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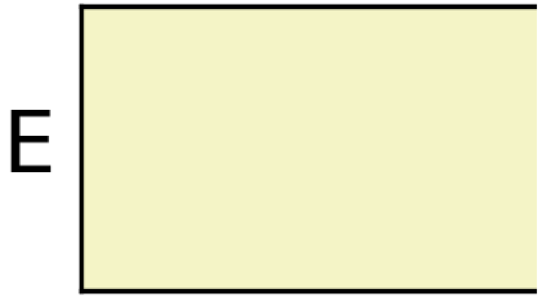
FOR CHEMISTRY

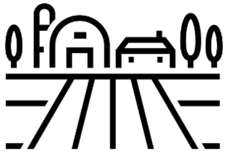
New insights on NO_x sources from the divergence of the mean NO_2 flux

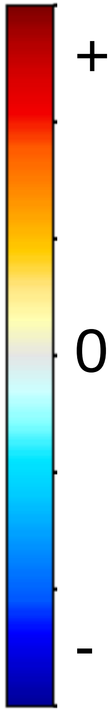
Steffen Beirle, Christian Borger, Steffen Dörner,
Vinod Kumar, Thomas Wagner

Synthetic data for illustration:

E: Emissions







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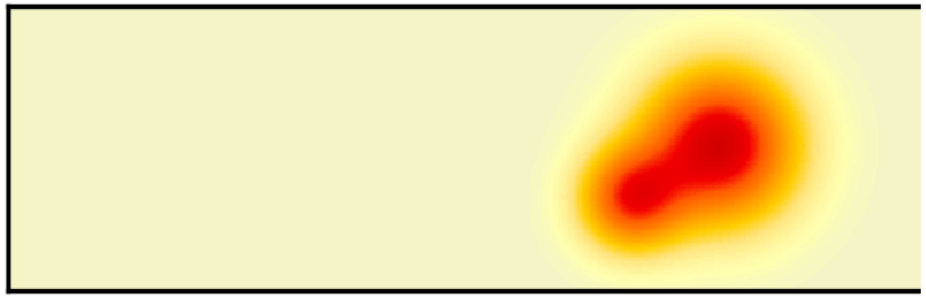
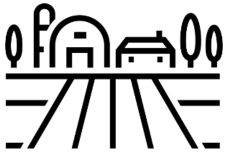
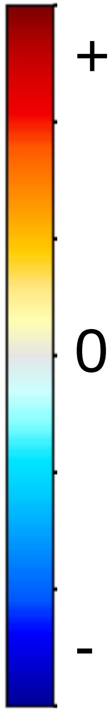




Created by Symbolon
from Noun Project

Created by Bence Bezeredy
from Noun Project



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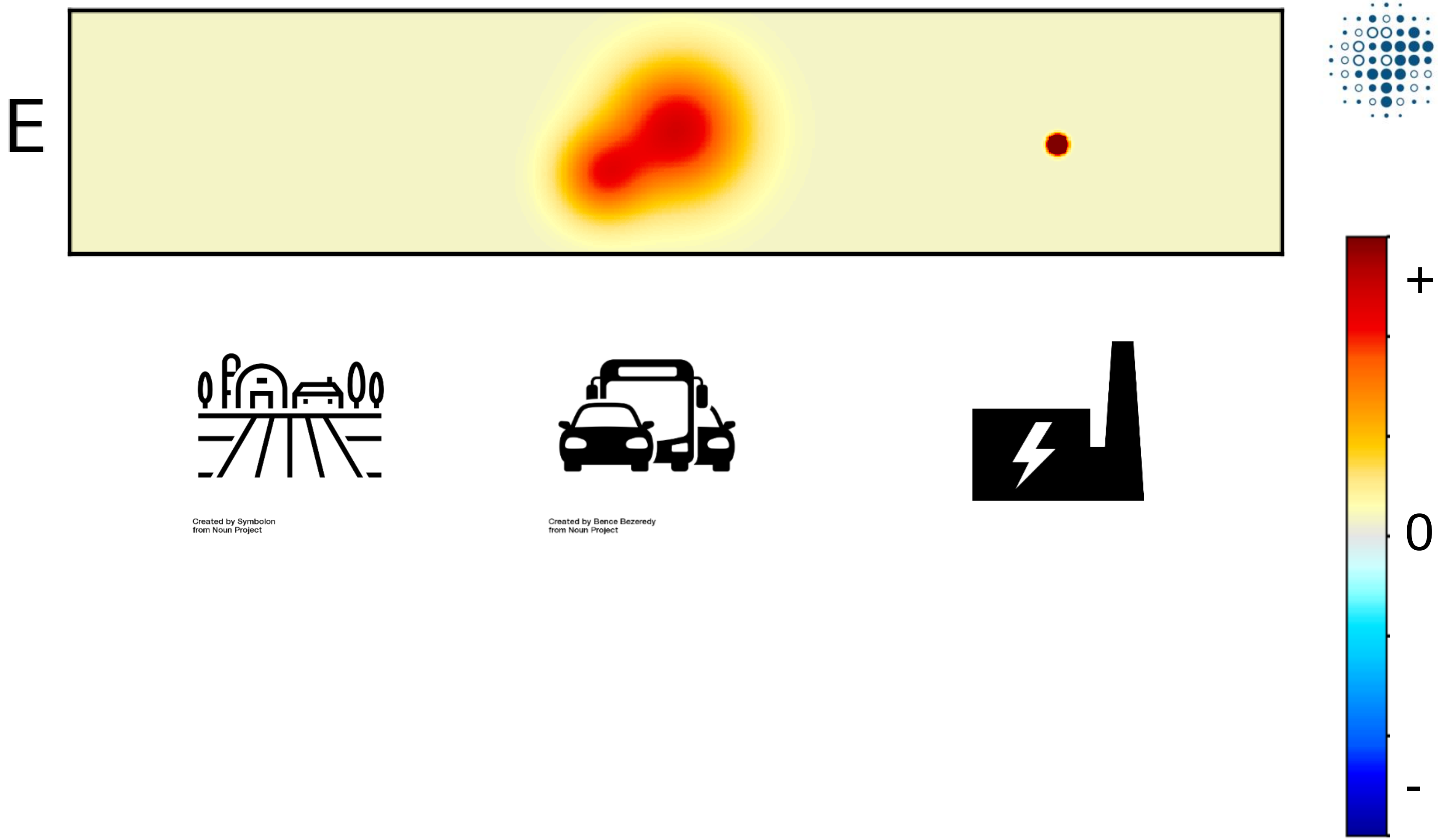

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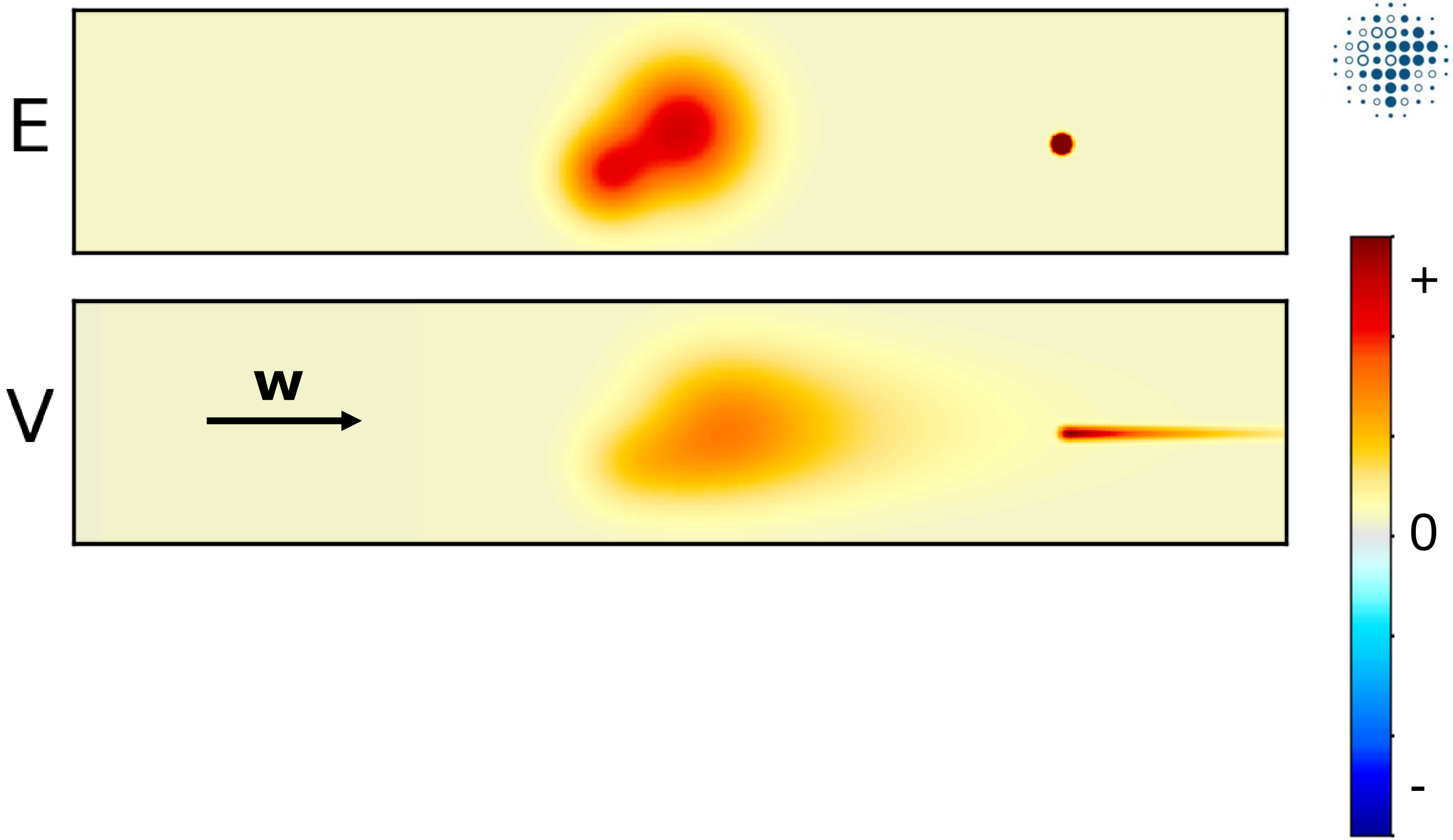
V: Vertical column

