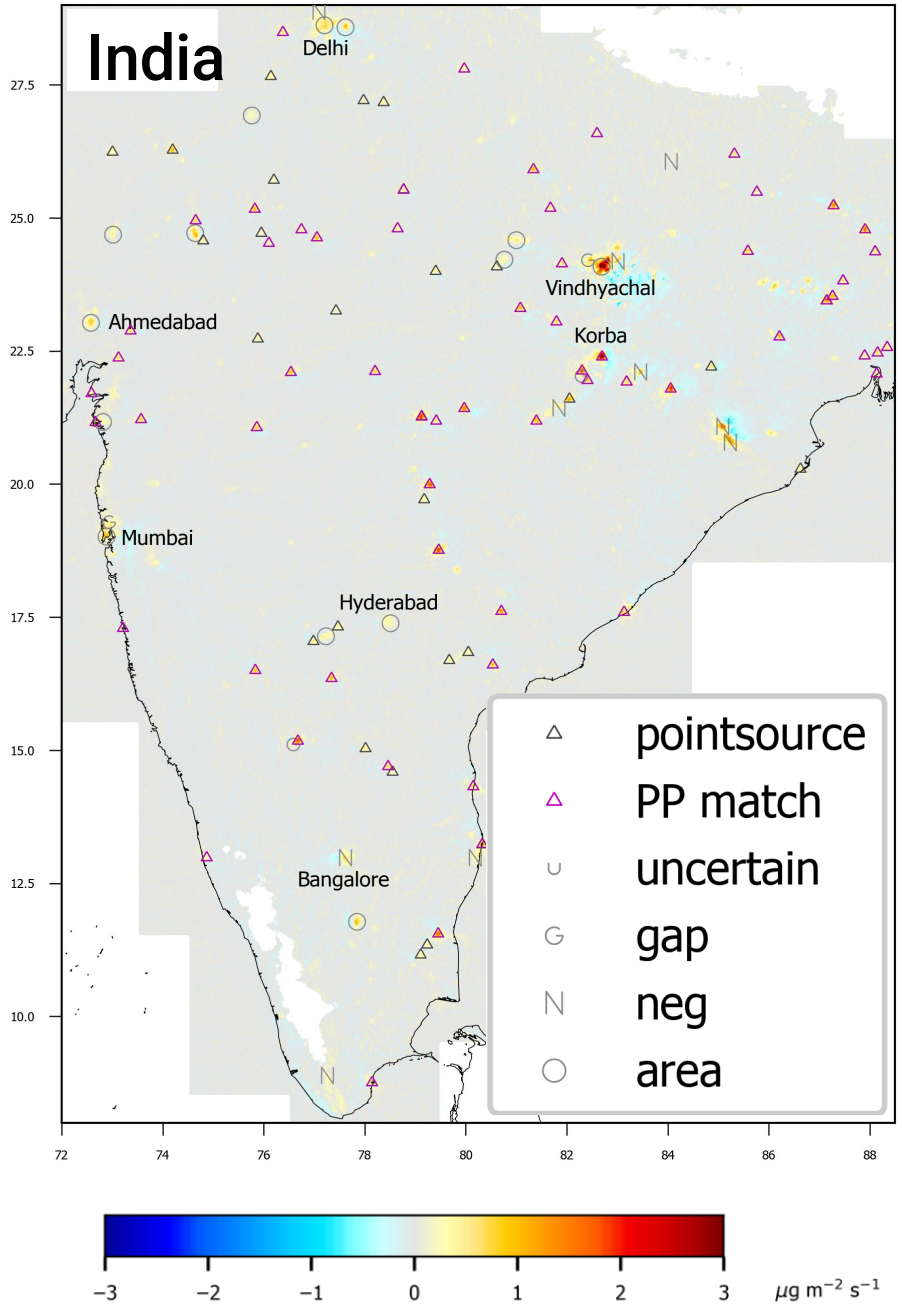
Catalog of NO_x emissions from point sources as derived from the divergence of the NO_2 flux for TROPOMI

Steffen Beirle[1], Christian Borger[1], Steffen Dörner[1], Henk Eskes[2], Vinod Kumar[1], Adrianus de Laat[2], and Thomas Wagner[1]

https://doi.org/10.5194/essd-13-2995-2021

Open Access Earth System Science Data

- 451 point sources detected by fully automated algorithm
  (power plants, cement plants, metal smelters, industrial areas, small cities)
- For 242 point sources:
  match in Global Power Plant Database within 5 km



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Open Access Earth System Science Data

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- Catalog lists NO_x point sources worldwide
- High accuracy of point source location

Remaining issues:

1. Catalog is incomplete:
   - Persistent gaps in input data
   - Noise in divergence / sampling issues, particularly for regions with frequent cloud cover
   - Systematic artefacts (input wind fields / mountains)
2. Emissions are biased low:
   - Missing lifetime correction
   - Wrong a-priori profile

A lot to be improved…

Towards v2 of the NO_x catalog: Applied and planned improvements (wip)

