Deriving Nitrogen Oxide emissions from inland waterway vessels using MAX-DOAS and in-situ measurements: First results from Koblenz, Germany

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MAX PLANCK INSTITUTE FOR CHEMISTRY

Max Planck Graduate Center mit der Johannes Gutenberg-Universität Mainz

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European Geosciences Union

Abstract

Sharing is encouraged

Motivation

- Negative air pollution impacts on human health
- **Nitrogen Oxides** (NO_x = NO + NO_2) – high temperature combustion processes
- Inland waterway vessels (IWVs) – **source of local air pollution**
- Inland ship impact on **air quality and human health**?

Rhine river at Boppard town, near Koblenz, Germany (Deutsche Welle, 2017)

Previous work

Deriving NO_x emissions from inland ships using MAX-DOAS measurements

How did we determine NO_x emissions from inland ships?

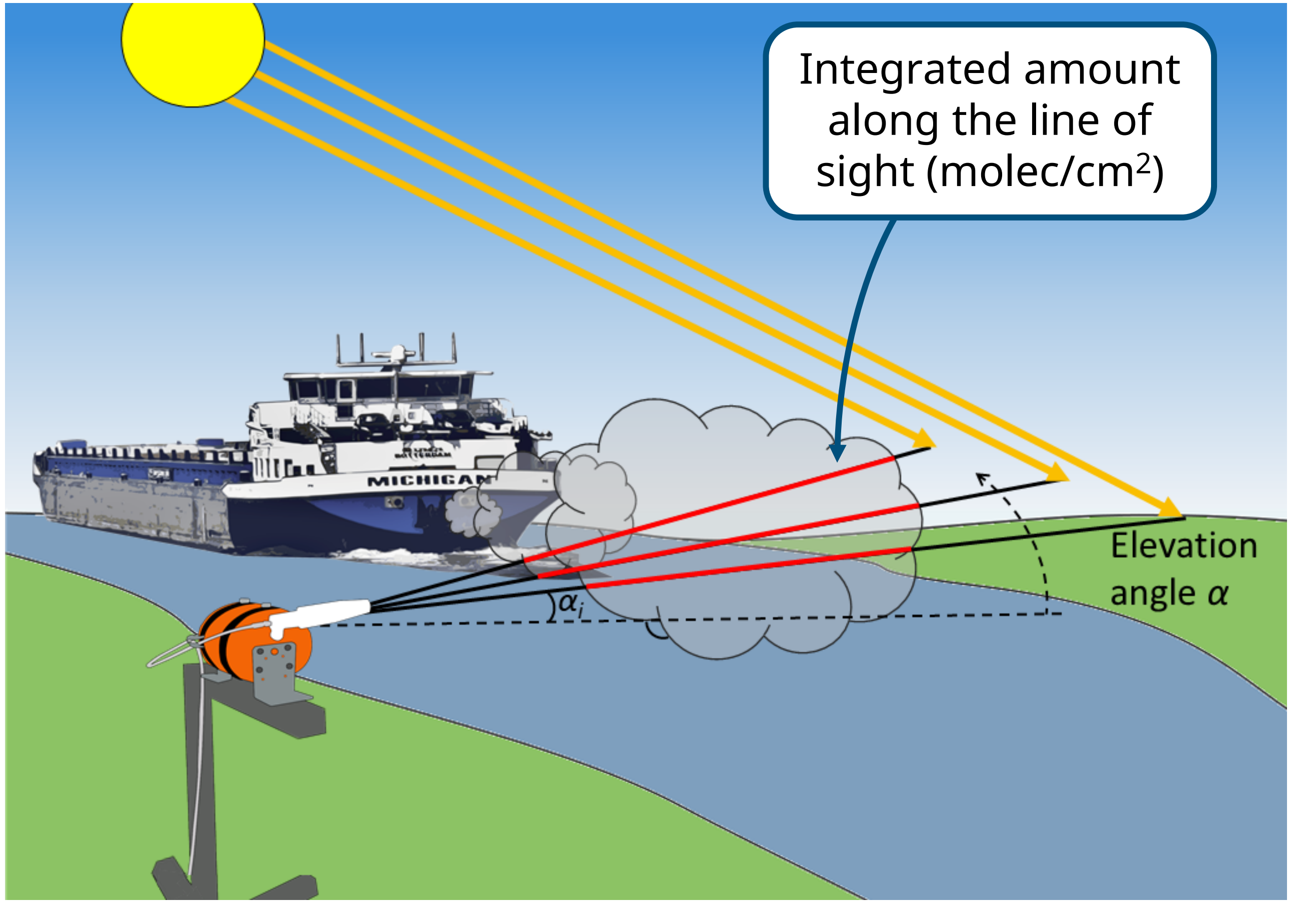
→

Ground based remote sensing technique **Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS)**

Previous work

Deriving NO_x emissions from inland ships using MAX-DOAS measurements

MAX-DOAS geometry for ship emission measurements



Adapted from Platt and Stutz (2008)

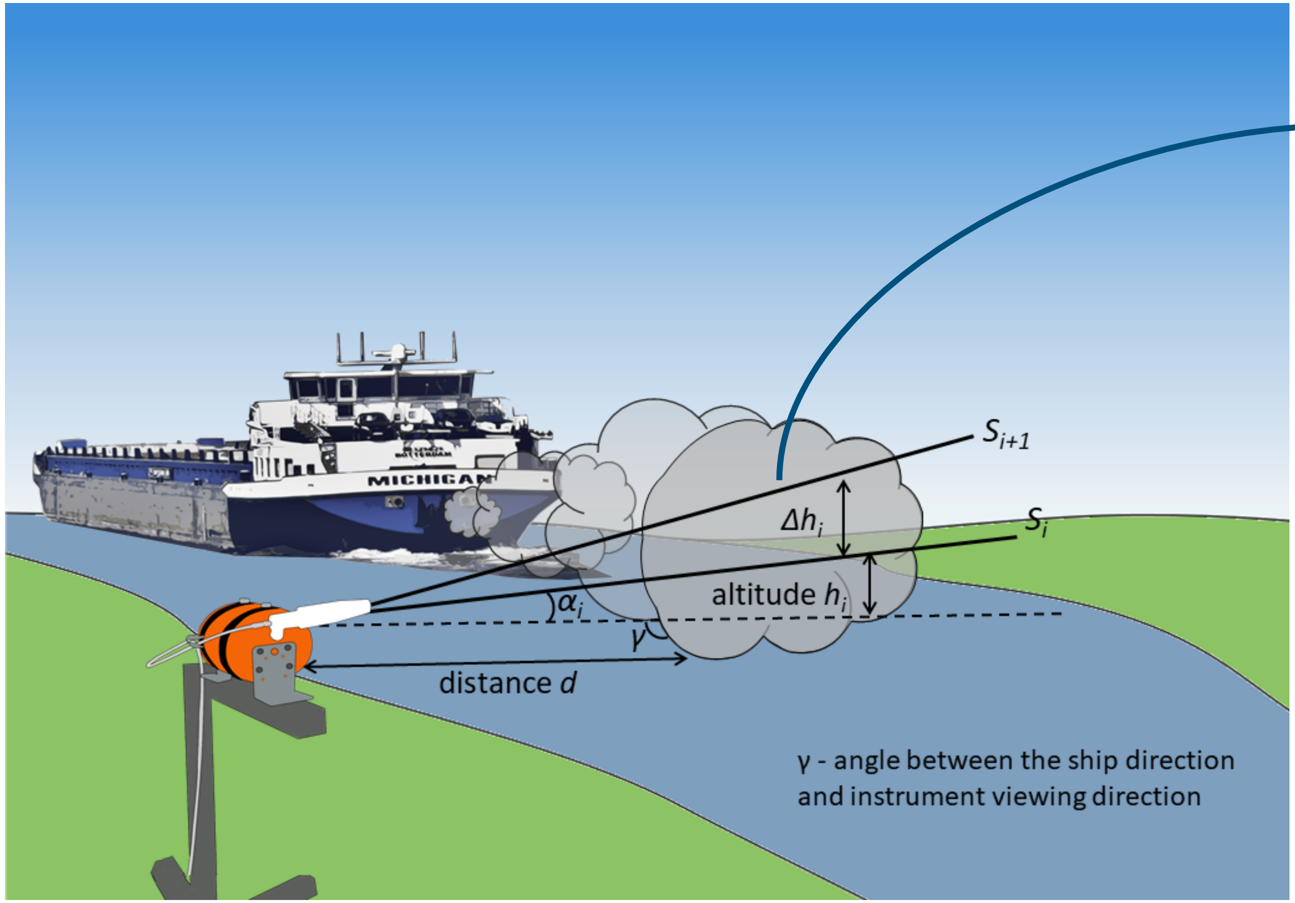
Ground based remote sensing technique **Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS)**

- ▶Always “sees” exhaust plumes
- ▶**Integrative** measurements
- ▶**Plume scans** → determine **emissions**

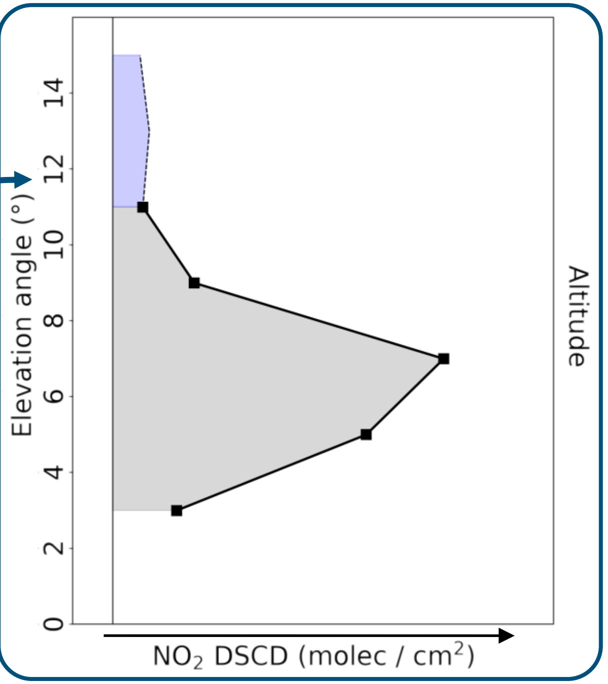
Previous work

Deriving NO_x emissions from inland ships using MAX-DOAS measurements

Integration of NO_2 amount in a ship emission plume



Adapted from Kern (2009)