w=(u, v): Wind

F = **w**·V : Flux



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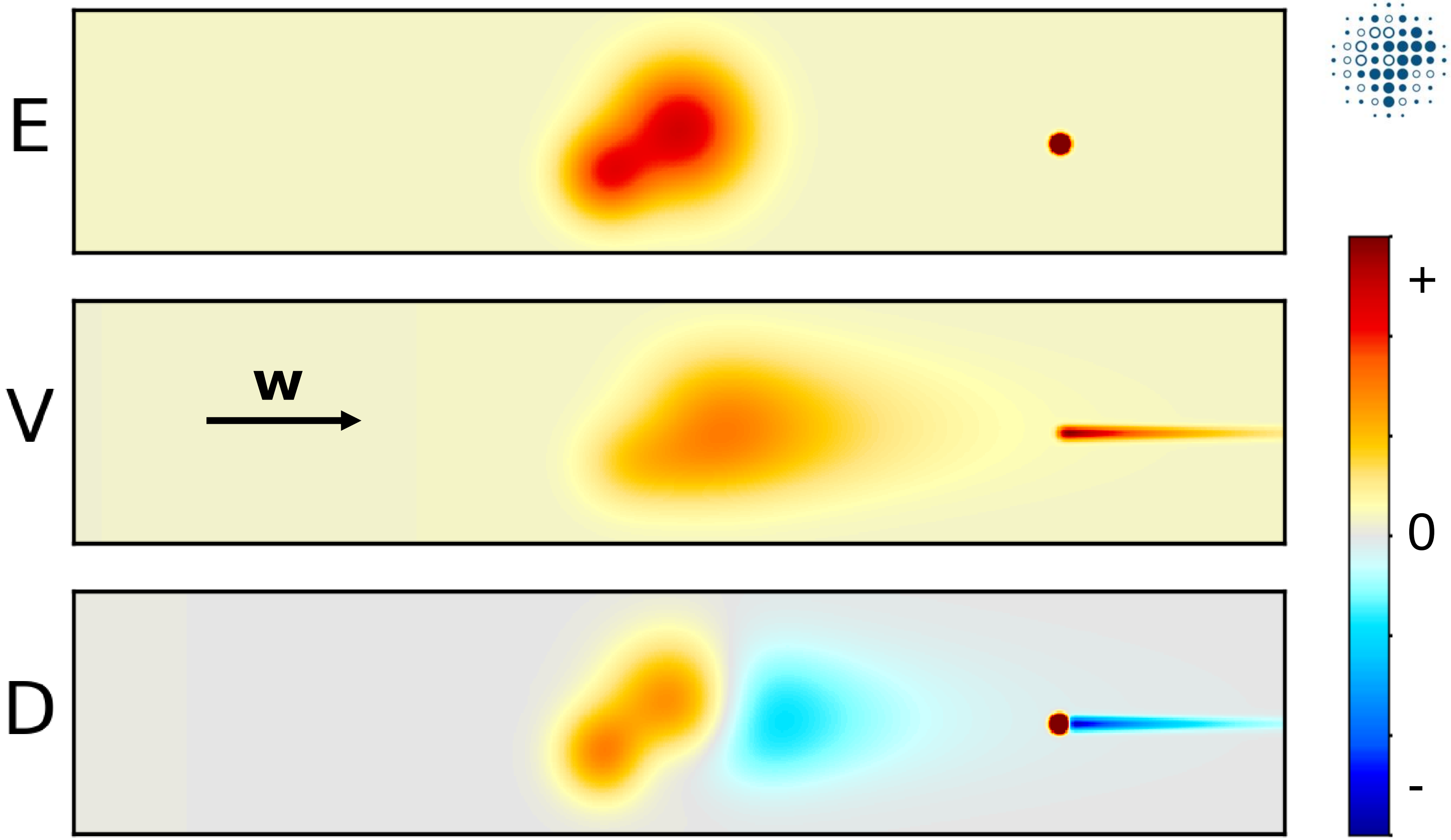
D = ∇·**F** : Divergence



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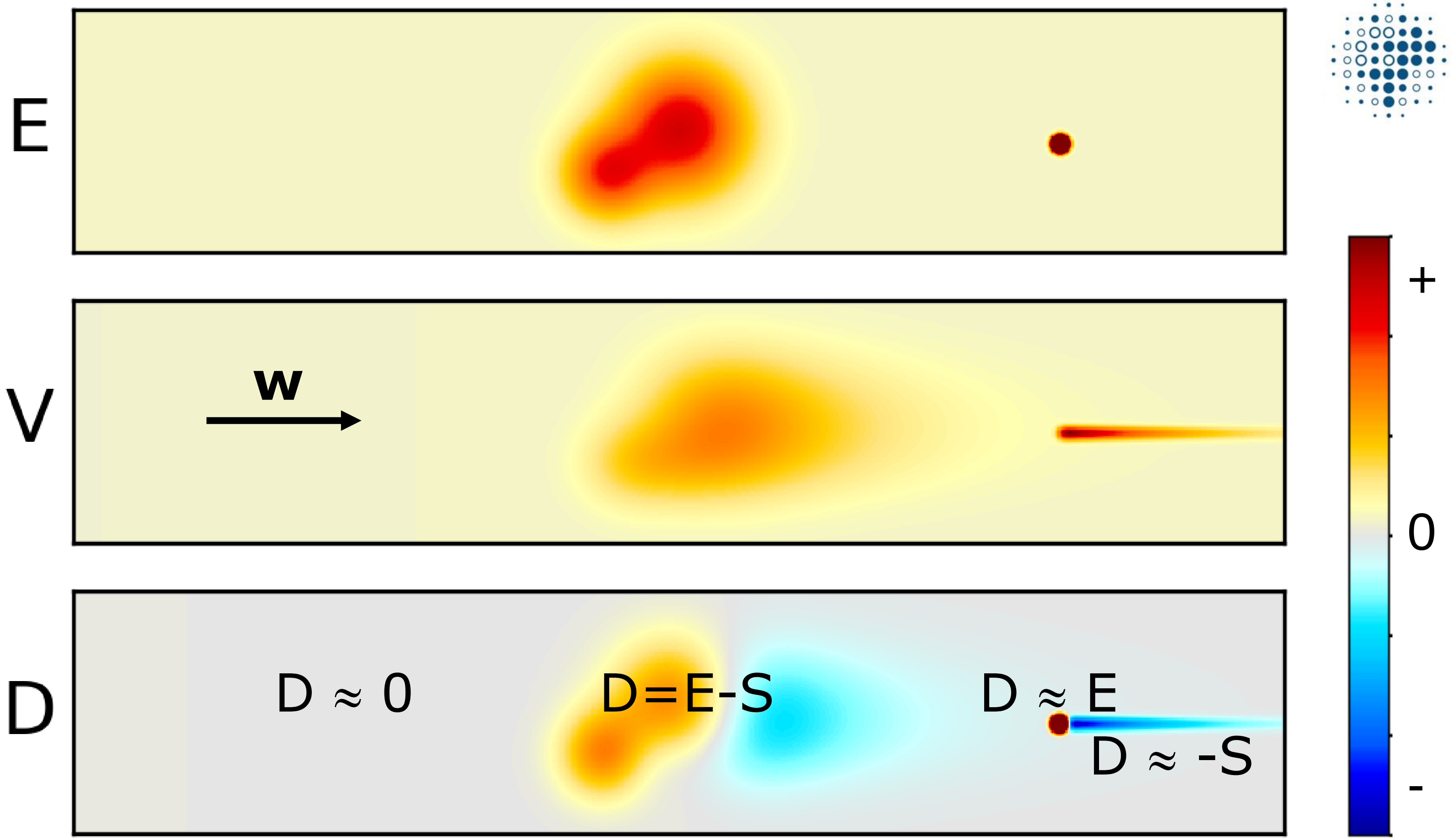