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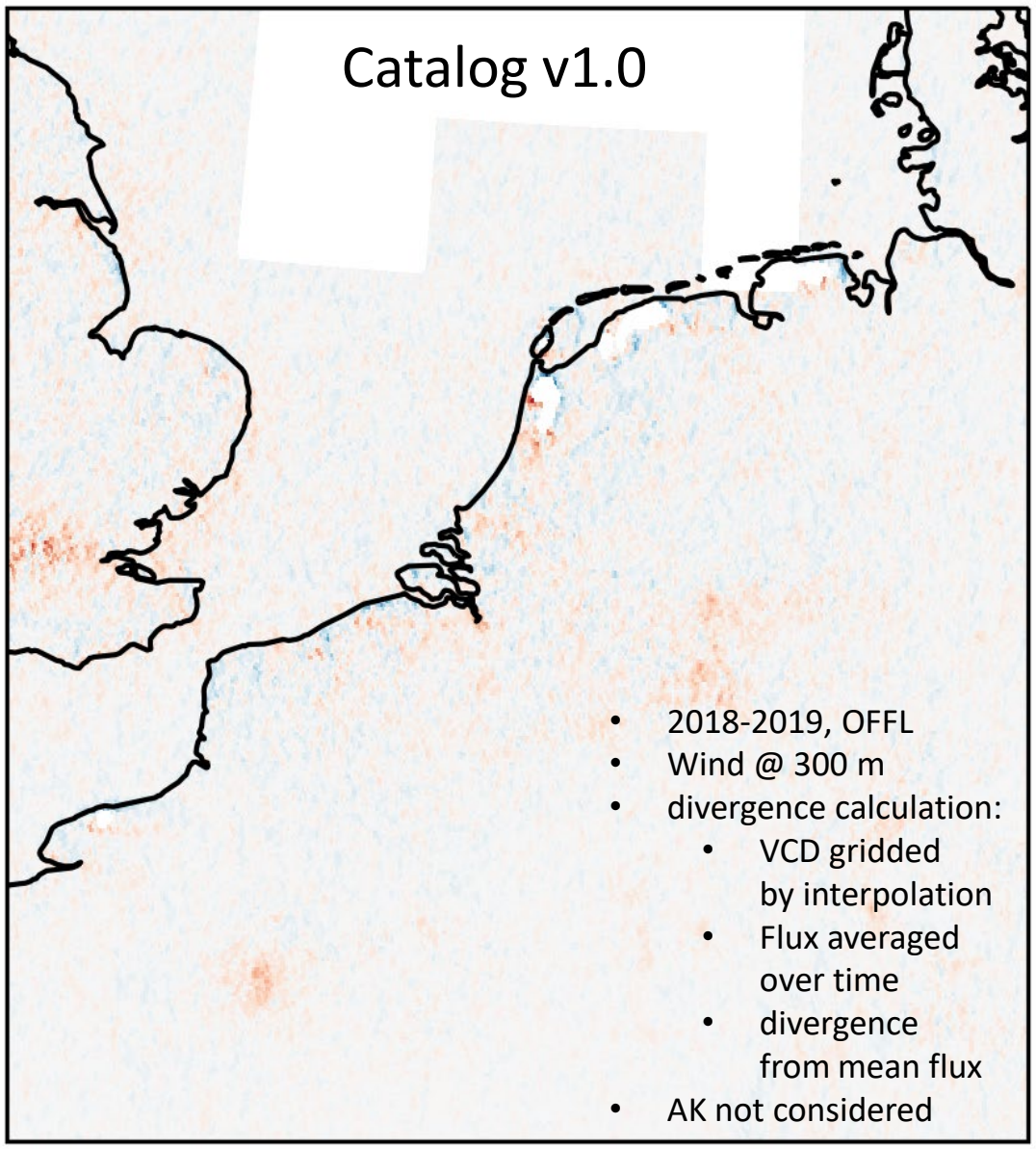
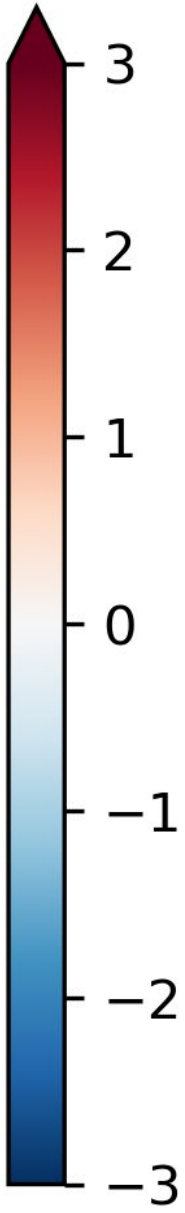
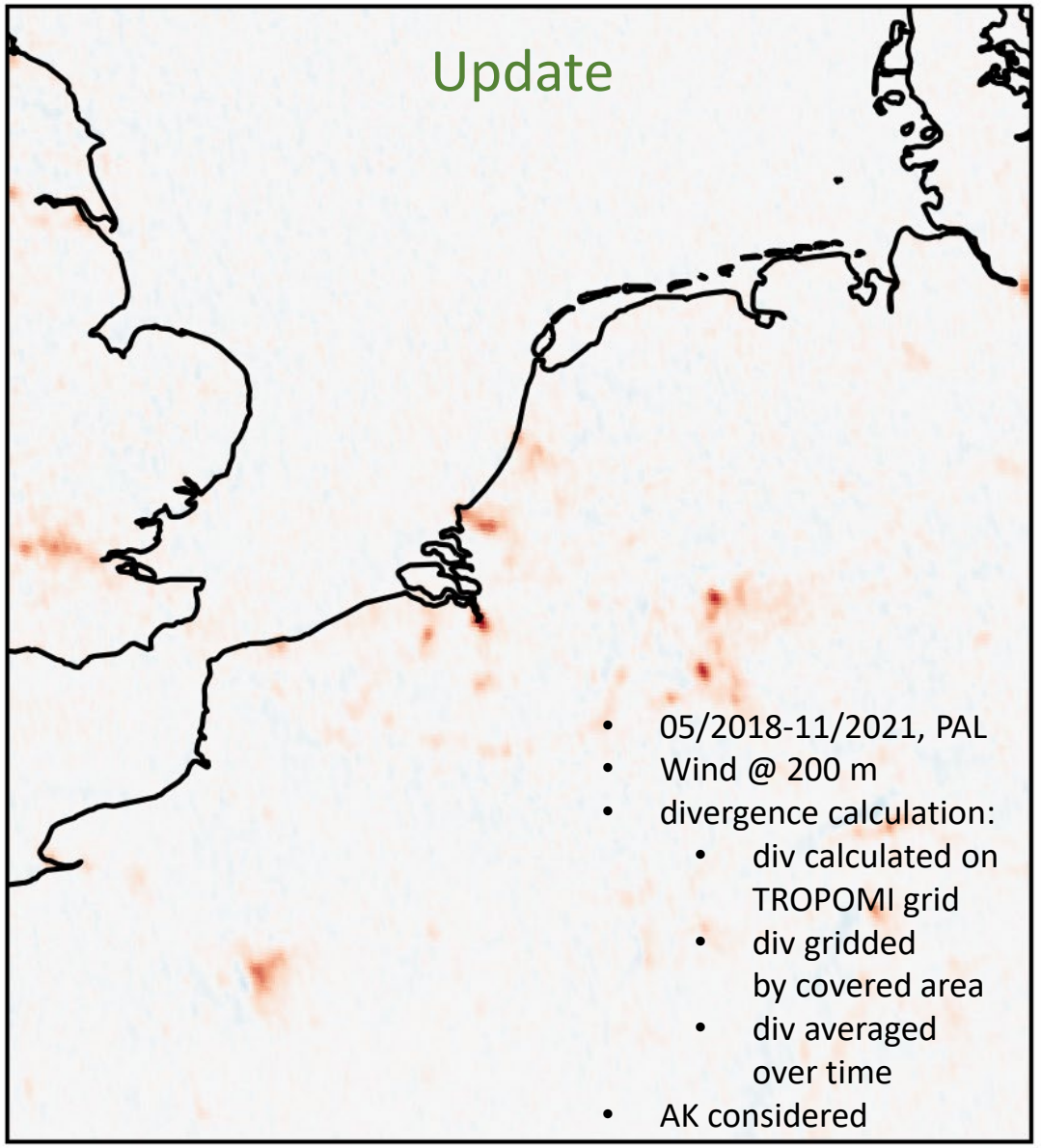
1. Catalog is incomplete:
   - Persistent gaps in input data
   - Noise in divergence / sampling issues, particularly for regions with frequent cloud cover
   - Systematic artefacts (input wind fields / mountains)

Update (wip):

- Use reprocessed data (PAL)
- Calculate divergence on TROPOMI grid (de Foy et al., 2022)
- Use high-res wind fields (not yet done – straightforward, but expensive)







Divergence [μg m^{-2} s^{-1}]

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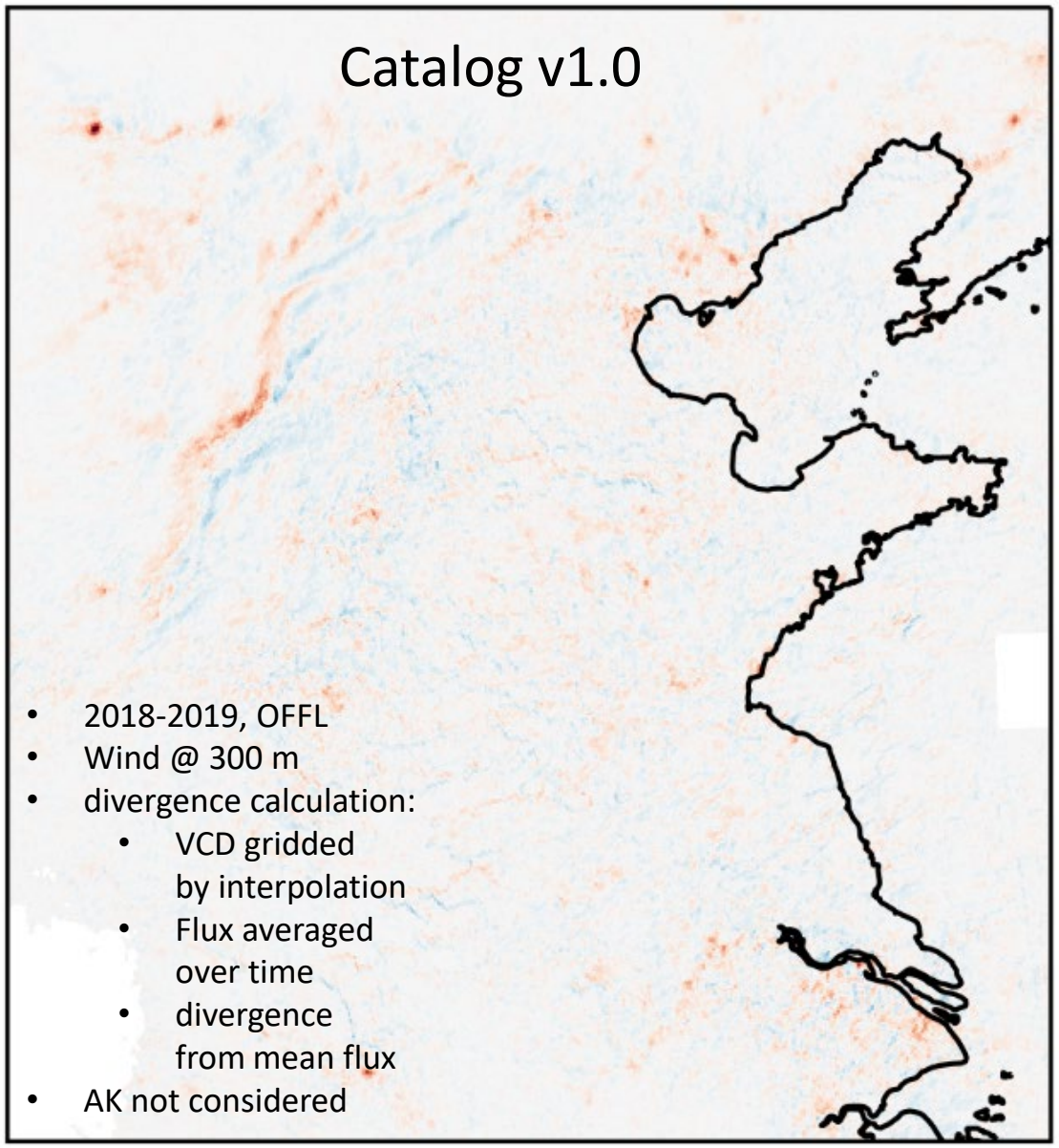