- ▶ NO_2 column densities

+

- ▶ Ship speed

+

- ▶ Wind speed

NO_x emission flux through the plume cross-section (molec/s)

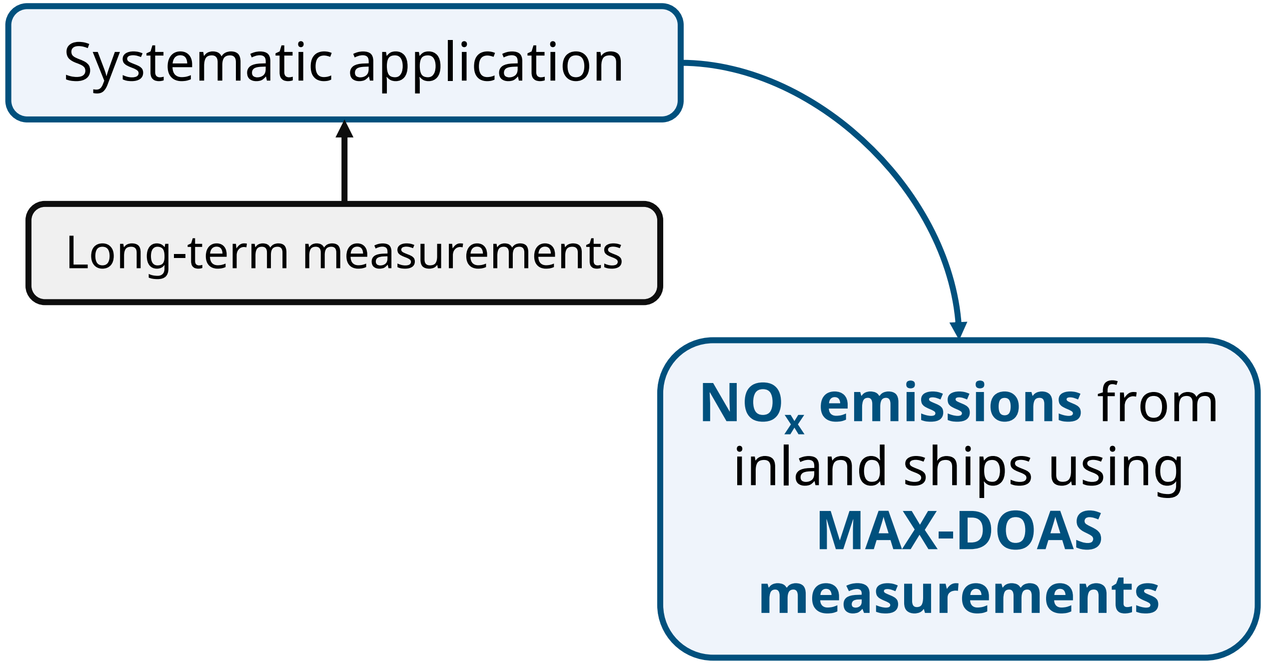
$$\Phi_{NO_x} = f \cdot X_{NO_2} \cdot v_{plume}$$

f – NO_2 to NO_x conversion factor

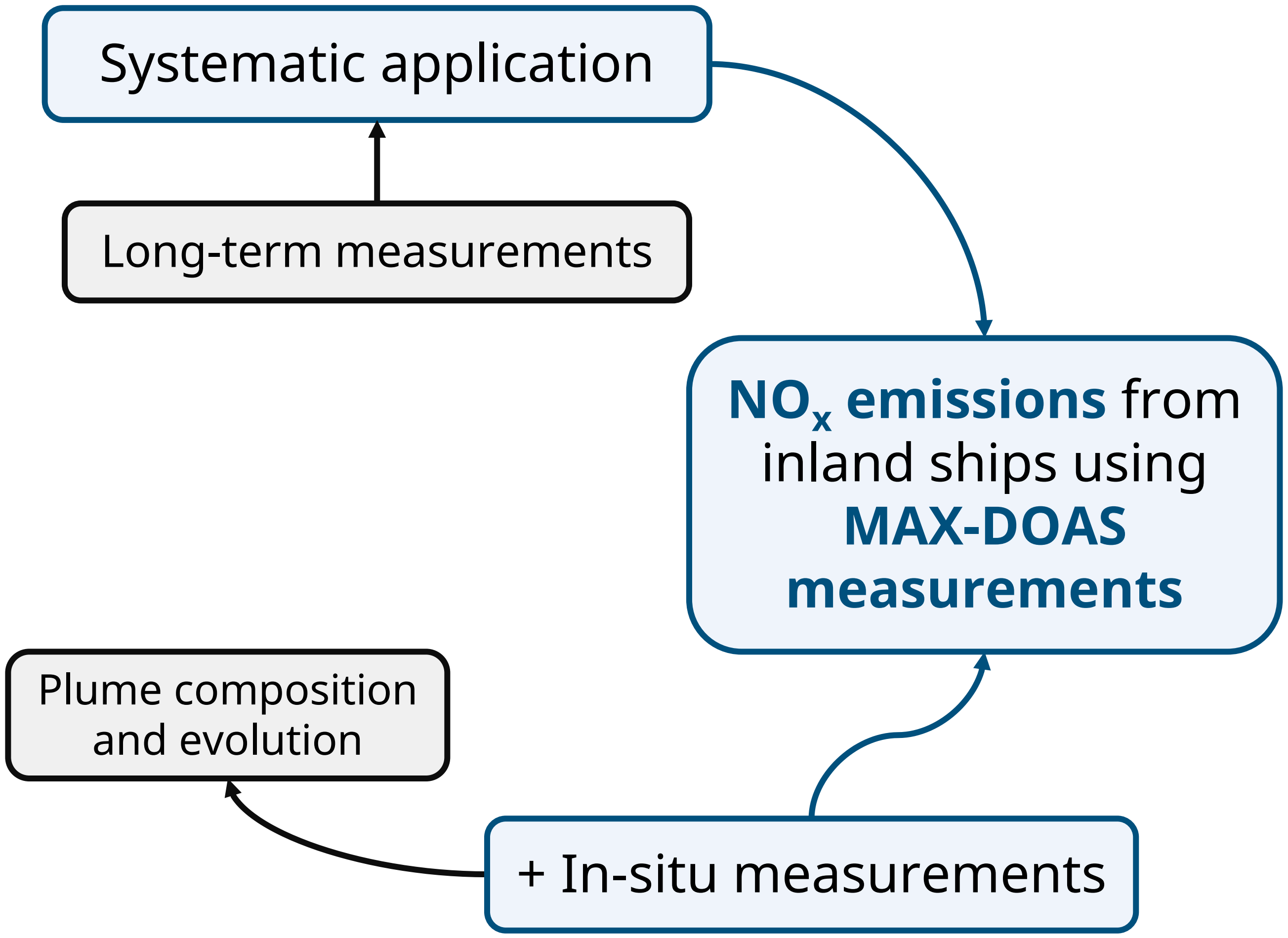
X_{NO_2} - integrated amount of NO_2

v_{plume} - plume transport velocity (v_{plume} - $v_{wind, \parallel}$)