Steady state:
D = E - S
S: Sinks
S = V/τ
E = D + S

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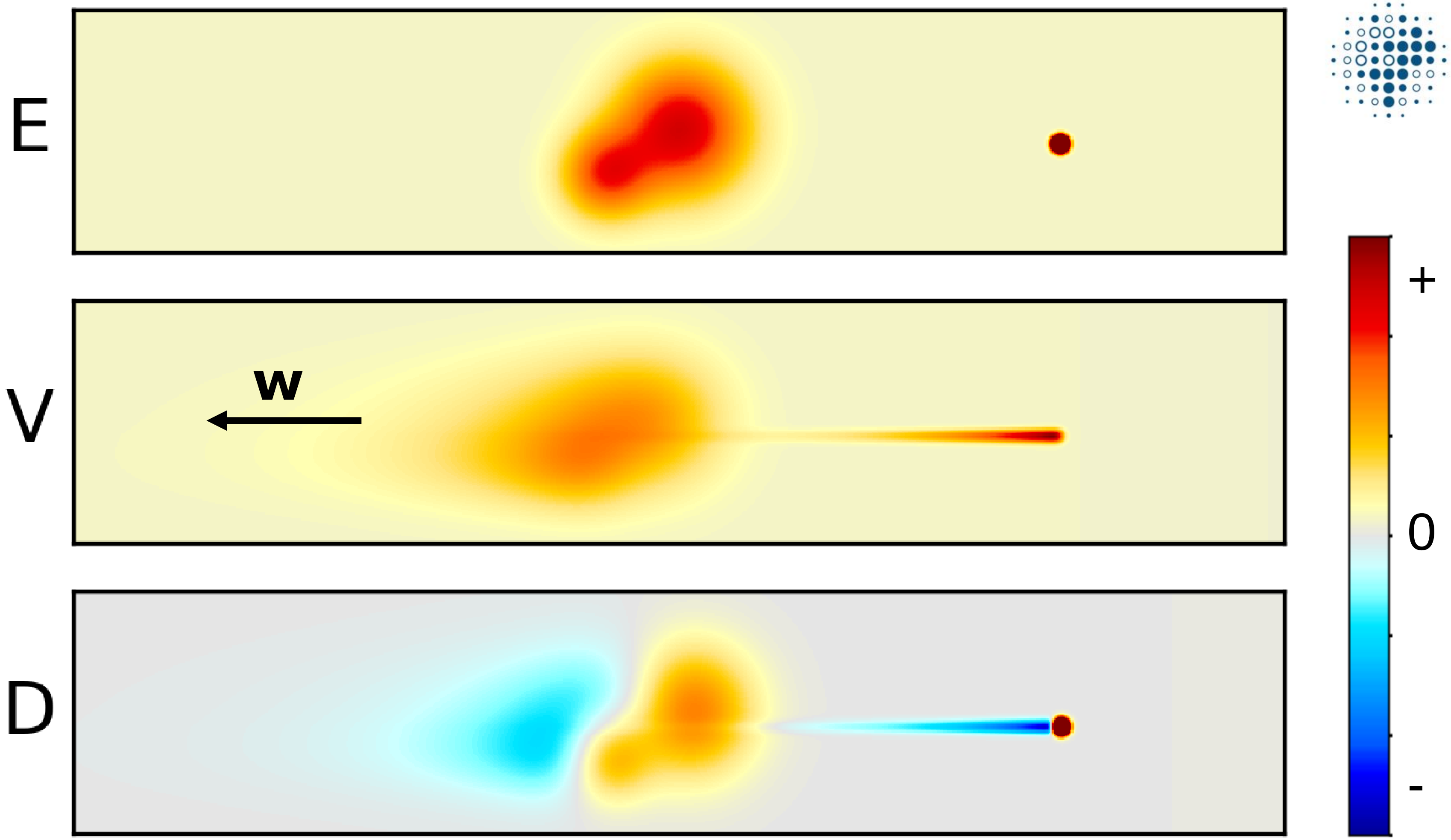

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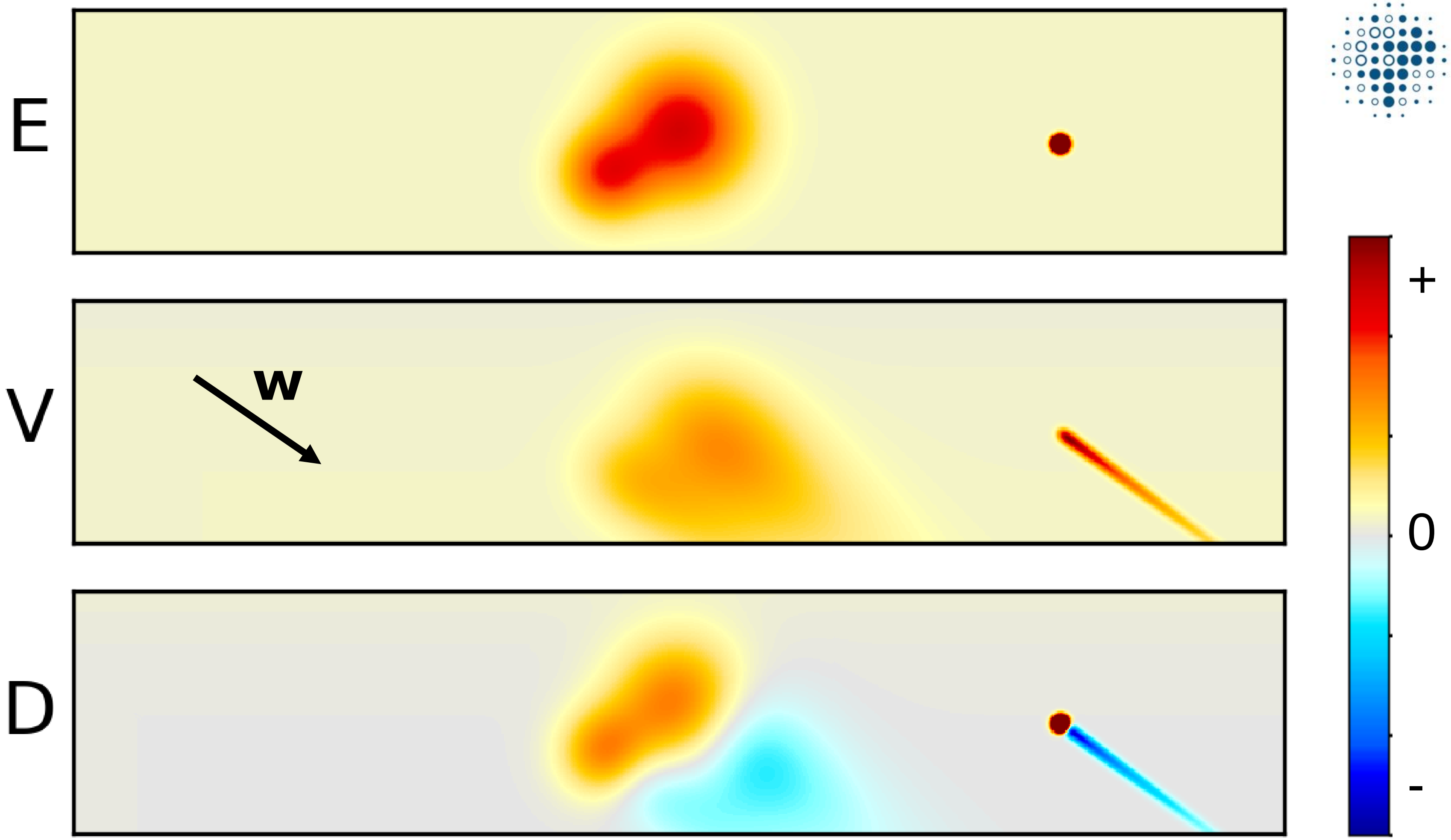