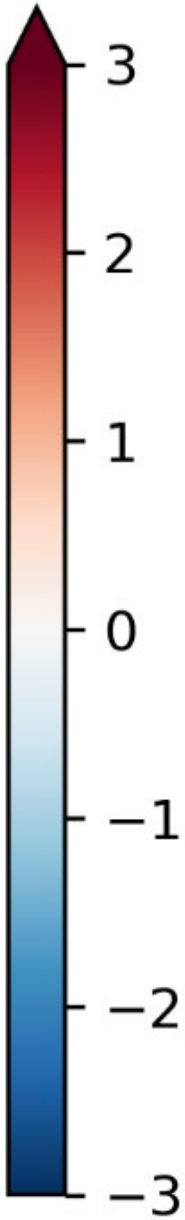

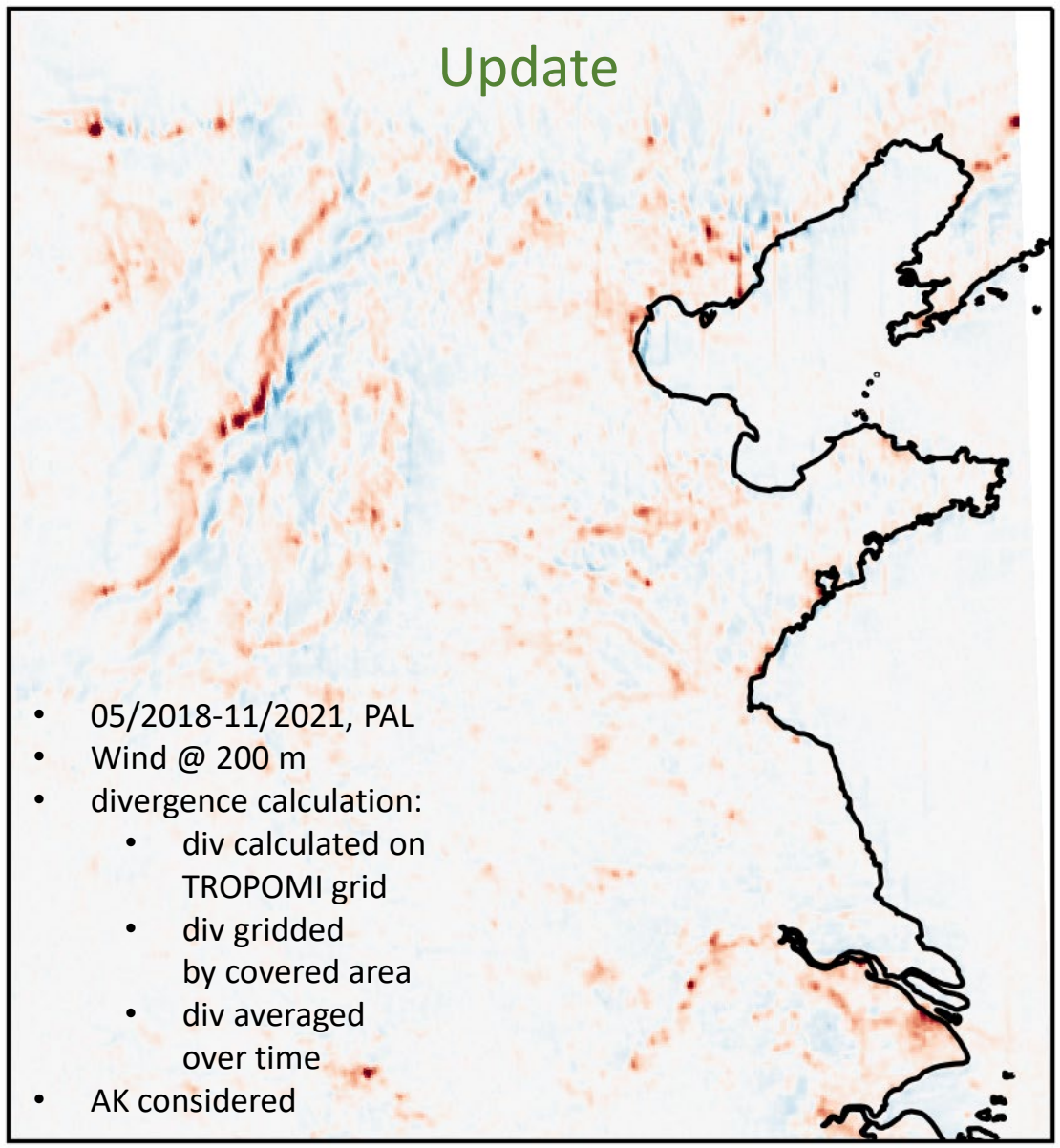

Divergence [μg m^{-2} s^{-1}]

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Towards v2 of the NO_x catalog: Applied and planned improvements (wip)

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2. Emissions are biased low:
   - Missing lifetime correction
   - Wrong a-priori profile

A-priori vertical profile

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- Needed for the calculation of air-mass factors
- Generally:
  - Complex
  - Not represented appropriately by global model on relatively coarse spatial resolution
- VCD can be corrected for actual profile via provided averaging kernels (AKs)

Synthetic data for illustration:

E: Emissions

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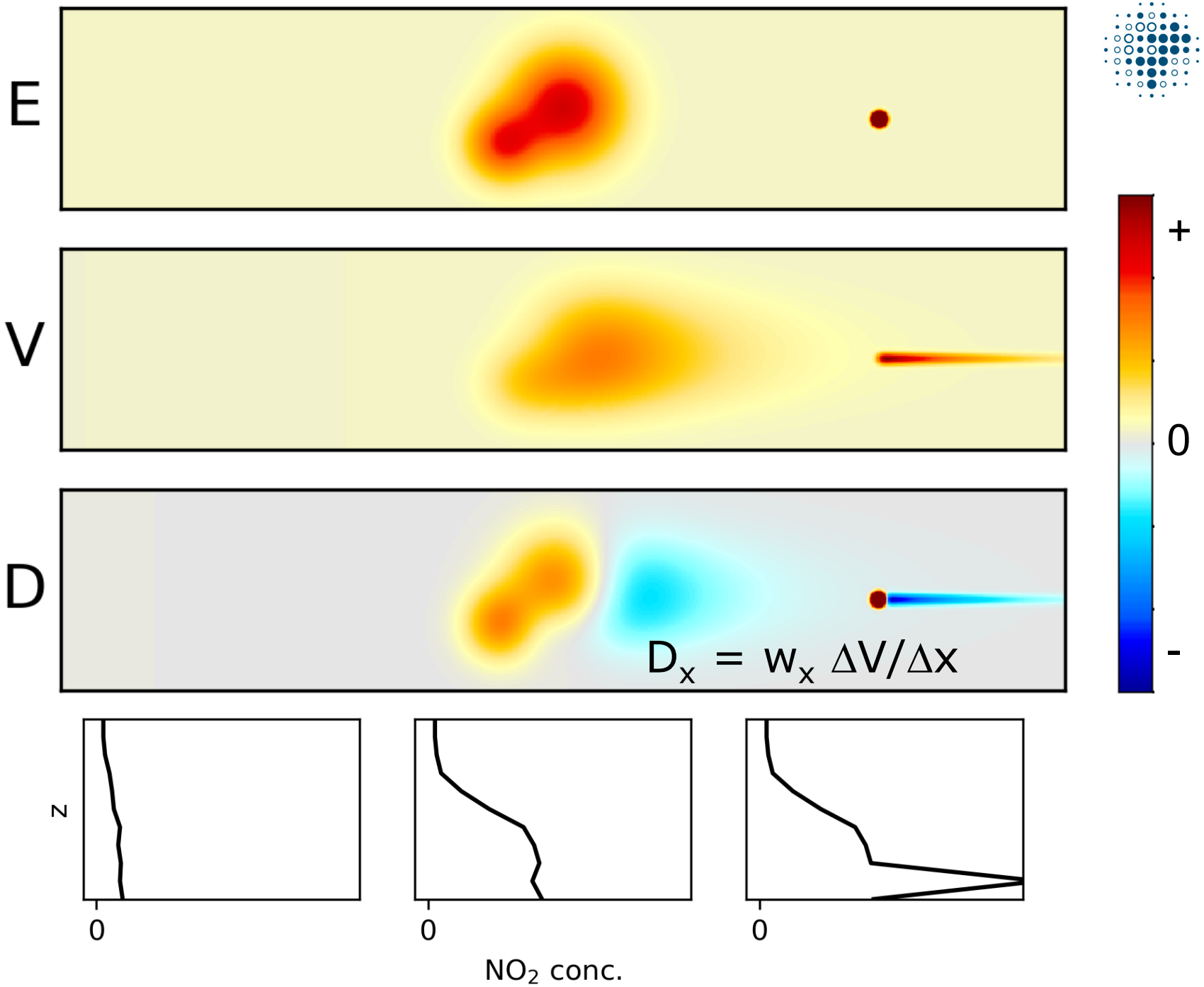
F = **w**·V : Flux

D = ∇·**F** :
Divergence

For correct V:
NO_2 profile required
(complex!)



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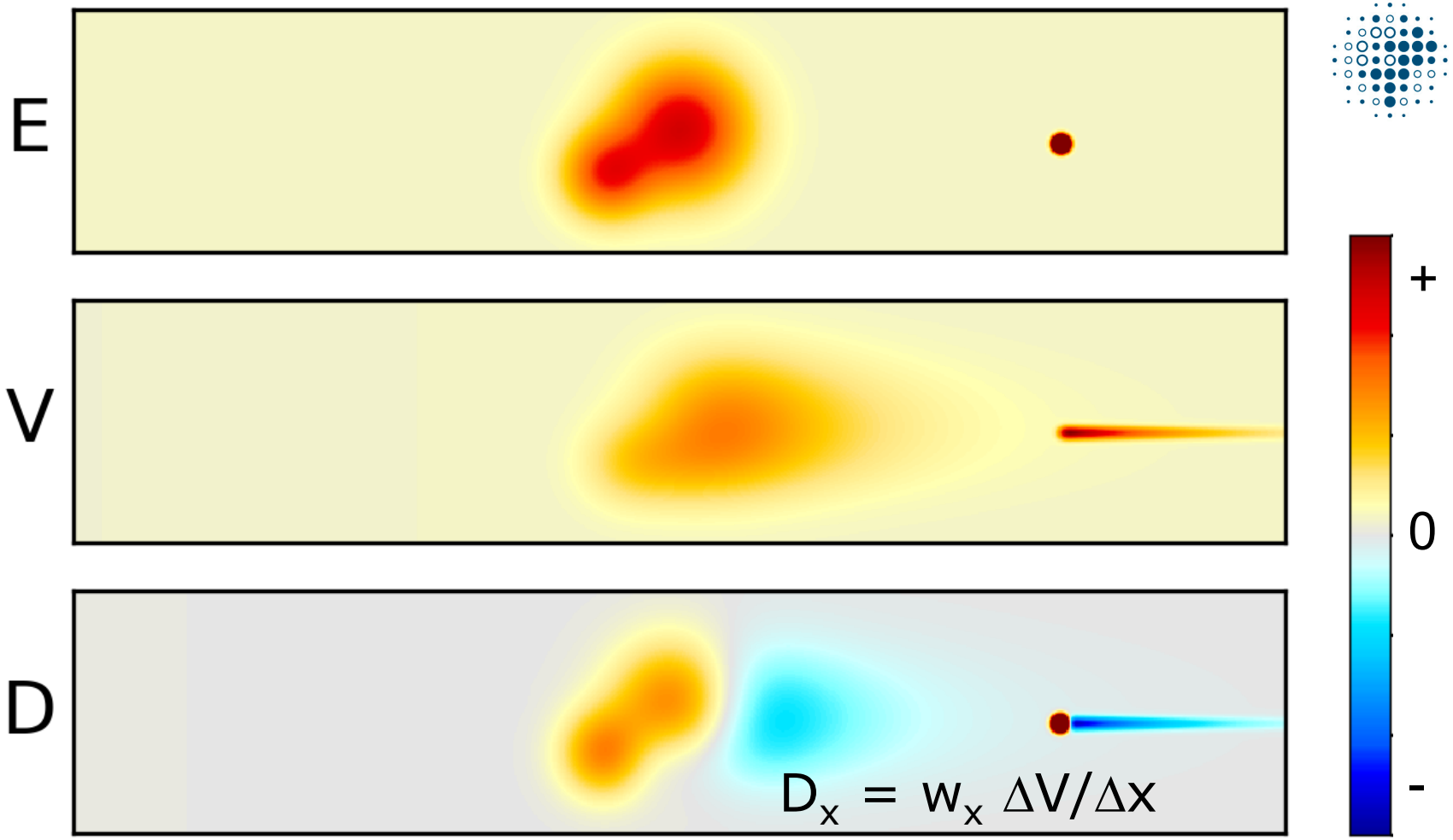
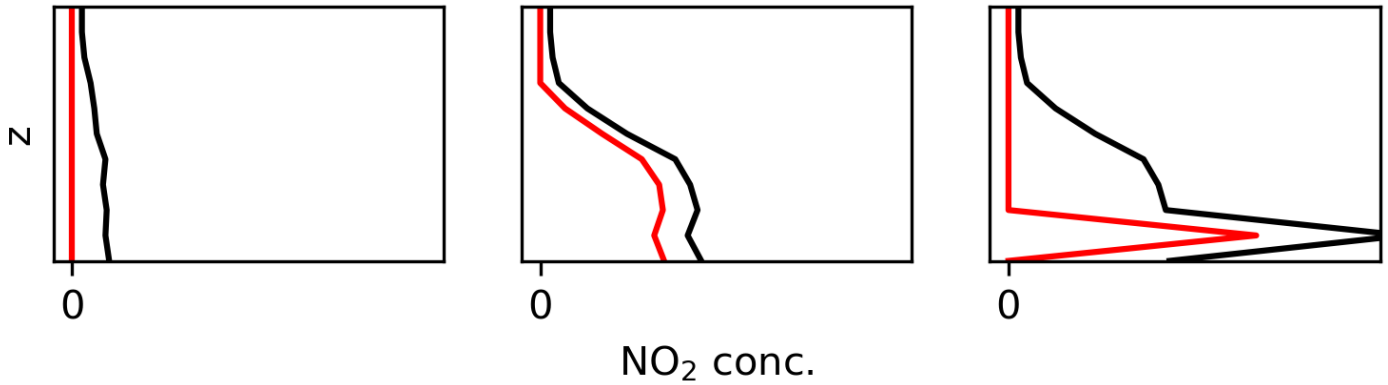


For correct V:
NO_2 profile required
(complex!)



For correct D:
NO_2 *excess* profile required
(simple!)