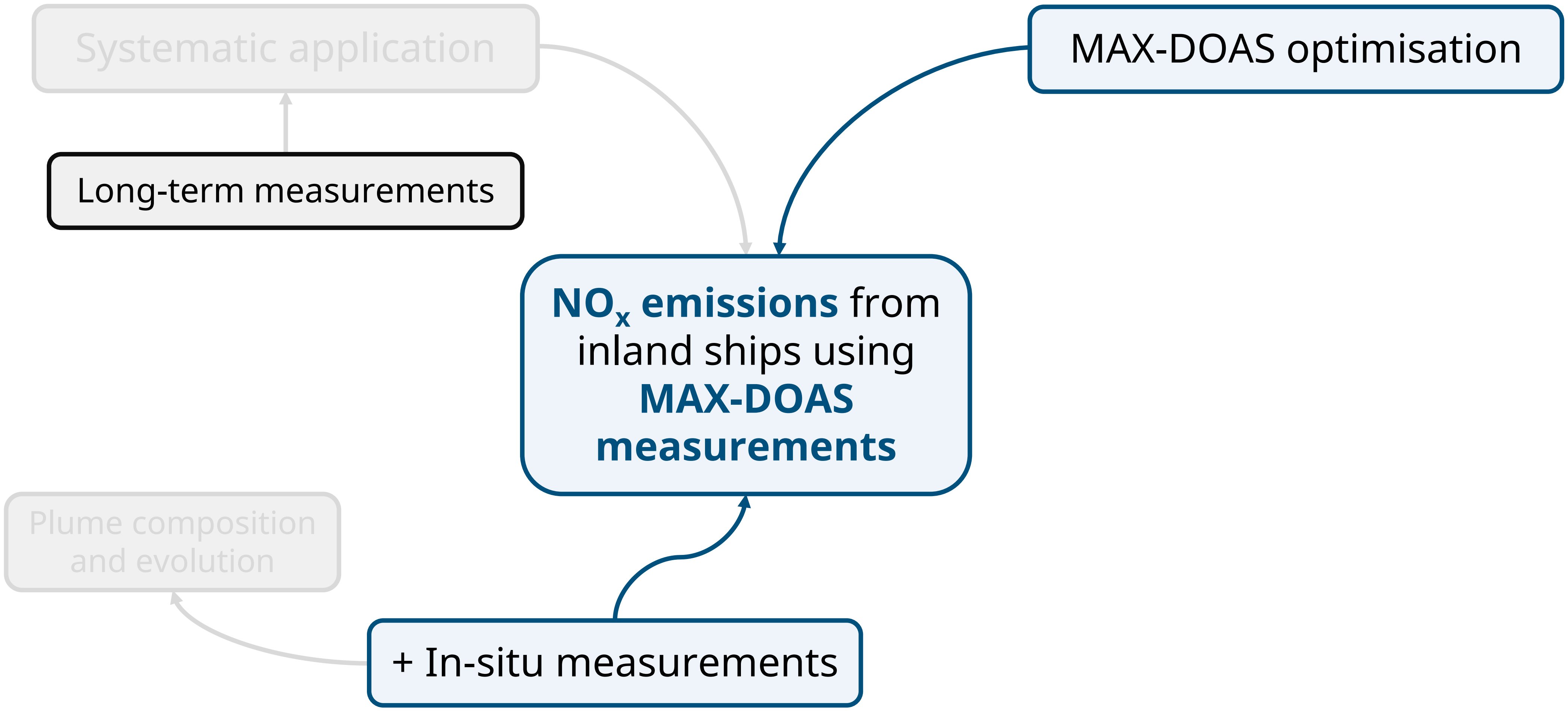
Current work and challenges



Current work and challenges



Current work and challenges



Current work and challenges

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Systematic application

Long-term measurements

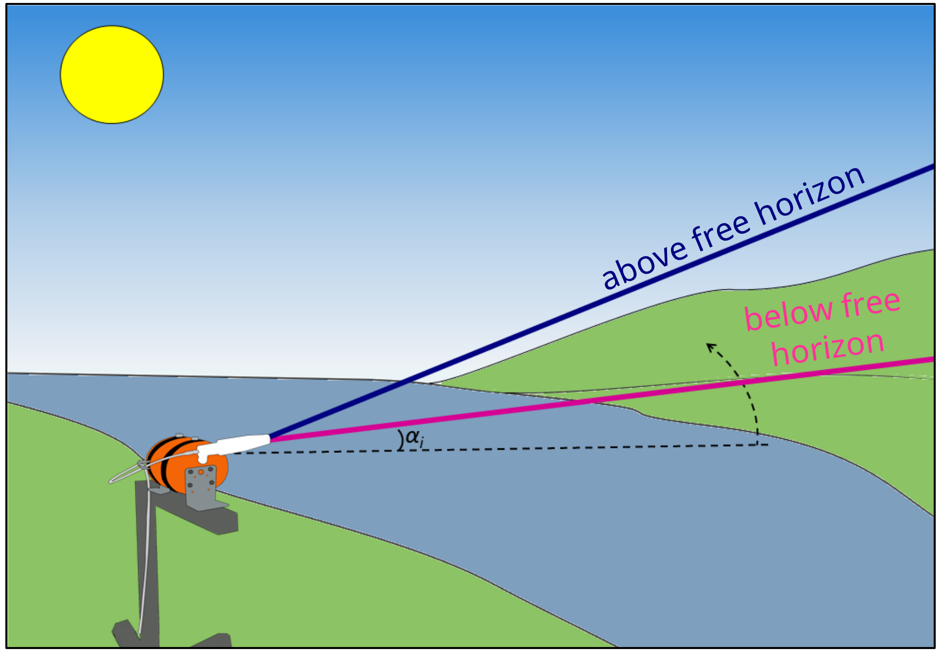
MAX-DOAS optimisation

open sky measurements + **surface reflection measurements**

NO_x emissions from inland ships using **MAX-DOAS measurements**

Plume composition and evolution

+ In-situ measurements



Current work and challenges

Systematic application

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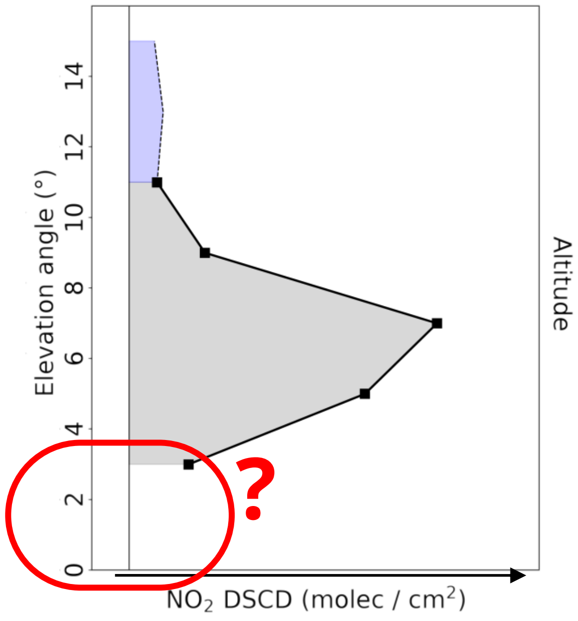
open sky measurements

+

surface reflection measurements

NO_x **emissions** from inland ships using **MAX-DOAS measurements**

Plume start



Plume composition and evolution

+ In-situ measurements

Current work and challenges

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Systematic application

Long-term measurements

NO_x emissions from inland ships using **MAX-DOAS measurements**

Plume composition and evolution

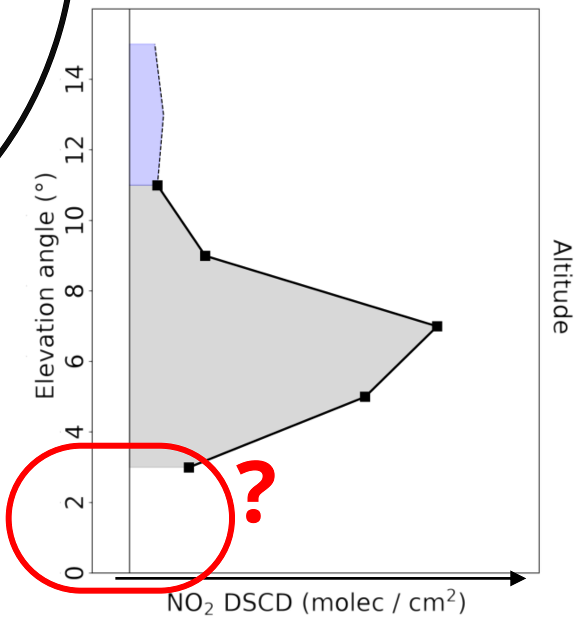
+ In-situ measurements

MAX-DOAS optimisation

open sky measurements + **surface reflection measurements**

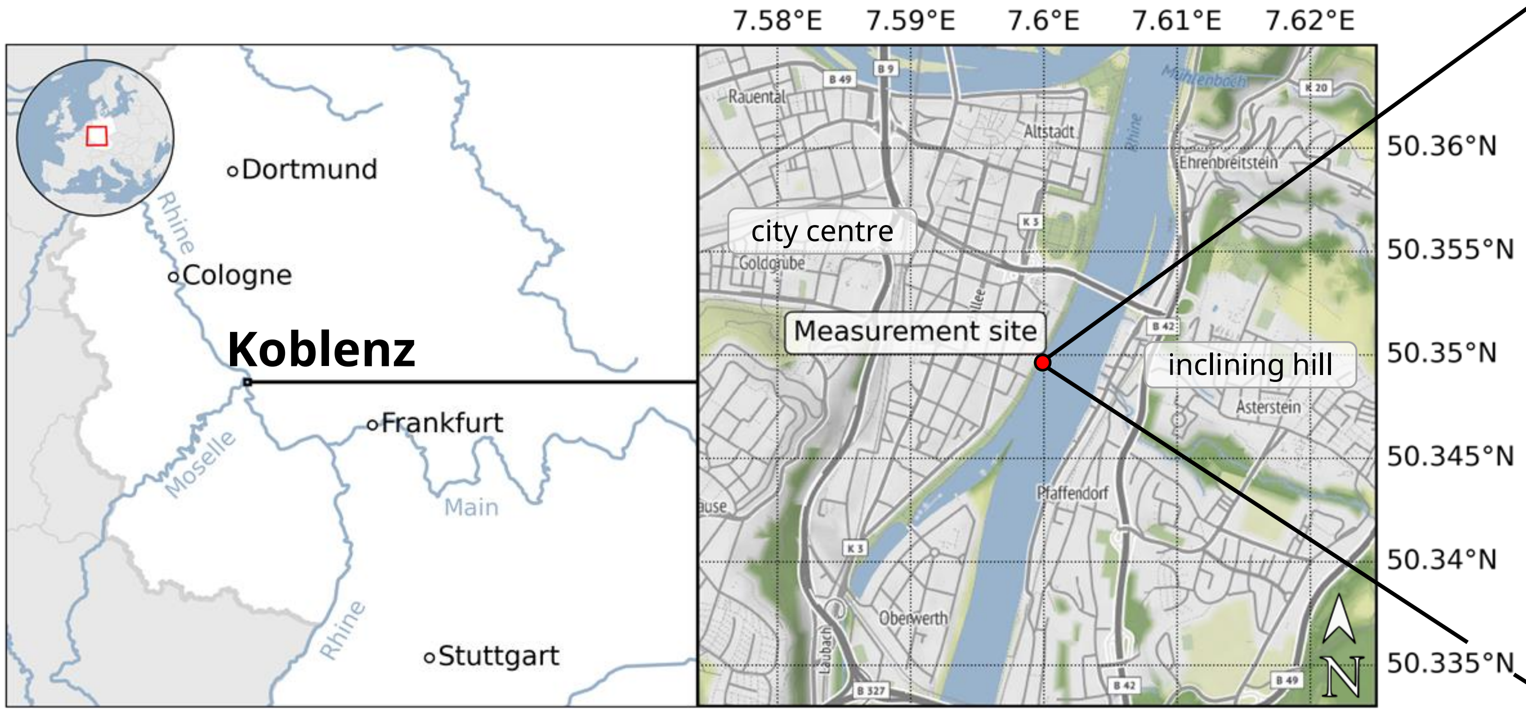
Plume start

More defined light path (like Target-DOAS)