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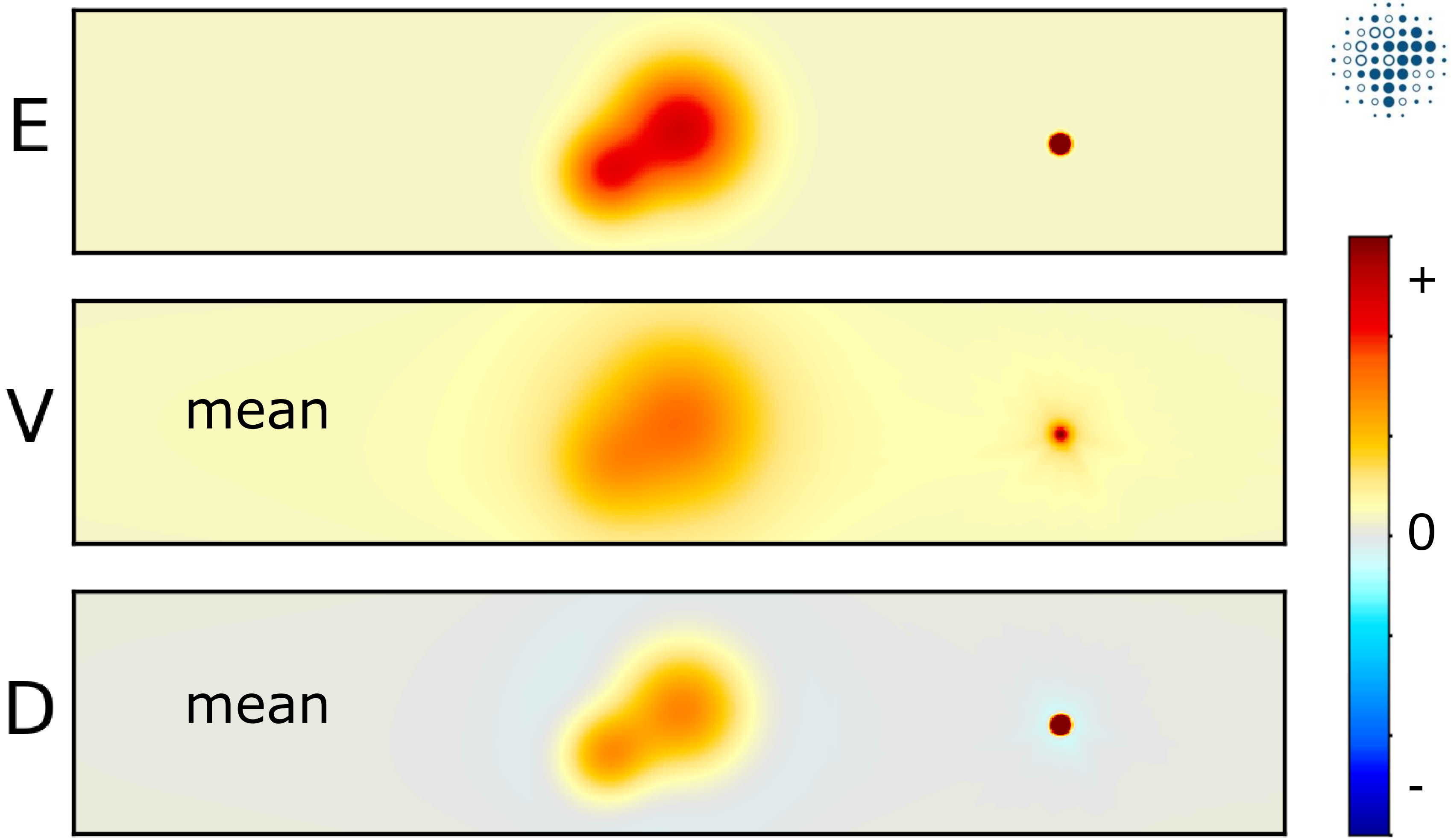

Steady state:

D = E - S

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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

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ATMOSPHERIC SCIENCE

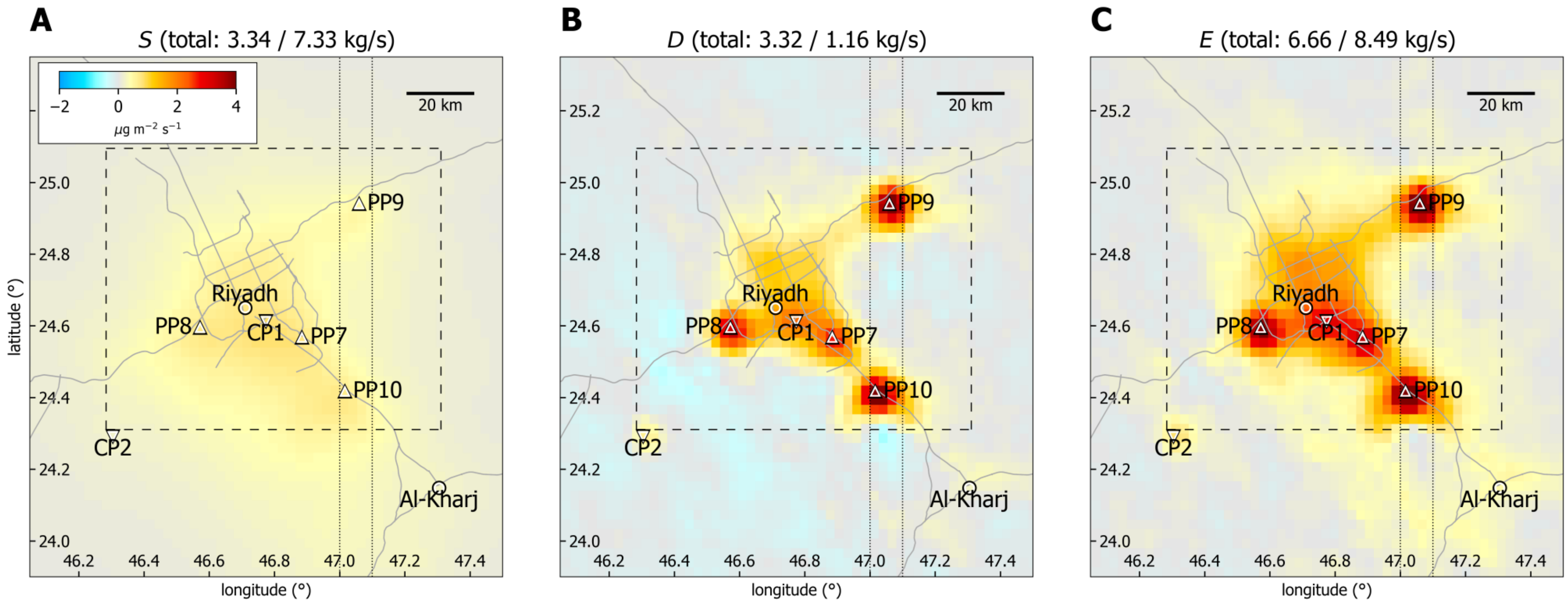
Pinpointing nitrogen oxide emissions from space