Towards v2 of the NO_x catalog: Applied and planned improvements (wip)

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2. Emissions are biased low:
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Update (wip):

- Apply lifetime correction
- Apply AK correction

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Emissions in kg/s

Power plant	EPA (2019)	Catalog v1 (2018-2019)
New Madrid	0.446	0.074
Colstrip	0.432	0.079
Miami Fort	0.360	0.053
Navajo	0.351	0.115
Hunter	0.333	0.040
Scherer	0.319	-
Martin Lake	0.301	-
Fort Martin	0.298	-
Intermountain	0.287	0.054
Thomas Hill	0.285	0.037

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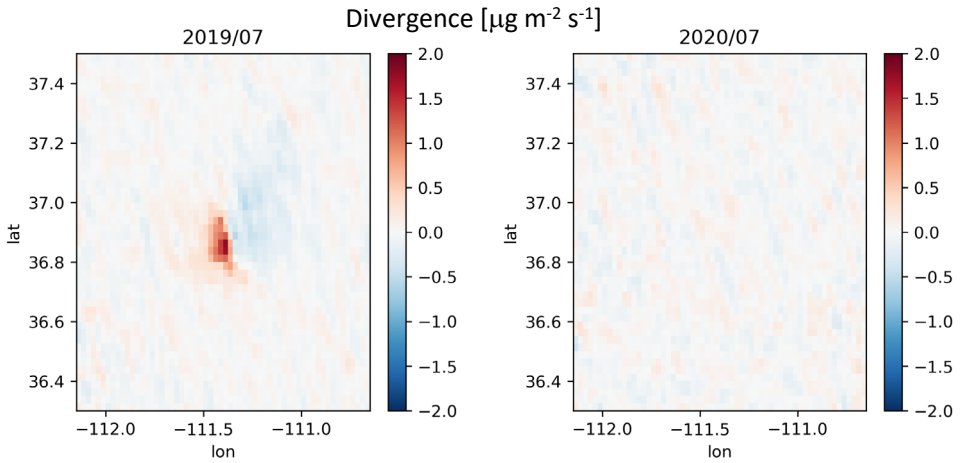
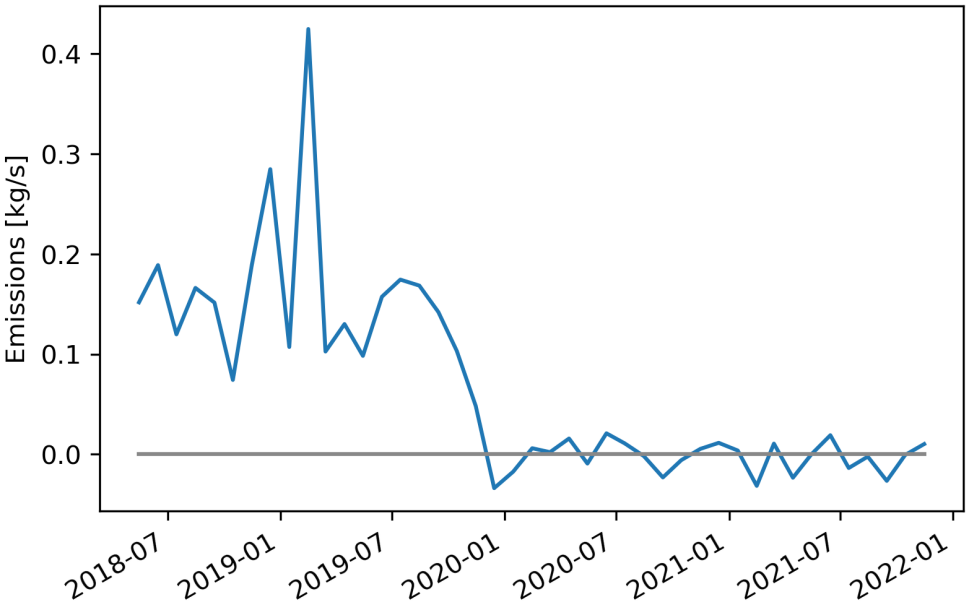
https://apnews.com/article/19487208f317460e9643f845e1440f65





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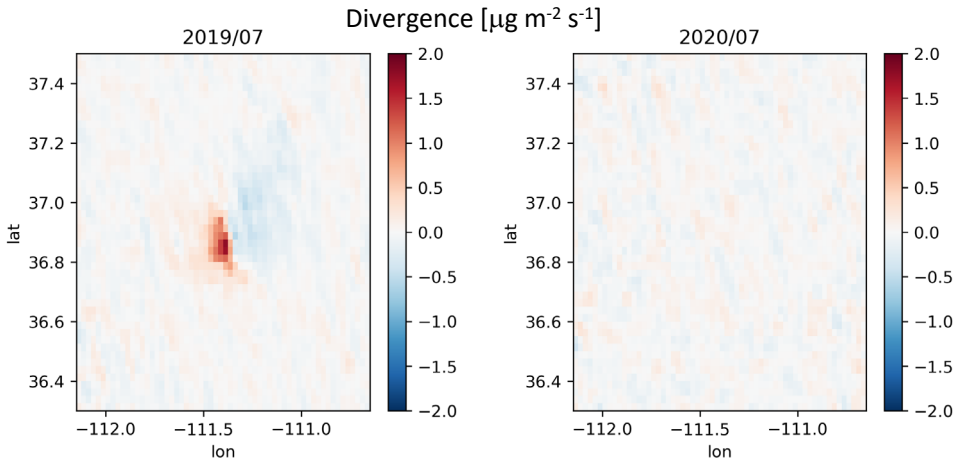
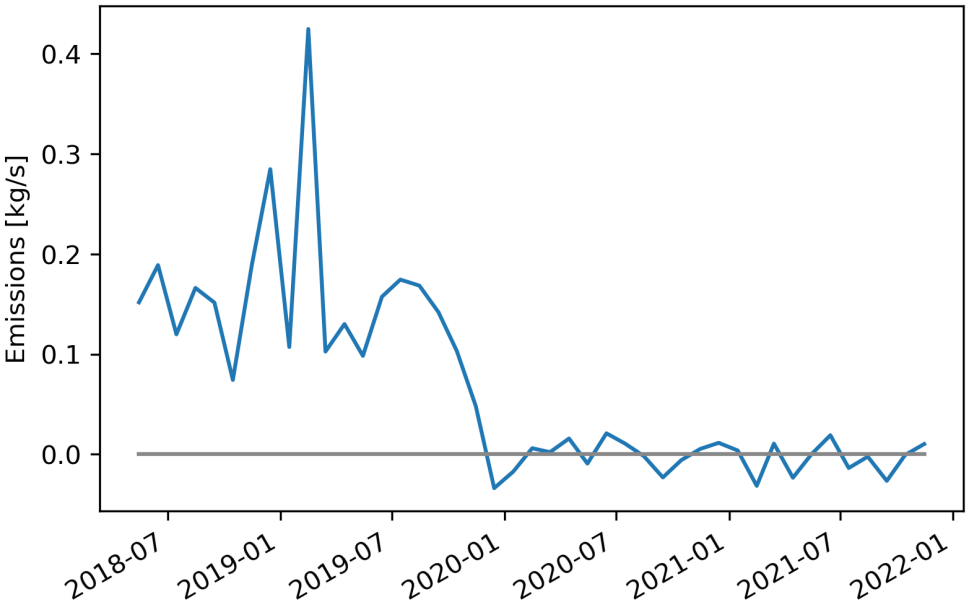
Long-running coal plant on Navajo Nation stops production

By FELICIA FONSECA November 19, 2019

https://apnews.com/article/19487208f317460e9643f845e1440f65





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Thomas Hill	0.285	0.037	0.096	0.103

Improved,
but still too low!

What is going wrong???