Measurement site

Continuous MAX-DOAS measurements since 26th of January 2024



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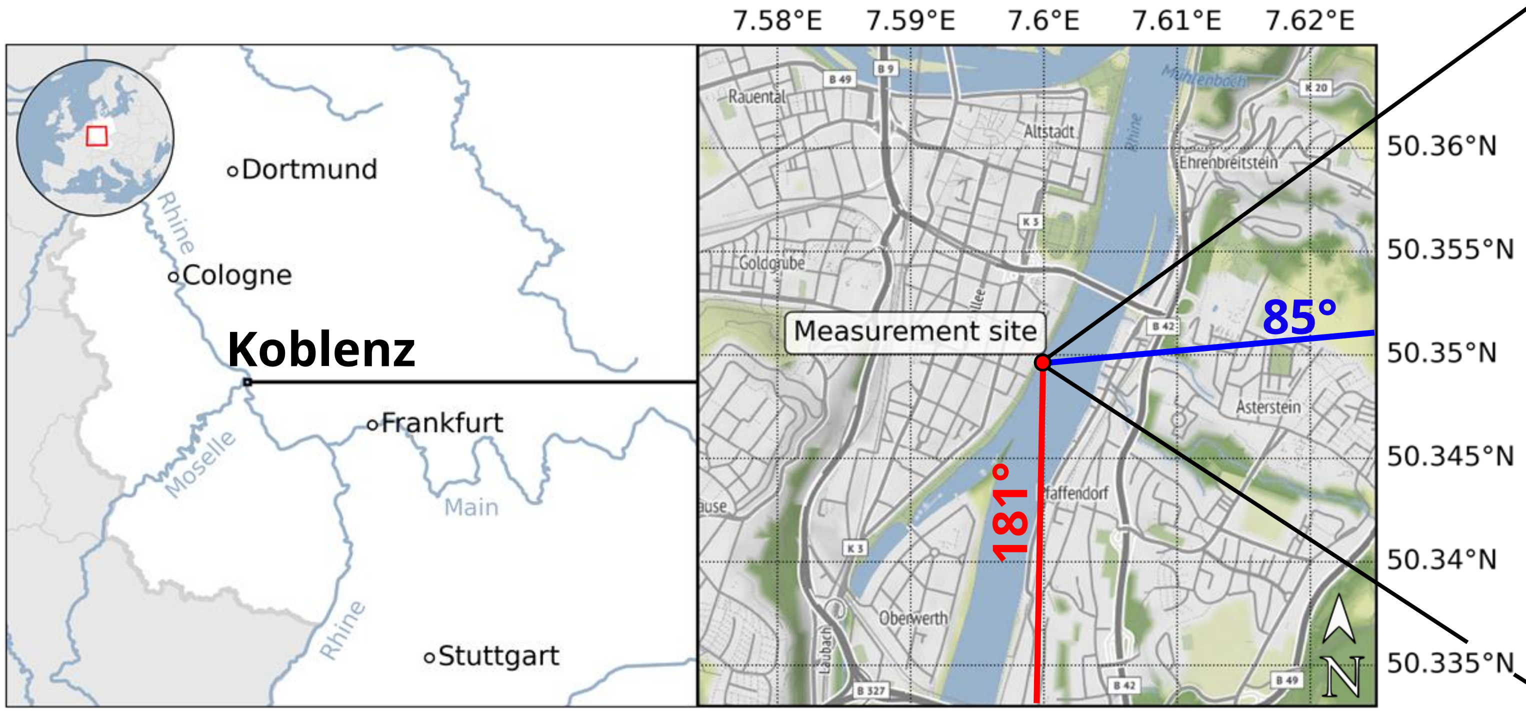
- ► **Rhine River in Koblenz**, west Germany
- ► **Pontoon** (Federal Institute for Hydrology) **on the river**

ICAD - Iterative Cavity-enhanced DOAS

- ► **Provided by Federal Institute for Hydrology:**
  - **ICAD** (Airyx) in-situ monitor data: **NO_2 /NO_x** and **CO_2**
  - **Weather** station data
  - Automatic Identification System (**AIS**) data

Measurement site

Continuous MAX-DOAS measurements since 26th of January 2024



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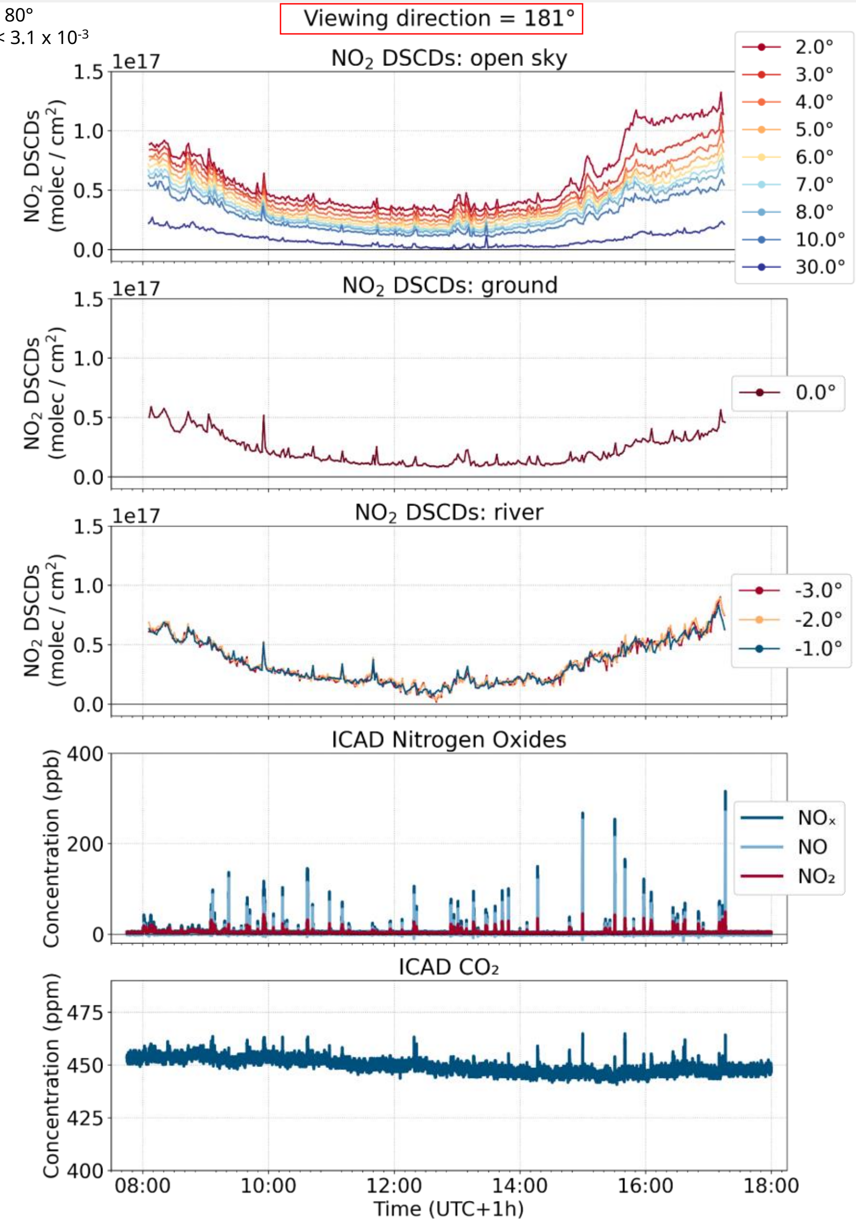
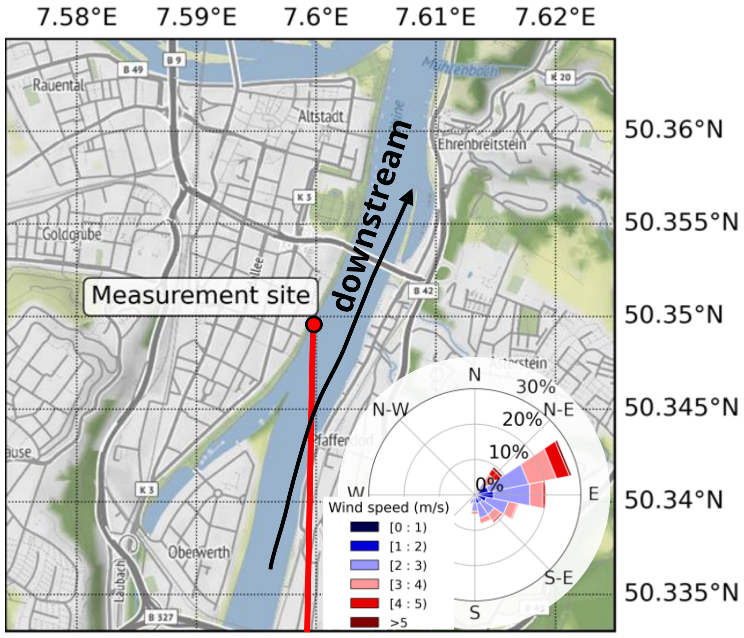
- Measurements every 6 seconds
- > 4000 spectra per day for instrument (increasing)

First results from Koblenz

Timeseries on 9th of March 2024

SZA < 80°
RMS < 3.1 x 10^{-3}





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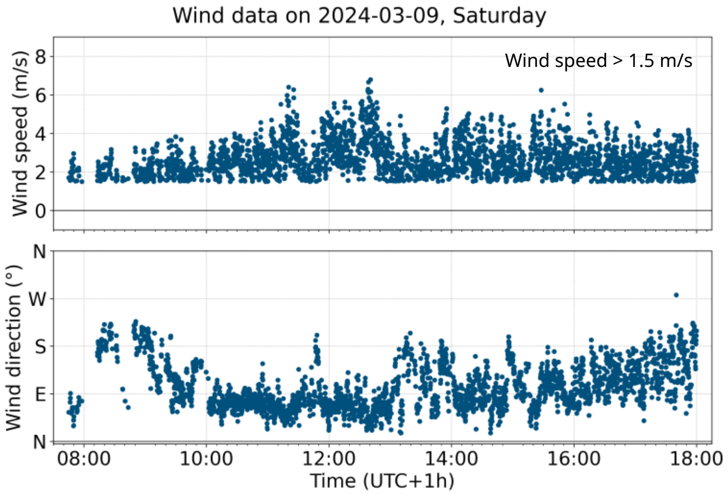