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

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

Riyadh



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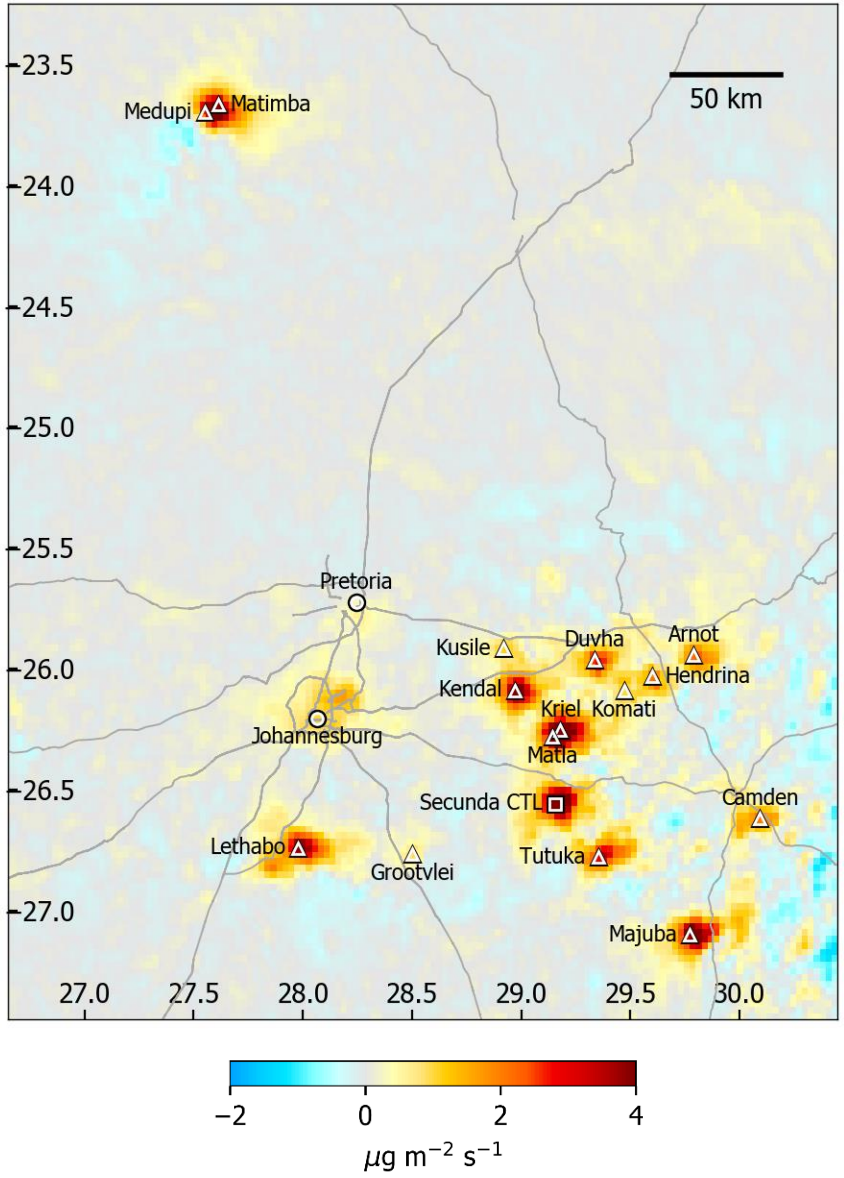

Highveld, South Africa

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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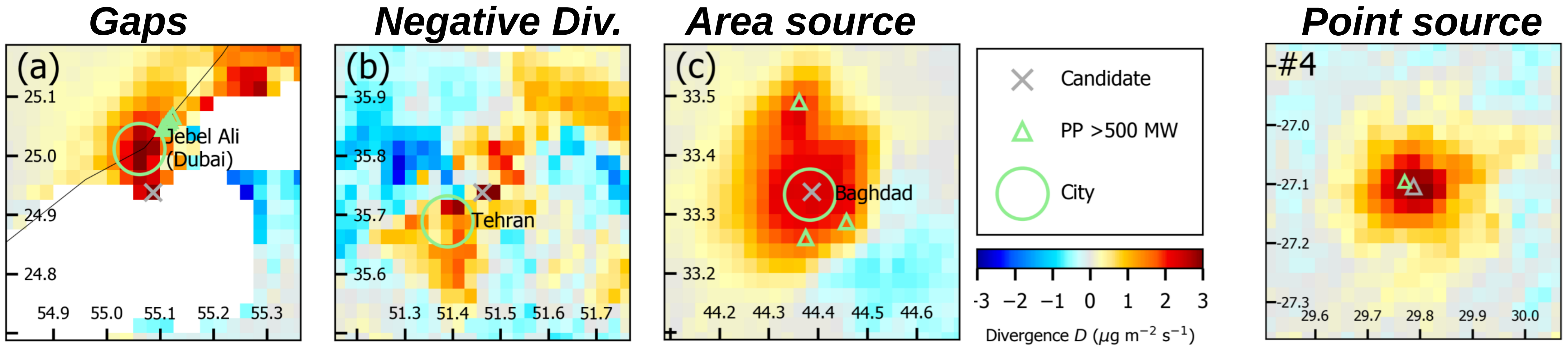
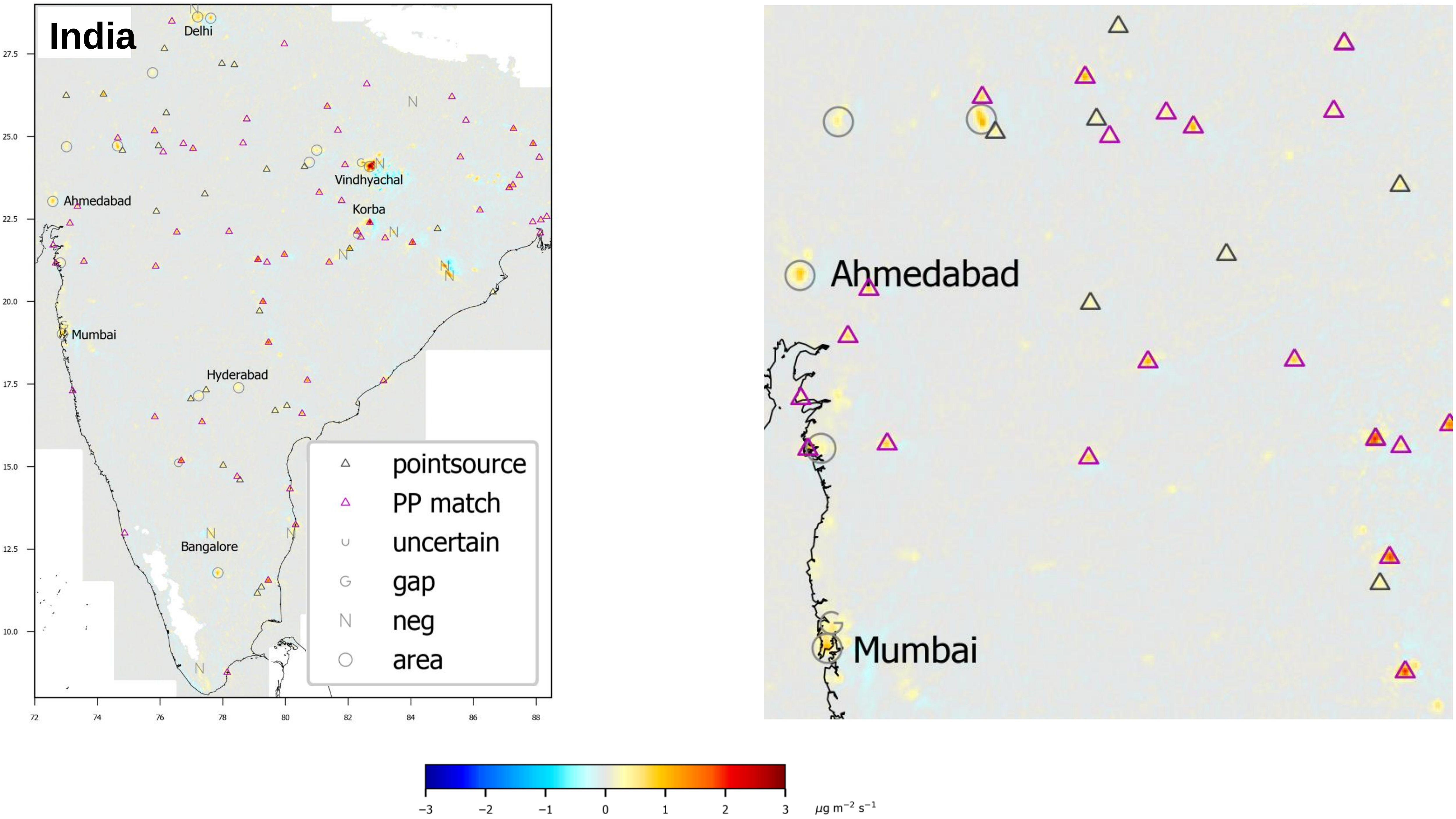
- 451 point sources detected
  (power plants, cement plants, metal smelters, industrial areas, small cities)
- For 242 point sources:
  match in Global Power Plant Database within 5 km
- Below:
  - method (short)
  - results (short)
  - limitations & potential improvements