Checking the general approach

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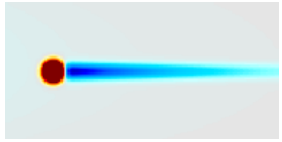
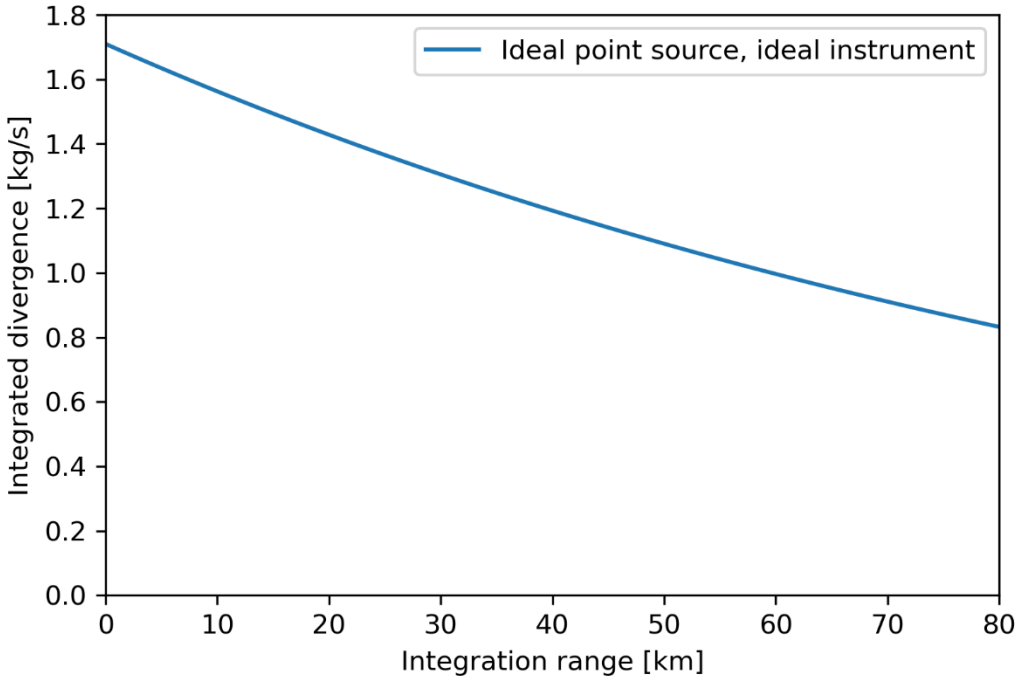
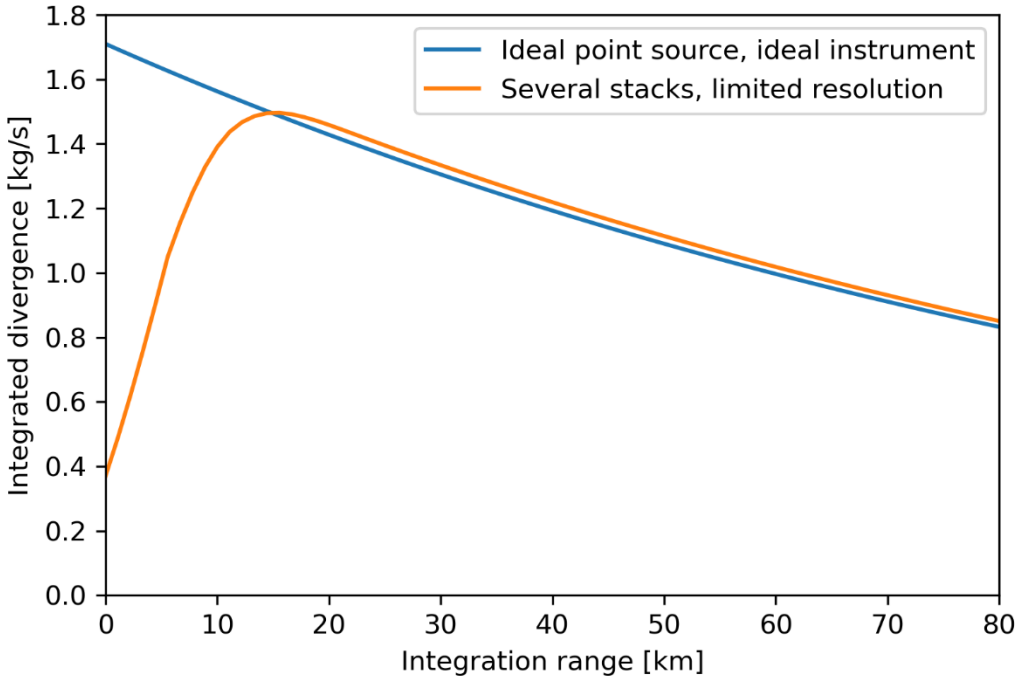
Divergence





Checking the general approach



Checking the general approach

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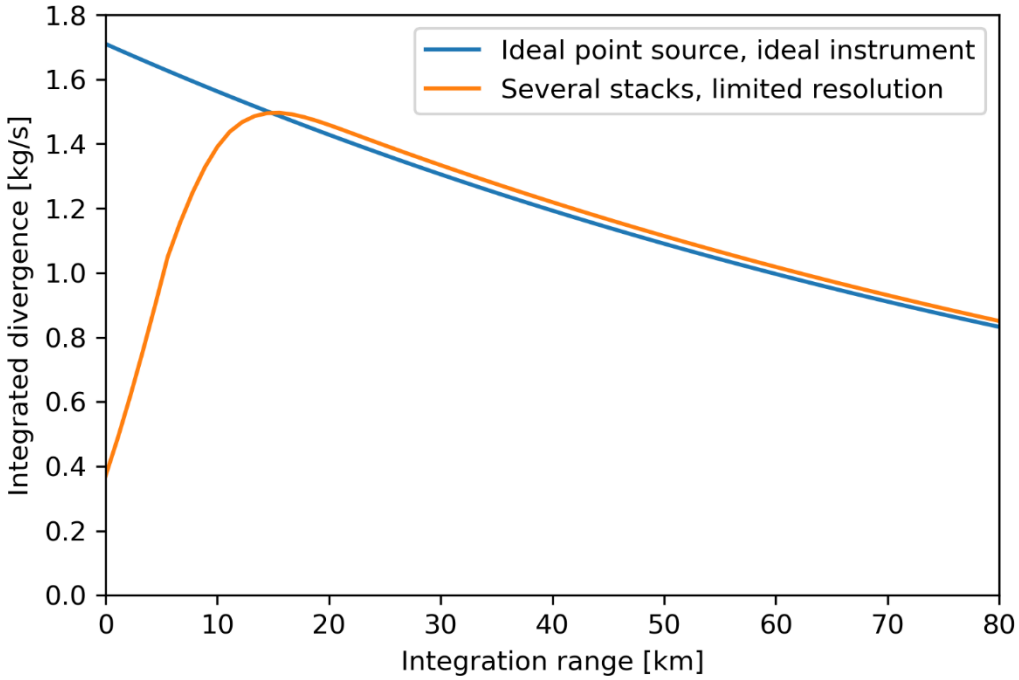
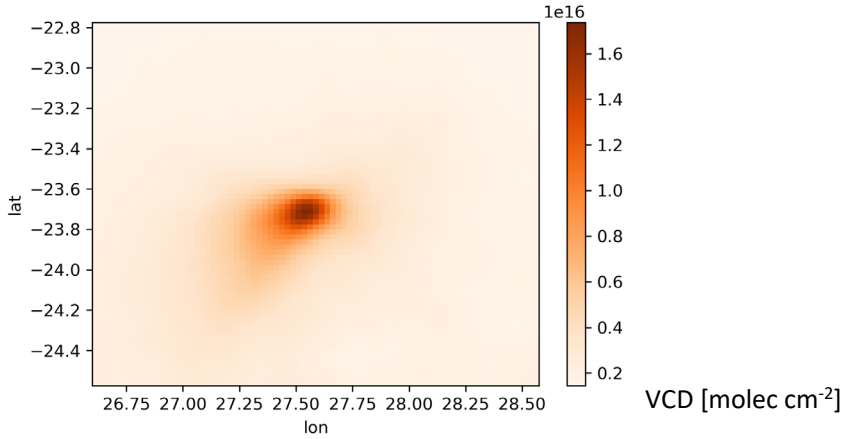
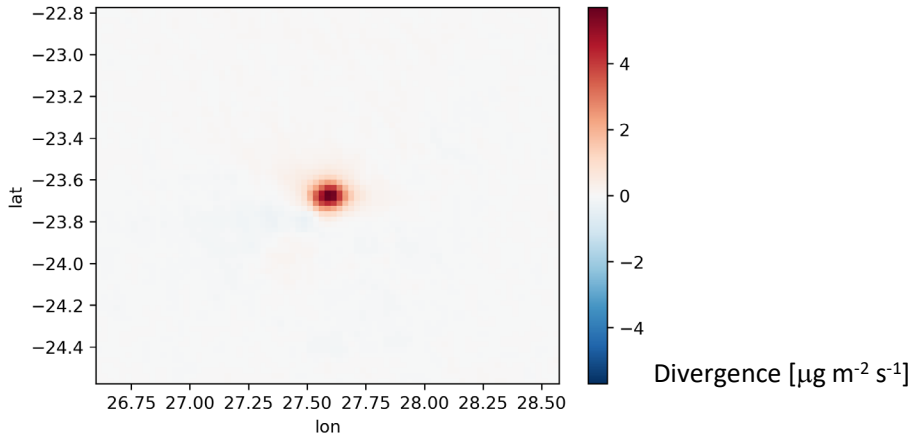