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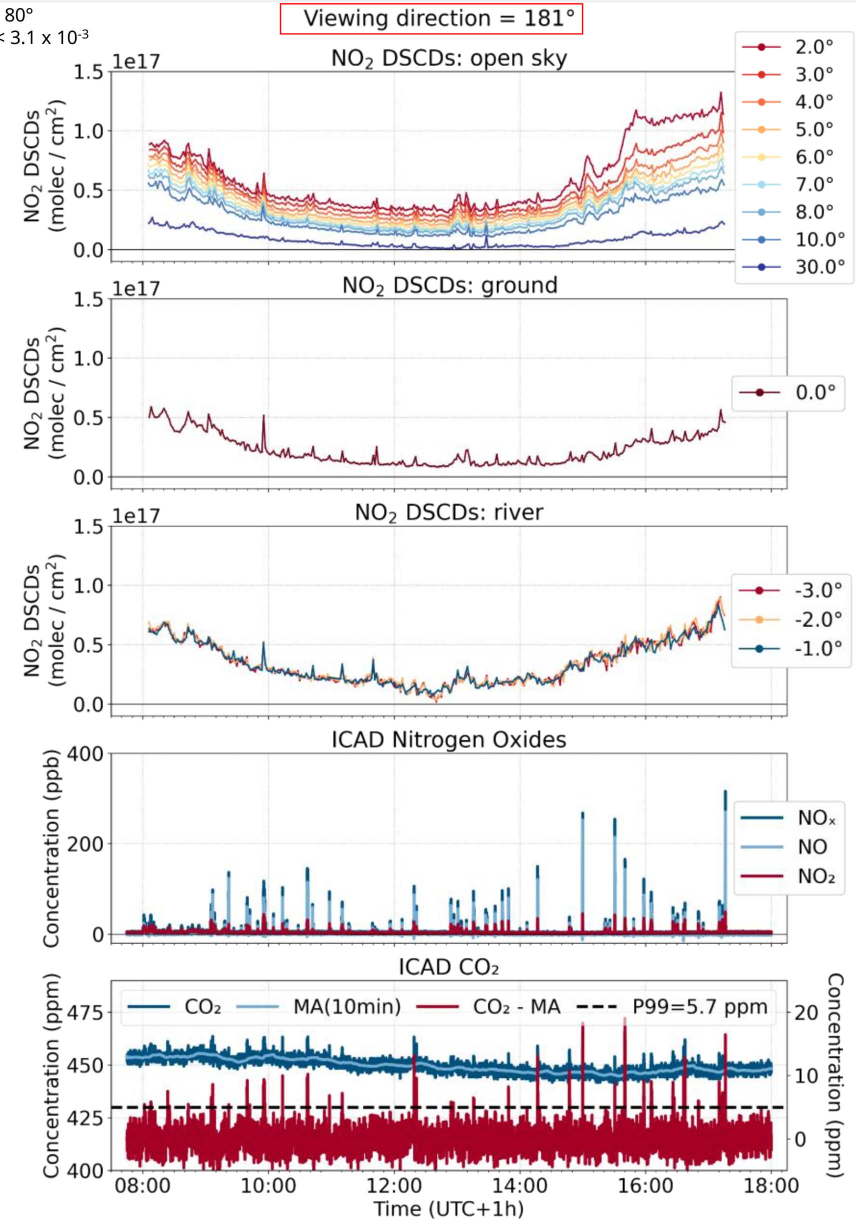

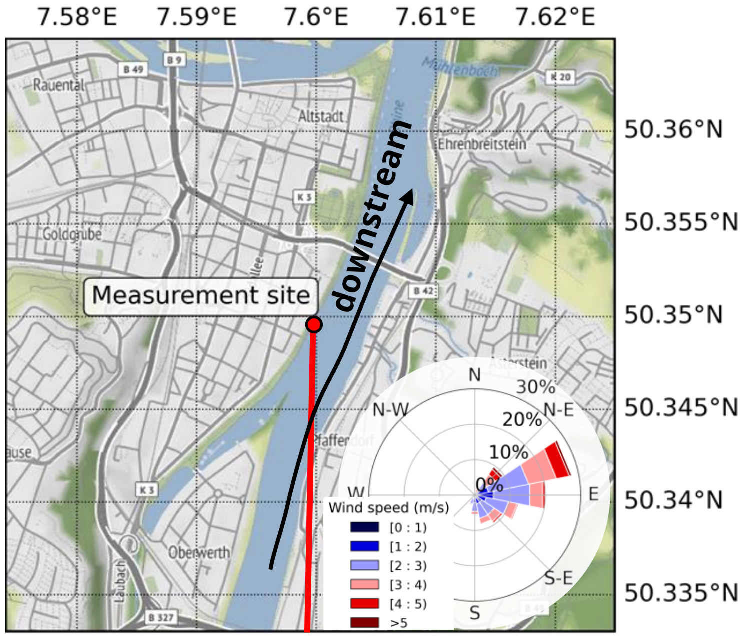

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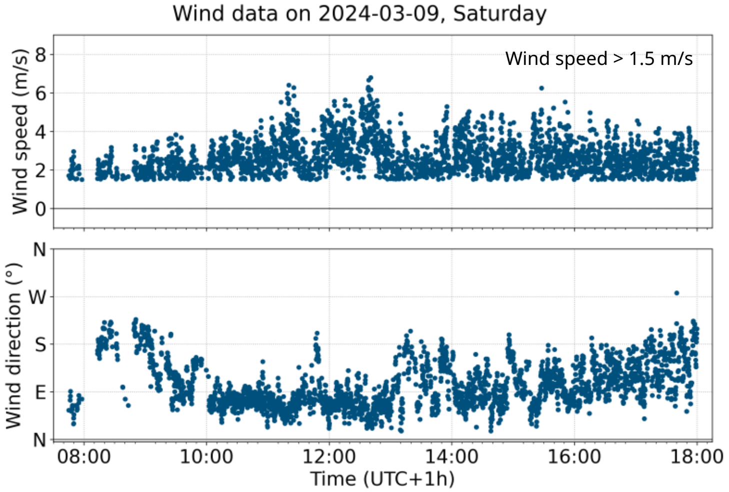

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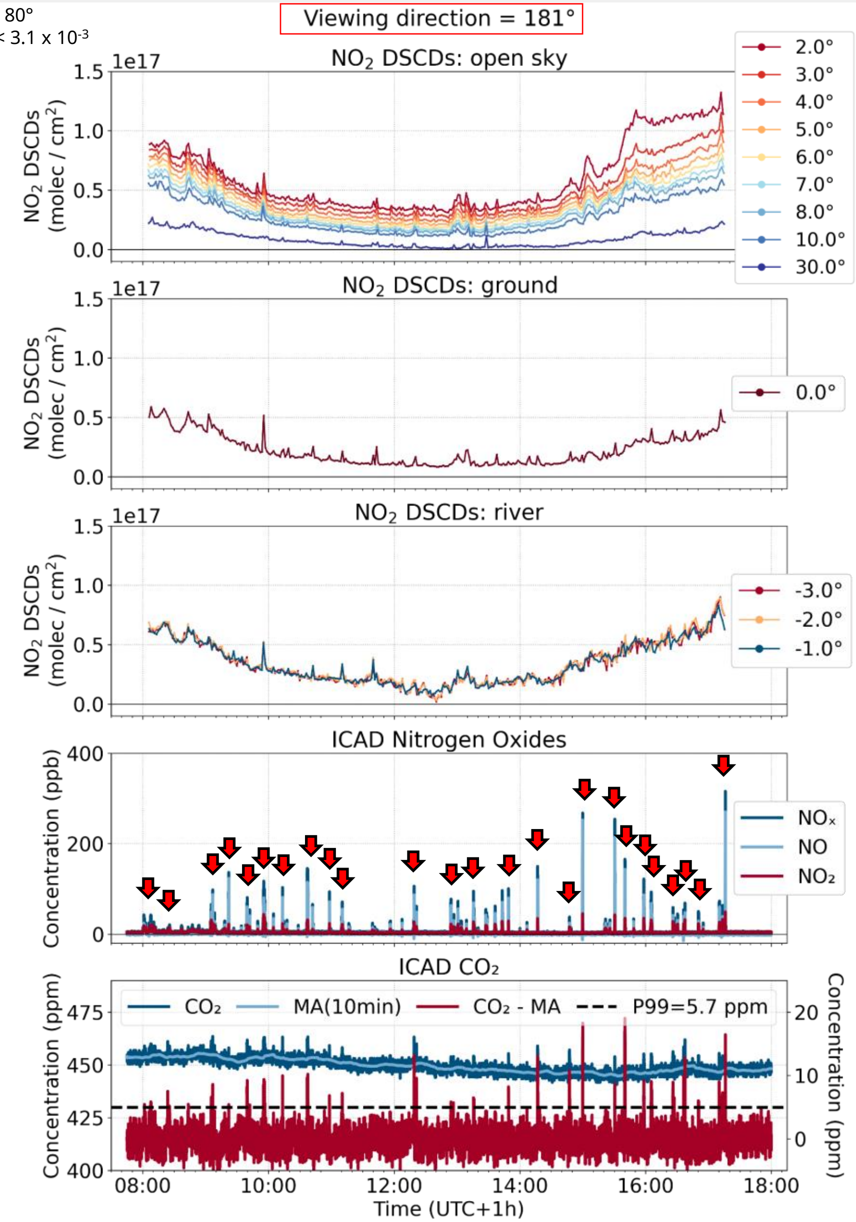