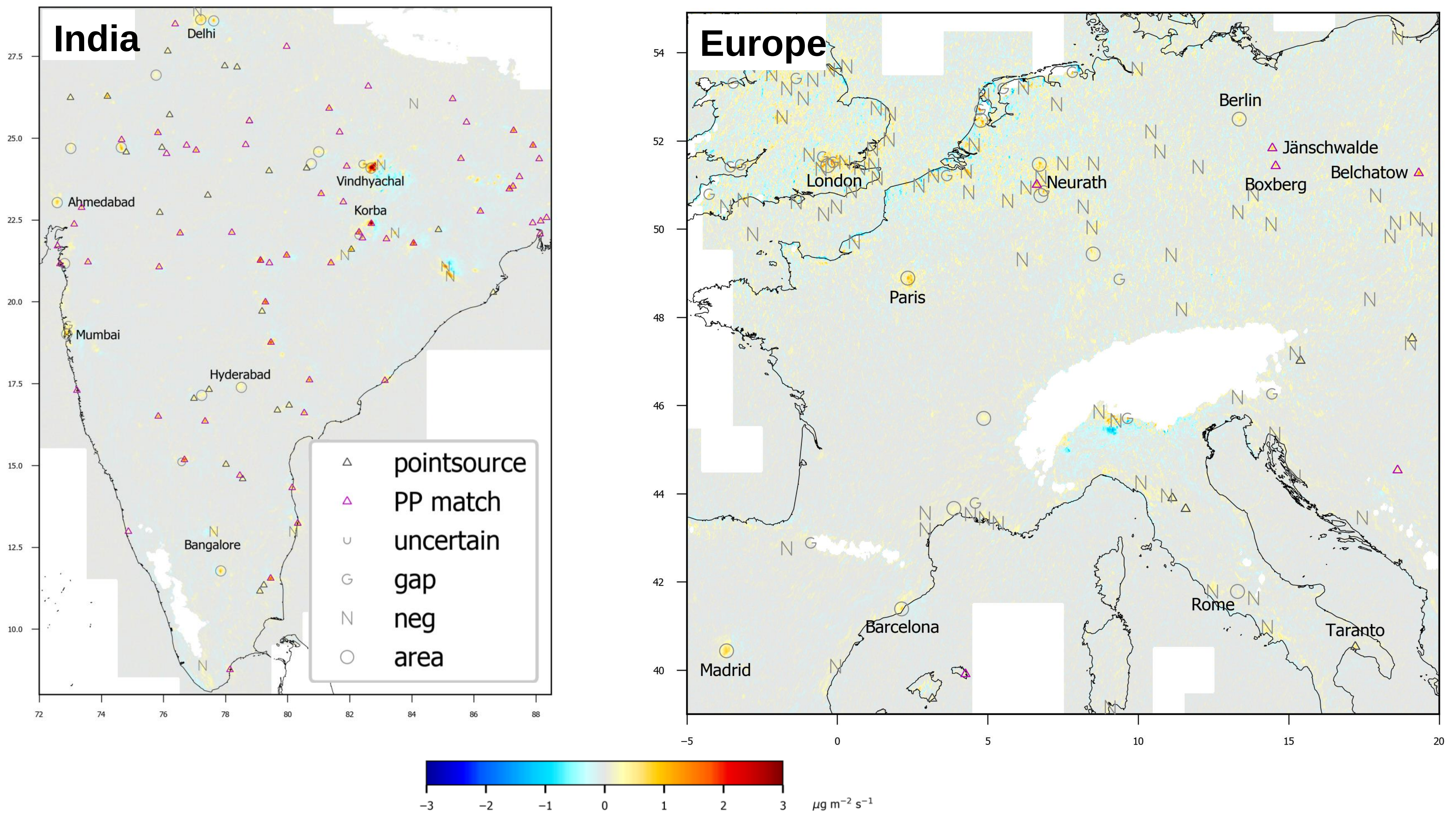
Method: Iterative peak fitting (fully automated)

- Point source candidate: maximum of D
- Classify artifacts and ambiguous cases:



- Fit 2D Gaussian to remaining candidates
- If fit succeeds: add candidate to catalog
- Add GPPD entries within 5 km
- Remove candidate from divergence map


India
Delhi
Vindhyachal
Korba
Ahmedabad
Mumbai
Hyderabad
Bangalore
pointsource
PP match
uncertain
gap
neg
area
27.5
25.0
22.5
20.0
17.5
15.0
12.5
10.0
72
74
76
78
80
82
84
86
88
Ahmedabad
Mumbai
−3
−2
−1
0
1
2
3
μg m−2 s−1


India
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Europe
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Boxberg
Belchatow
London
Neurath
Paris
Rome
Barcelona
Madrid
Taranto
μg m^{-2} s^{-1}

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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
- Catalog is incomplete:
    - Persistent gaps in input data
    - Noise in divergence
    - Systematic artefacts (input wind fields / mountains)
- Emissions are biased low
- Possible reasons:
    - Lifetime correction
    - NO_x/NO_2 ratio
    - A-priori profile / averaging kernel (AK)

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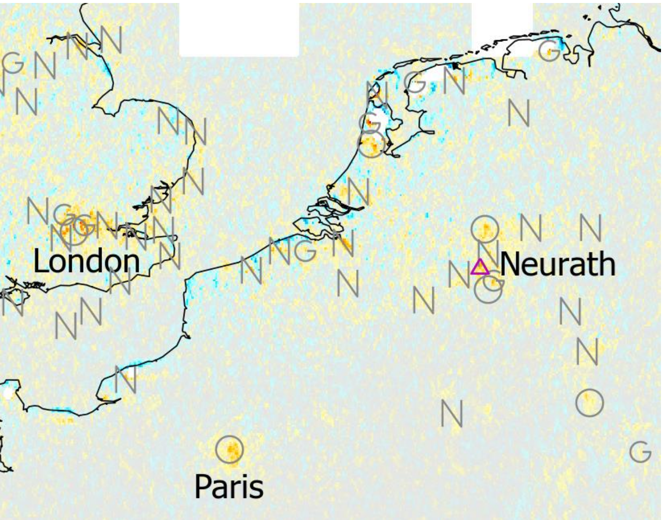
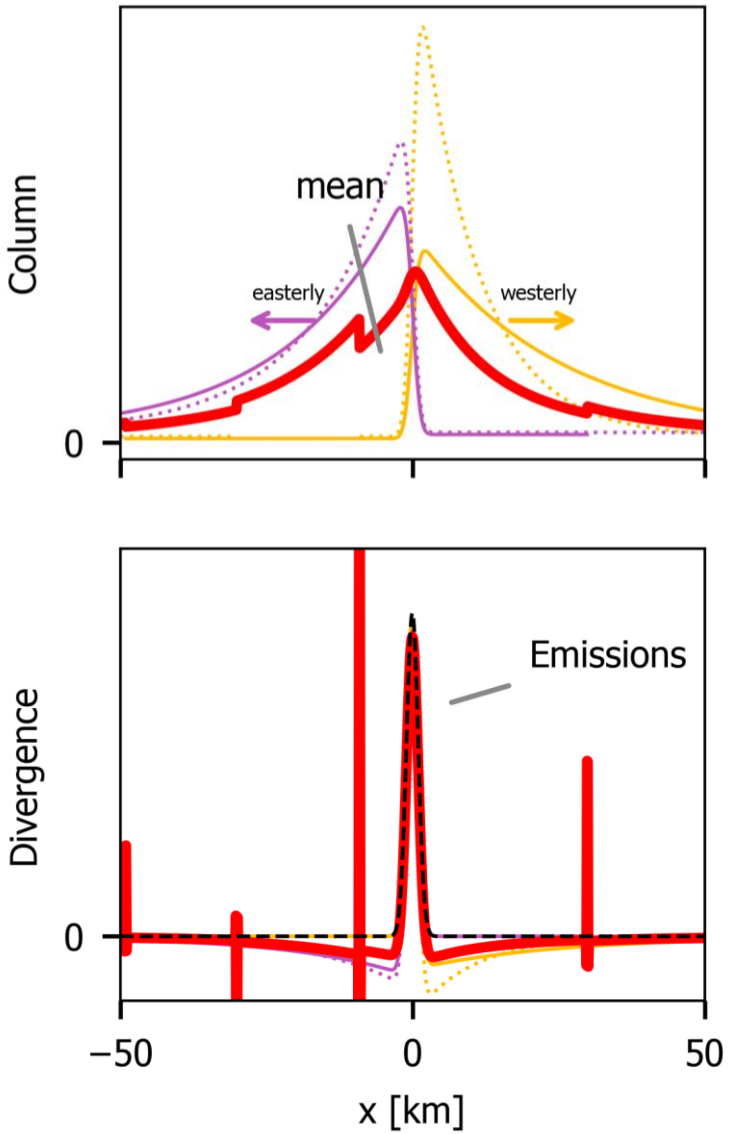
Noise in divergence