Isolated point source:
Medupi / Matimba
(South Africa)





Checking the general approach

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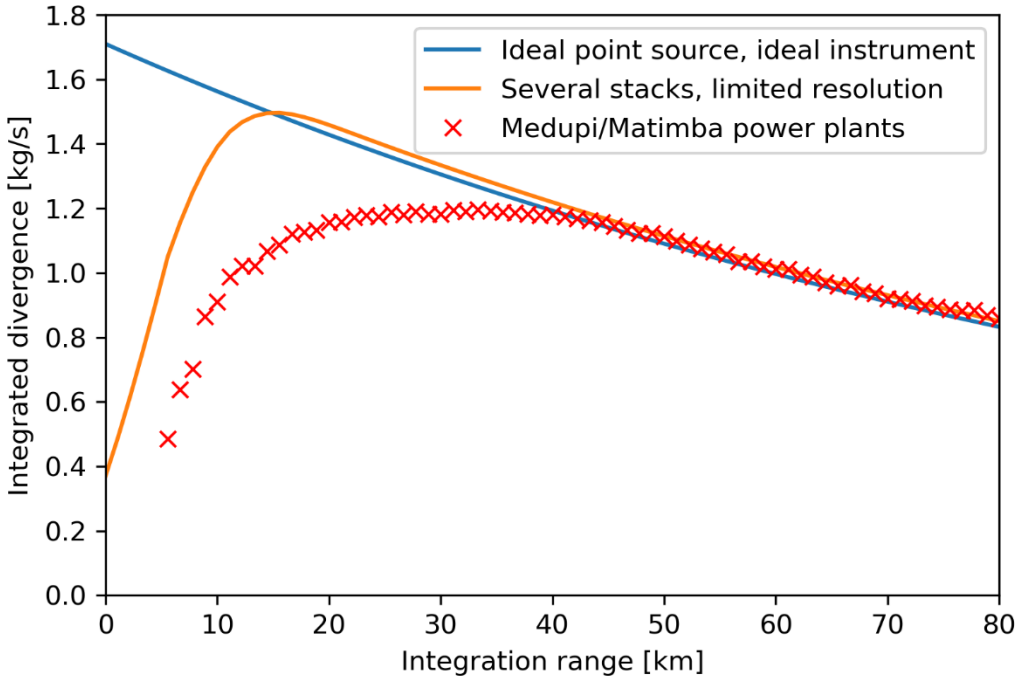
- Virtual source term ~20-40 km around the point source
- NO to NO_2 conversion?
- 3D effects on AMF (see Wagner et al., 11:25)
- Any other idea?



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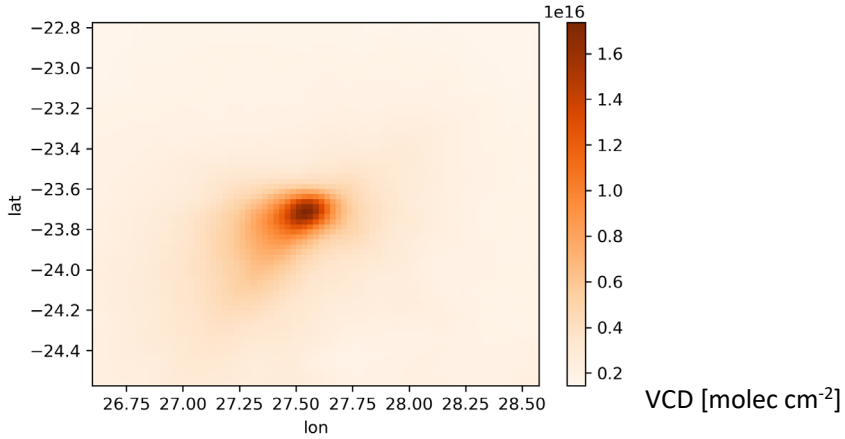

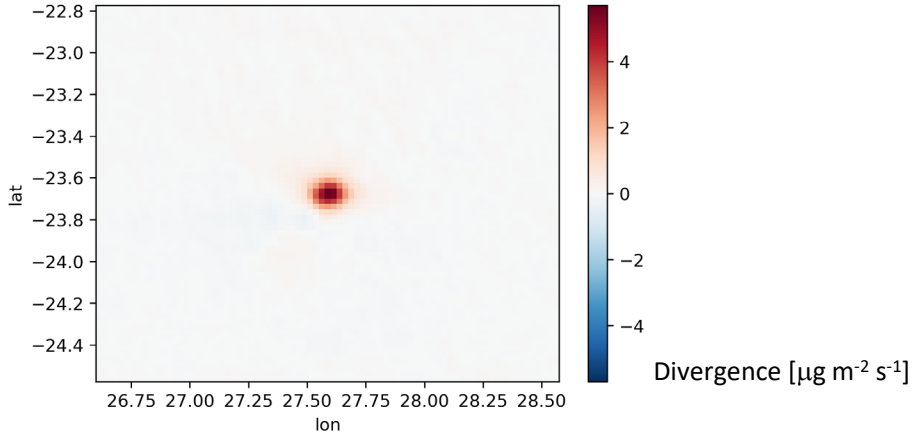

Conclusions

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- Divergence of NO_2 flux yields balance of NO_x sources and sinks
- Method is particularly sensitive for point sources:
  - Accurate localization
  - Detection of switch on / switch off on monthly basis
- Quantifying emissions:
  - Still tricky, work in progress
  - To start with: empirical correction factors?

Within the **ESA World Emission** project:

- Compile NO_x point source catalog v2
- Compile SO_2 point source catalog

World Emission

Contact: steffen.beirle@mpic.de

Supplement

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Noise in divergence

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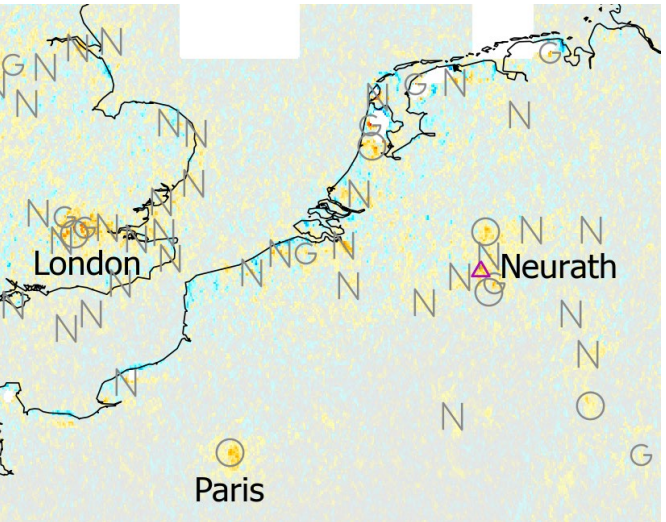
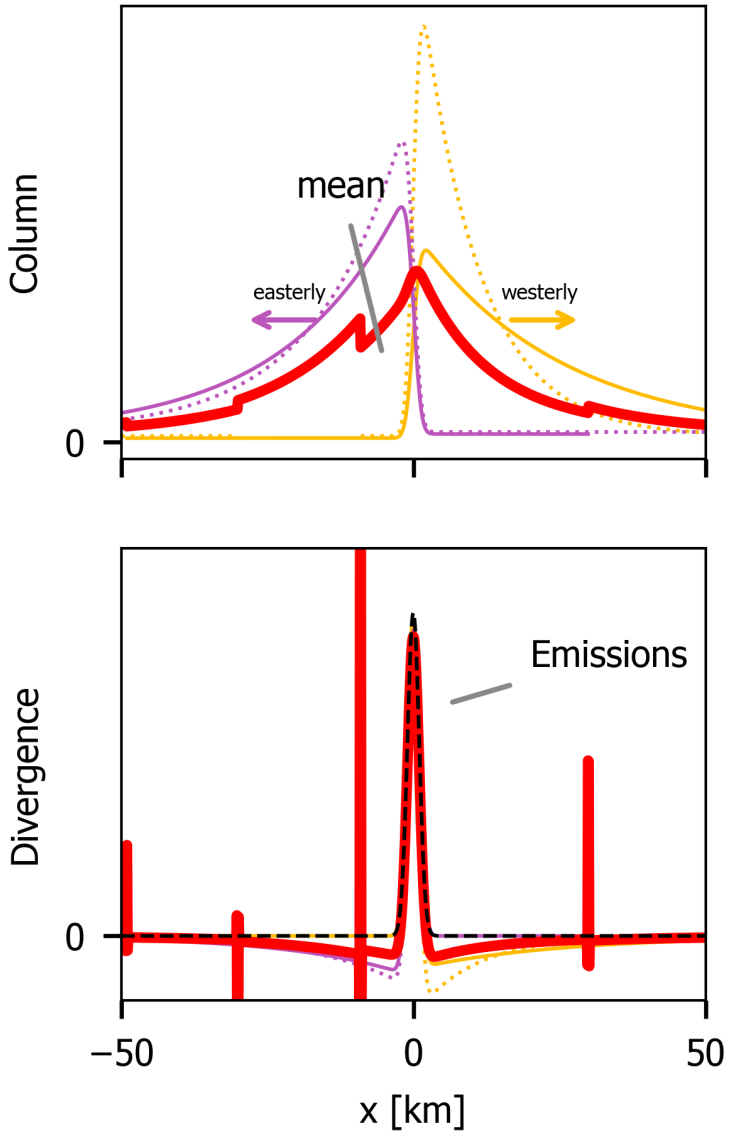
- Gaps due to cloud masking cause „jumps“ in mean VCD & mean flux
- Divergence (spatial derivative) results in spikes
- Effect stronger for
  - frequent cloud occurence
  - polluted background
- Poor performance over e.g. Western Europe or China
- Longer time periods needed





Catalog of NO_x emissions from point sources as derived from the divergence of the NO_2 flux for TROPOMI

Steffen Beirle[1], Christian Borger[1], Steffen Dörner[1], Henk Eskes[2], Vinod Kumar[1], Adrianus de Laat[2], and Thomas Wagner[1]

https://doi.org/10.5194/essd-13-2995-2021

Open Access Earth System Science Data

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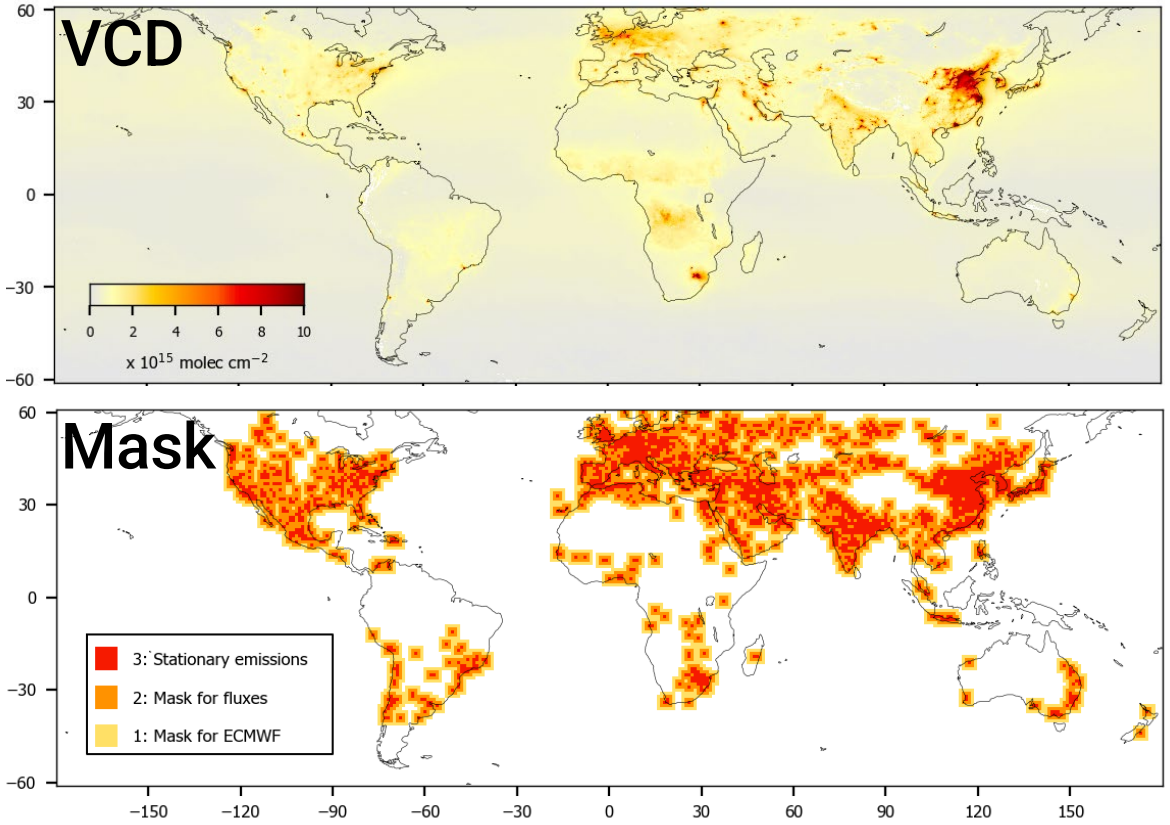
Method:

- Mask for potential stationary emissions
- Calculate mean fluxes and divergence
- Peak classification and point source emission fit by fully automated algorithm



NO_x/NO_2 ratio

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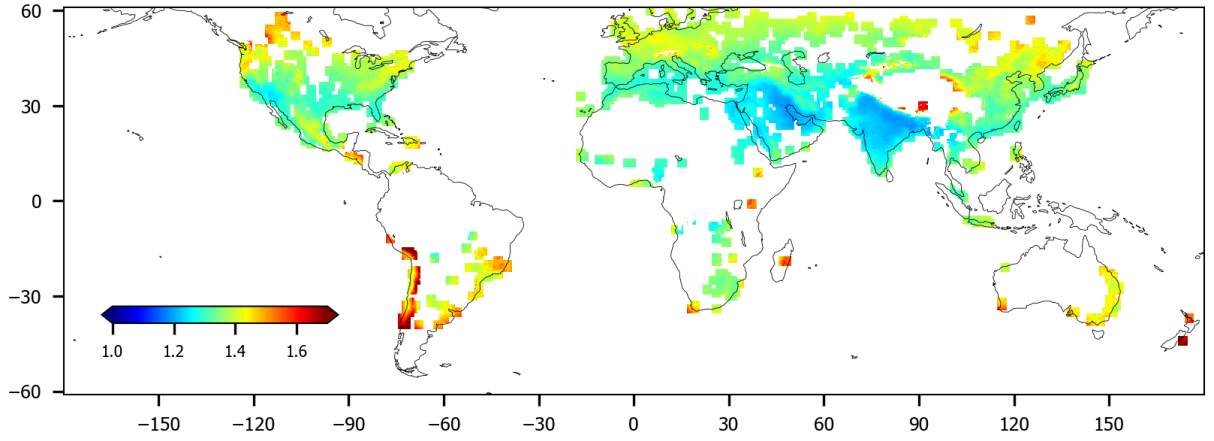
- For quantification of NO_x emissions, information on the NO_x/NO_2 ratio is needed.
- In Beirle et al., 2019: constant (1.32)
- In Beirle et al., 2021: calculated from
  J = f(SZA) and
  $[O_3]$ from model climatology
- Only moderate spatial variability:
  Cloud free conditions around noon,
  SZA < 65°



- In-plume NO_x/NO_2 ratio might be considerably higher (Ozone titration)
- In this case, the divergence method will „notice“ the NO_x source as soon as the NO is converted to NO_2, i.e. the peak in D would be shifted downwind
- For quantification of complete plume: „background“ ratio is appropriate
- On TROPOMI spatial resolution, we do not observe such a shift