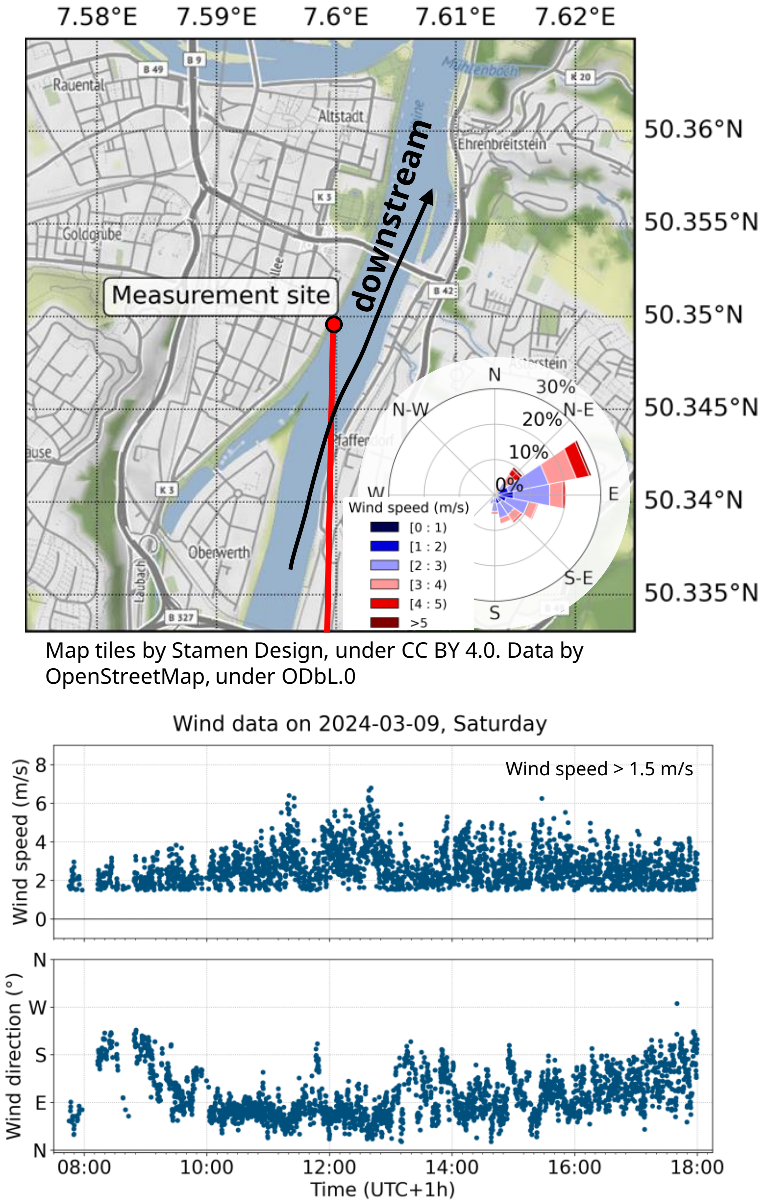

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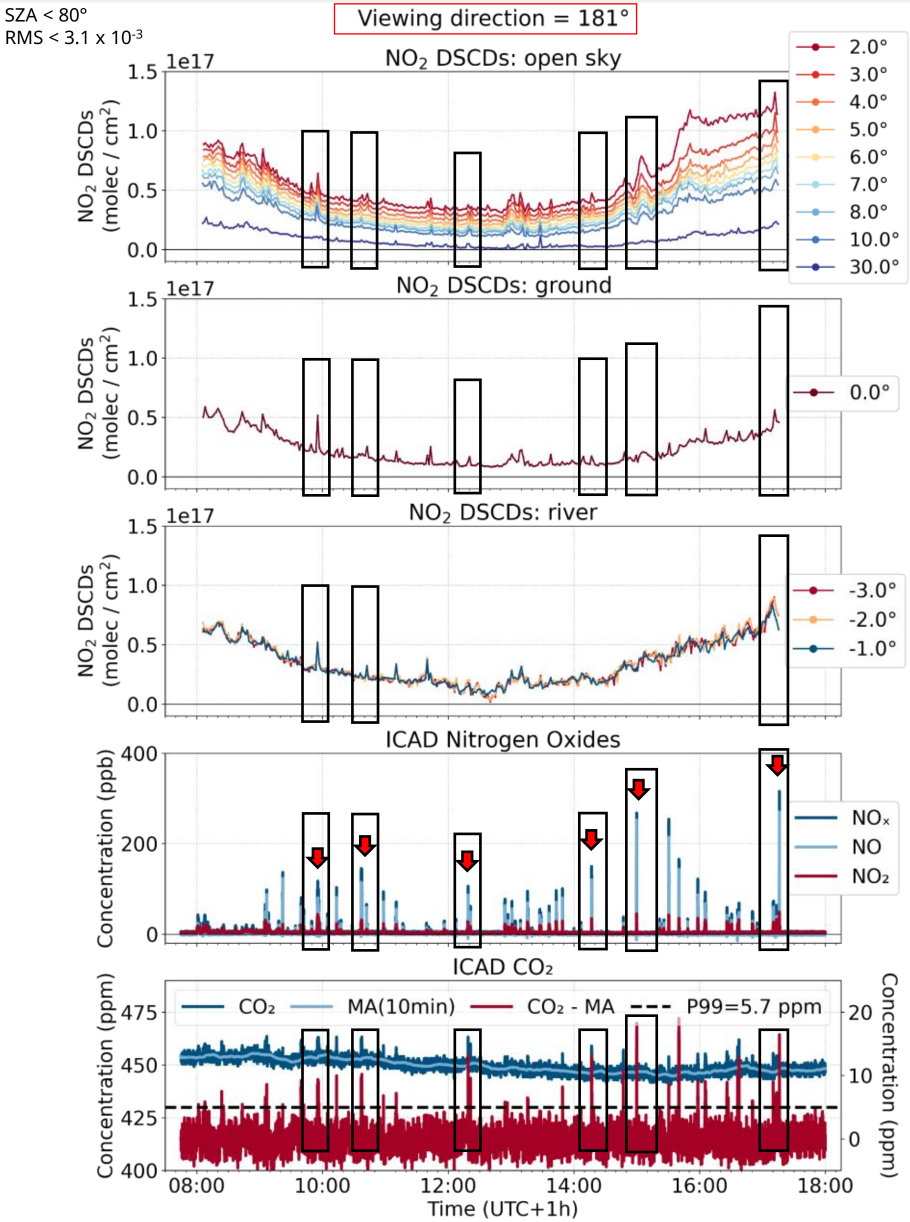
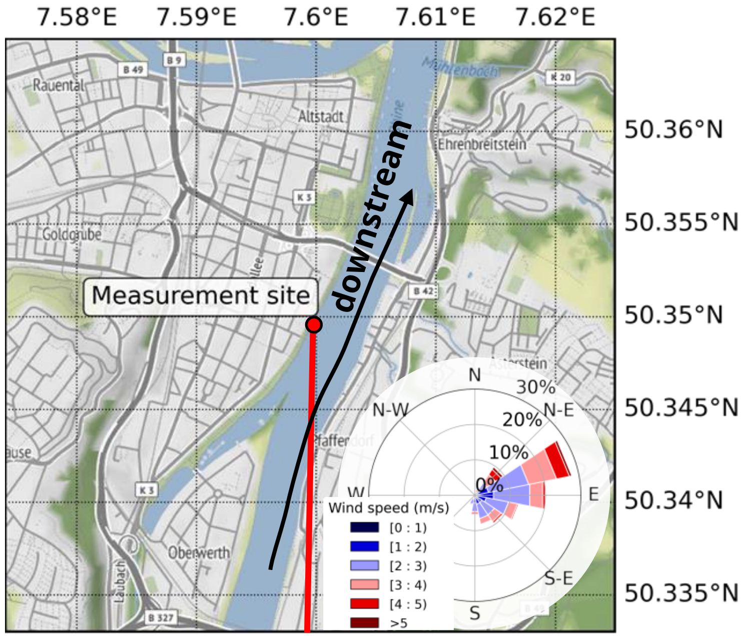
Timeseries on 9th of March 2024





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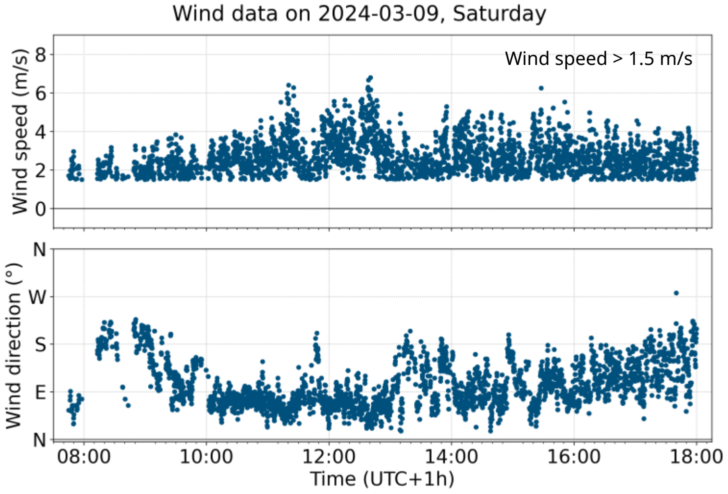
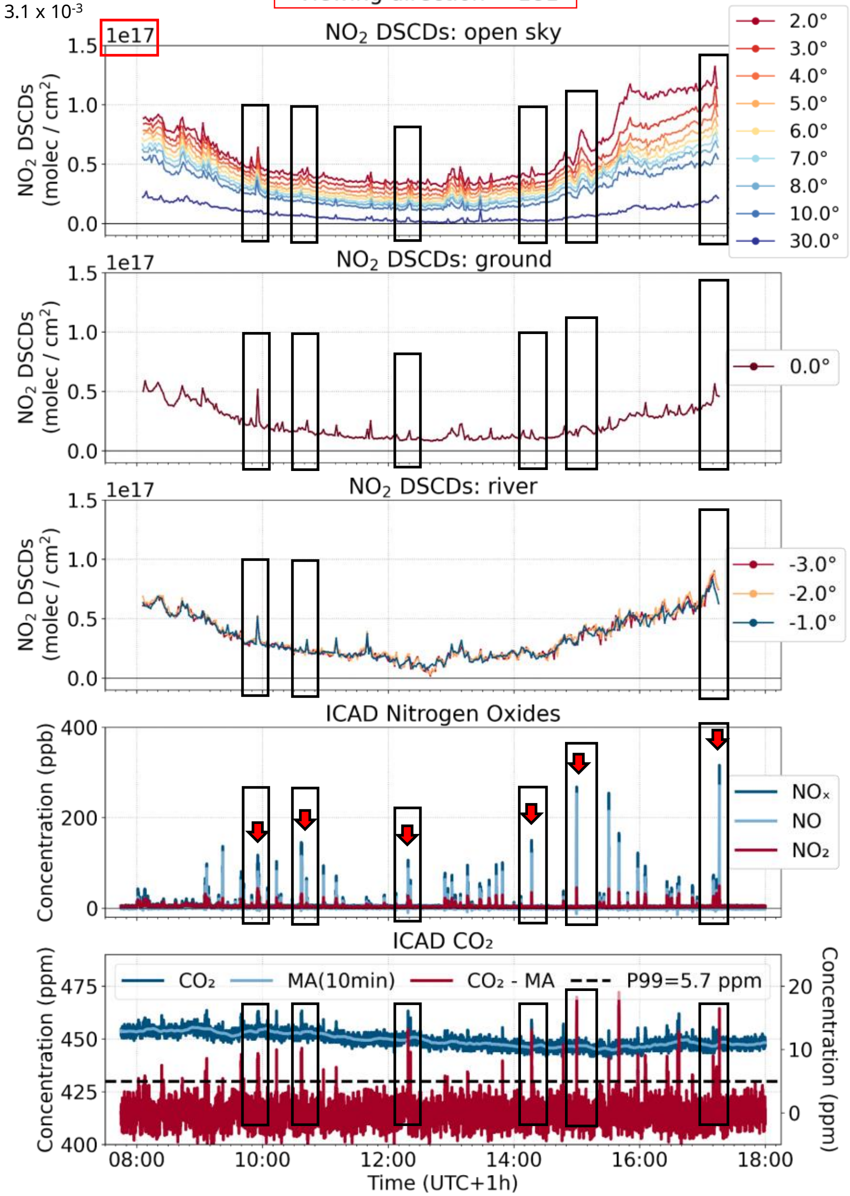
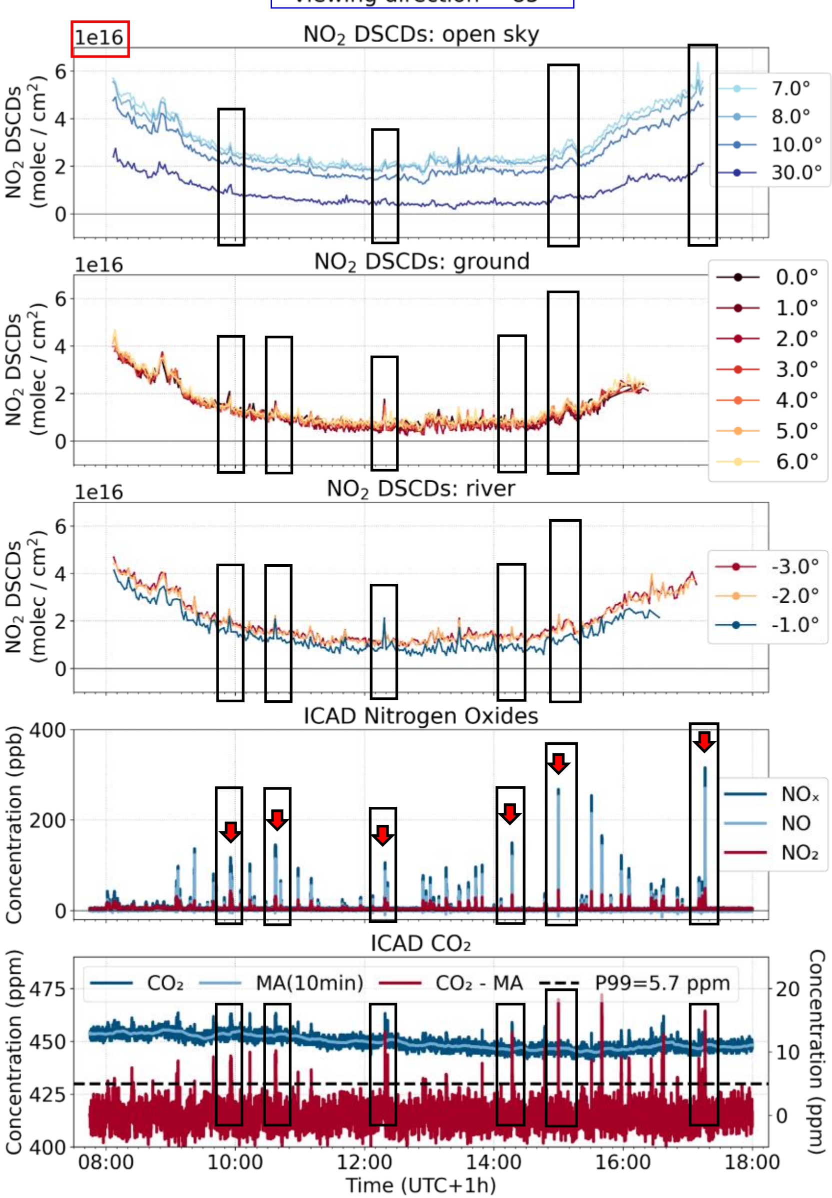