- 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





NO_x/NO_2 ratio

- 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 for each TROPOMI pixel (1.35±0.08) (using J = f(SZA) and $[O_3]$ from model climatology)
- 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

A-priori vertical profile

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

Synthetic data for illustration:

E: Emissions

V: Vertical column

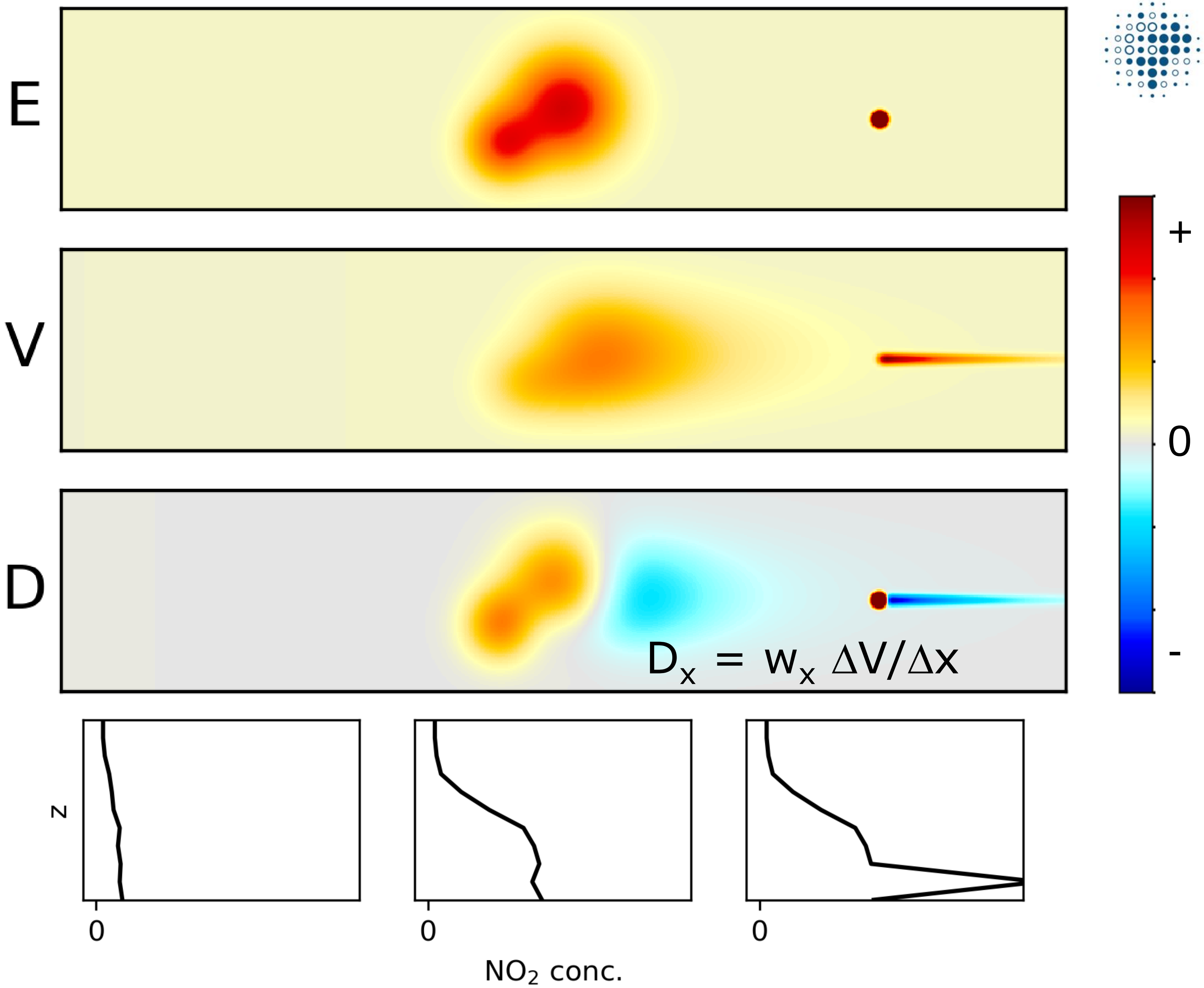
w=(u, v): Wind

F = **w**·V : Flux

D = ∇·**F** : Divergence

For correct V:

NO_2 profile required (complex!)



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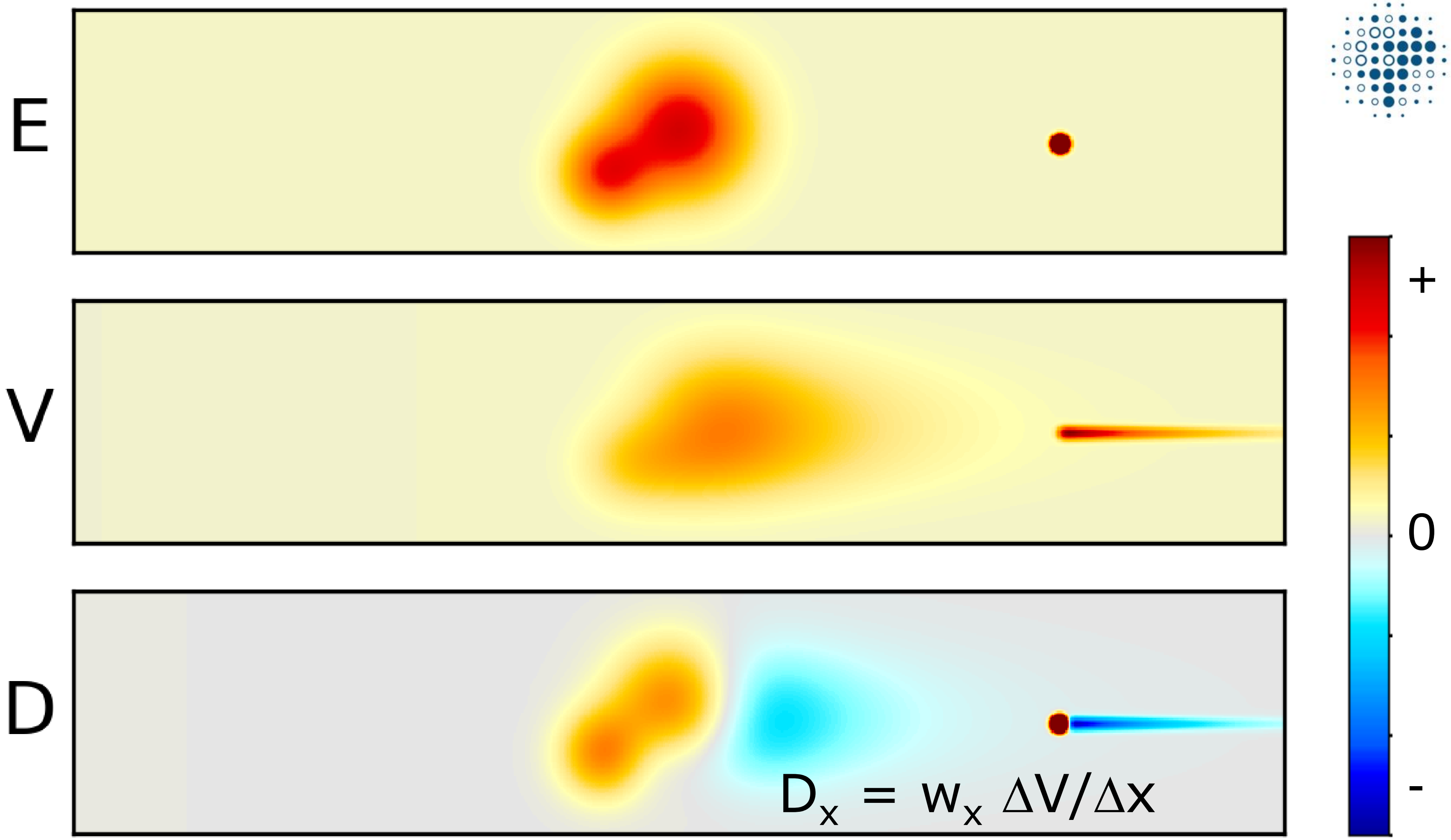
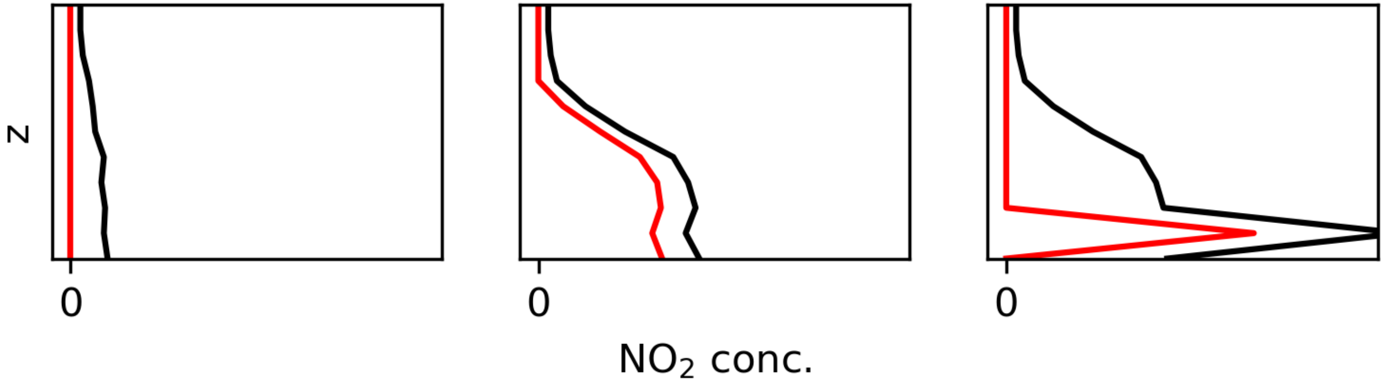
$\mathbf{w}=(u, v)$: Wind