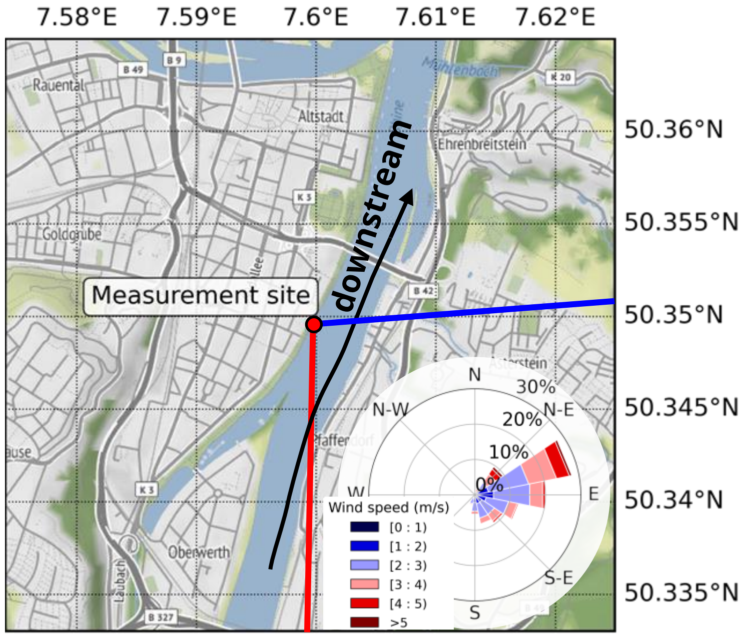
First results from Koblenz

Timeseries on 9th of March 2024

SZA < 80°
RMS < 3.1×10^{-3}







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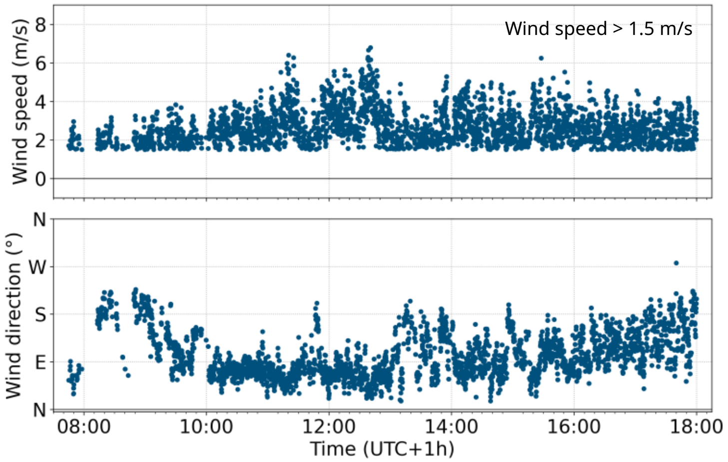
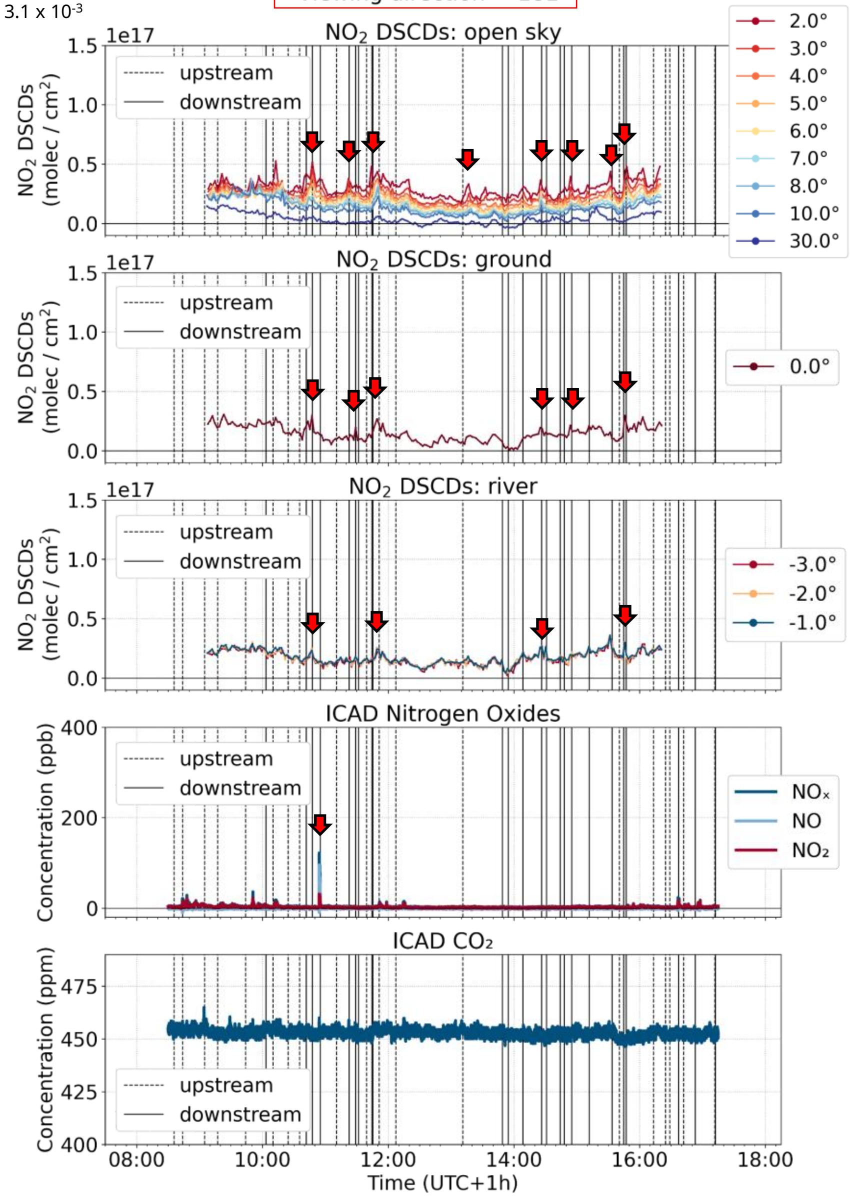