$\mathbf{F} = \mathbf{w} \cdot V$: Flux

$D = \nabla \cdot \mathbf{F}$:
Divergence



For correct V:
NO_2 profile required
(complex!)



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

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Earth System Science Data (Open Access)

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- Catalog is incomplete:
  - Persistent gaps ➢ Improved in TROPOMI NO_2 update
  - Noise in divergence ➢ Consider longer time periods
  - Mountains ➢ Use wind fields with better resolution
- Emissions are biased low:
  - Lifetime correction ➢ To be applied
  - NO_x/NO_2 ratio ➢ „Background” ratio is appropriate
  - A-priori profile / averaging kernel (AK) ➢ Apply AK for stack height (lowest model layer)

Conclusions

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- Divergence of NO_2 flux yields balance of NO_x sources and sinks
- Divergence is linear operator: applicable to mean flux
- Method is particularly sensitive for point sources
- Allows very accurate localization of point sources
- Clouds are crucial:
  - a strict cloud masking is necessary for accurate emission estimates
  - cloud gaps increase noise in divergence
- Quantifying emissions: only *excess* column matters → profile is known!
- Method also applicable to other trace gases: e.g. SO_2
  (Jost et al., P2.4, Thursday afternoon)
- Detection of point sources can support CO_2 satellite missions
- High potential for possible future missions like NITROSAT

Supplement

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Divergence of the NO_2 flux

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- Direct mapping of emissions: $E = D+S$
- Linear operation: can be applied to mean fluxes
- For area sources (cities): lifetime has to be considered
- Strong sensitivity for point sources
- Requirements:
  - VCDs on high spatial resolution with low noise (i.e. TROPOMI)
  - Cloud free conditions
  - Windy conditions
  - Wind fields (at relevant altitude) as input

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Open Access Earth System Science Data

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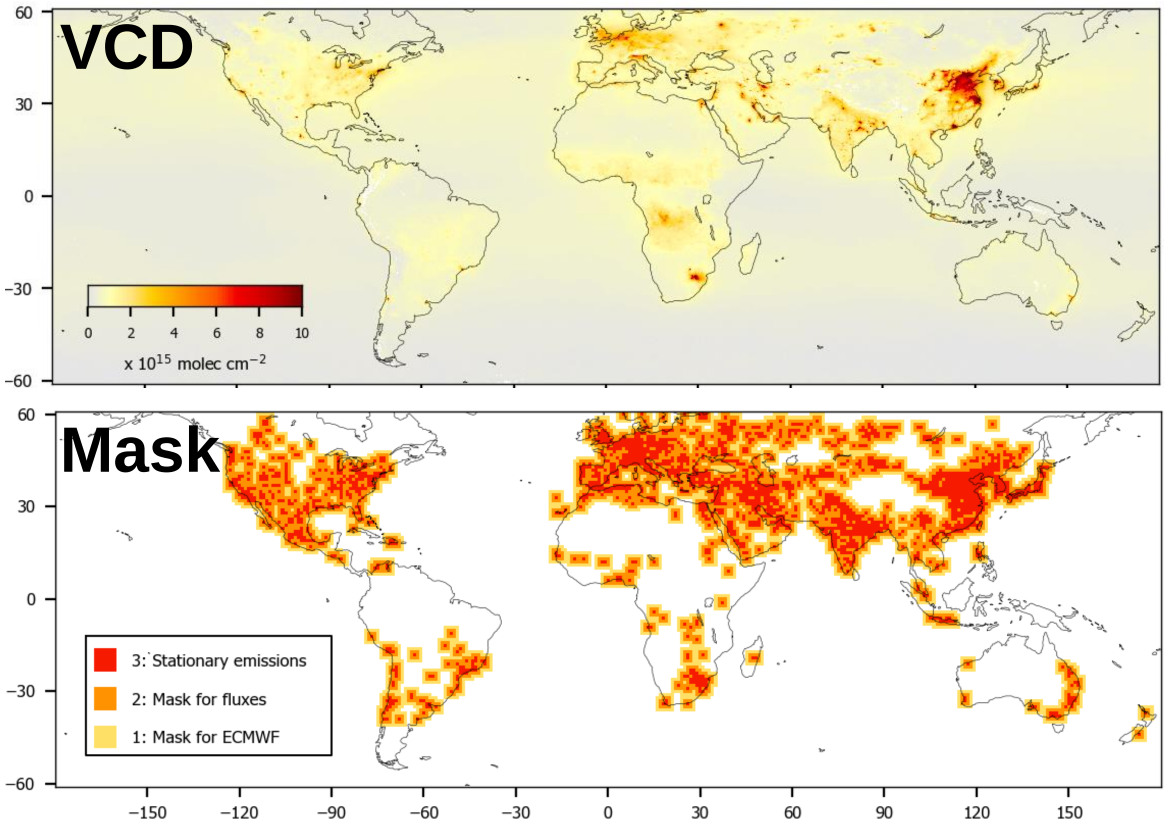
Method:

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



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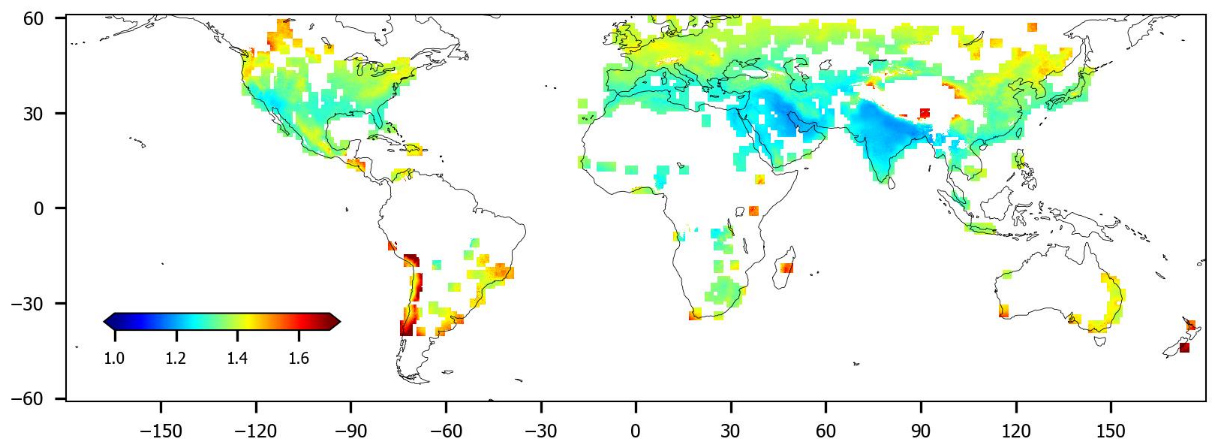

- Only moderate spatial variability: Cloud free conditions around noon, SZA < 65°
- In-plume NO_x/NO_2 ratio might be considerably higher (Ozone titration)
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- For quantification of complete plume: „background“ ratio is appropriate
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