First results from Koblenz

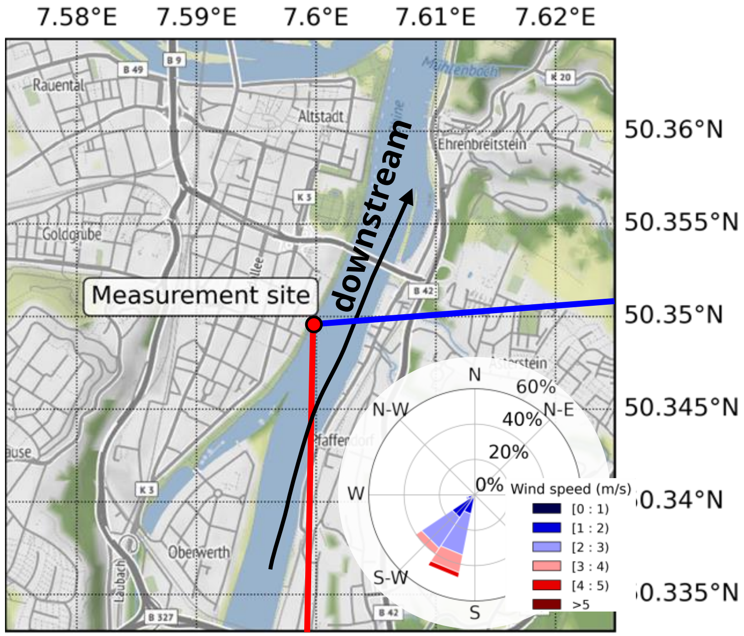
Timeseries on 11th of February 2024

SZA < 80°
RMS < 3.1 x 10^{-3}

Viewing direction = 181°



No data for viewing direction = 85°



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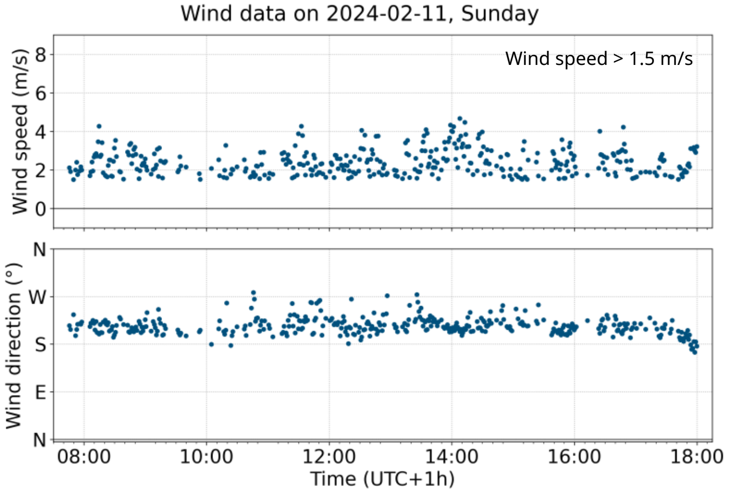

Conclusions and outlook

- Continuous **MAX-DOAS (two instruments)** measurement site at the **Rhine River in Koblenz** since the beginning of this year
- Additional **in-situ NO_x** and **CO_2** data
- Measurements **below the horizon** → information about the **plume start (elevation)**
- **Matching in-situ CO_2 and NO_x peaks** during favourable wind conditions
- **Enhancements in NO_2 DSCDs** for most of the elevation angles regardless of wind direction

- Emissions will be calculated using the shown method
- More data during spring and summer (lower background NO_2 levels)

Abstract

Thanks for your attention!

Special thanks to Philipp Eger and Steffen Ziegler

For questions, comments and suggestions please contact:
Simona Ripperger-Lukošiūnaitė:
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References

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- ►Kern C. Spectroscopic measurements of volcanic gas emissions in the ultra-violet wavelength region. PhD thesis, 2009. Doctoral Dissertation
- ►Platt U. and Stutz J. Differential absorption spectroscopy. In Differential Optical Absorption Spectroscopy. Springer, 2008

Extra slides

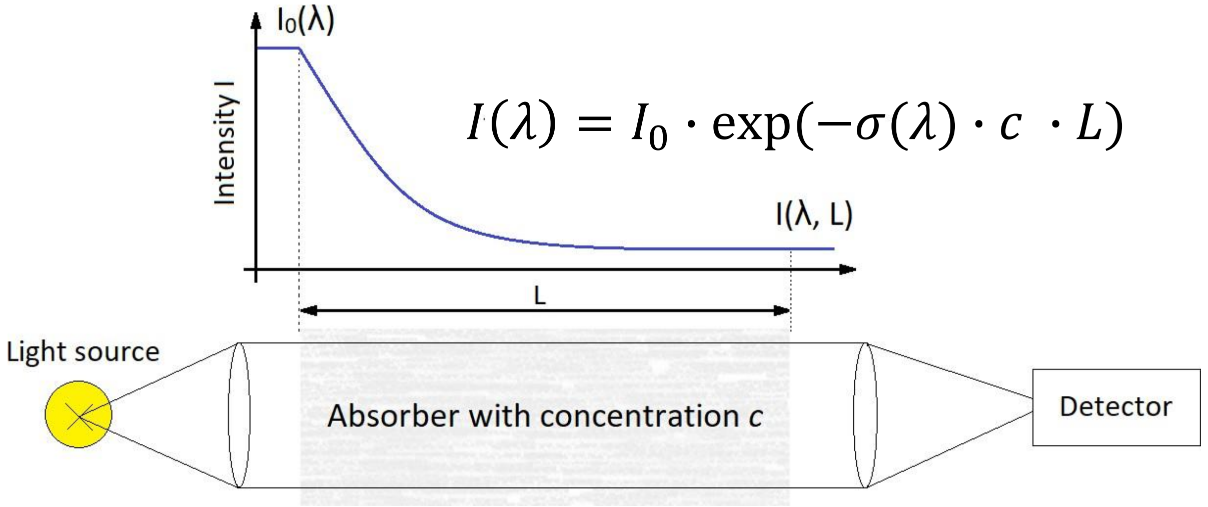
- Differential Optical Absorption spectroscopy (DOAS)
- Multi-AXis DOAS (MAX-DOAS)
- Example of NO_2 fit
- Horizon scans

Differential Optical Absorption spectroscopy (DOAS)

- ▶ Based on Beer-Lambert law

- ▶ BUT: Open atmosphere:
  - multiple trace gases (ci , σi)
  - scattering (Rayleigh, Mie)
  - non-homogeneous distribution

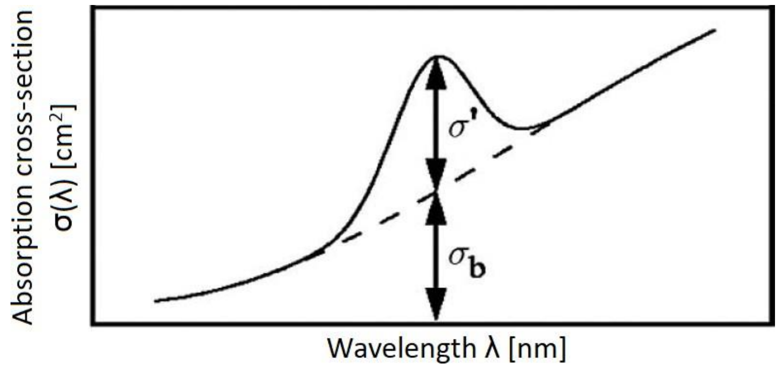
- ▶ Key DOAS idea → separation of σi(λ):
  - broad-band structures $\sigma_{i,b}(\lambda)$
  - narrow-band structures $\sigma'_i(\lambda)$ **(characteristic for certain trace gases**)



Adapted from Platt and Stutz (2008) and IUP Bremen (2020)

Known from laboratory measurements

$$\ln\left(\frac{I(\lambda,L)}{I_0(\lambda)}\right) = -\sum_{i=1}^{N} \mathrm{SCD}_i \cdot \sigma_i'(\lambda) + \sum_{\mathrm{p}} c_{\mathrm{p}} \cdot \lambda^{\mathrm{p}}$$



Adapted from Platt and Stutz (2008)

Retrieved quantity → **Slant Column Density:** $\mathrm{SCD}_i = \int_0^L c(s)ds$ (molec/cm²)

Backup slides

Multi-AXis DOAS (MAX-DOAS)

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- ► Ground-based passive DOAS application (uses natural light source)

- ► Measures **scattered sunlight** spectra in
- ► **different** viewing **directions**

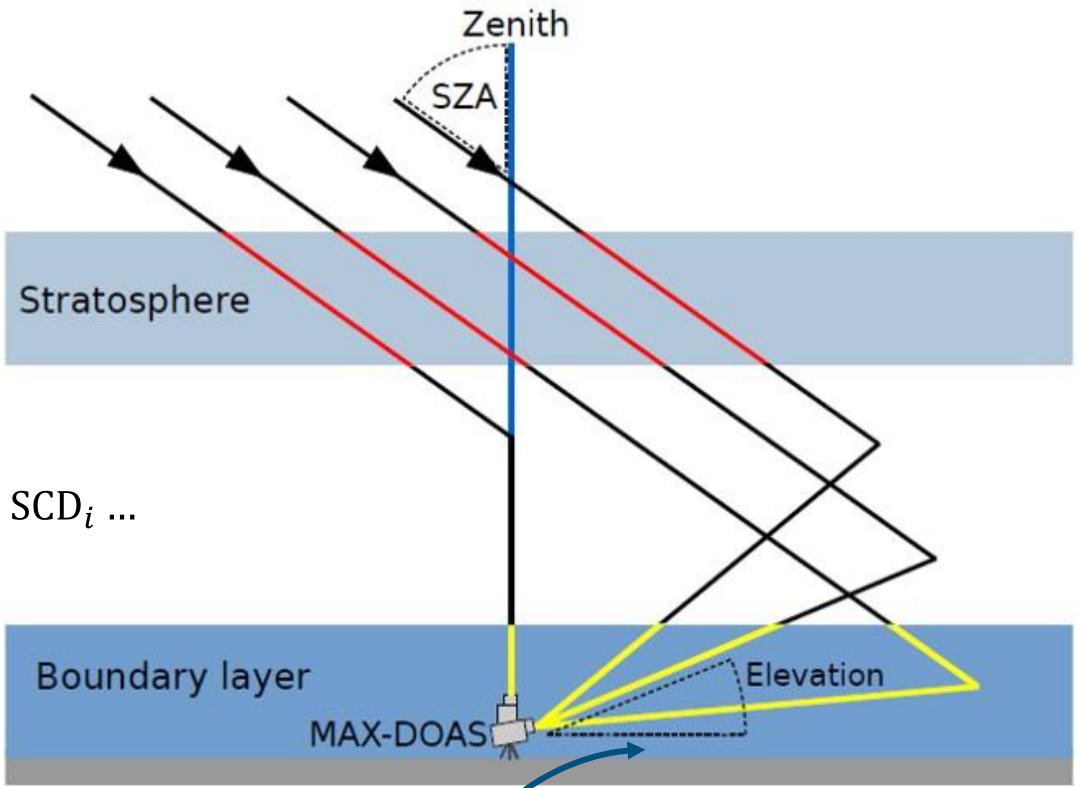
- ► To retrieve SCD, we need:
  - Spectrum with absorption
  - Spectrum without absorption ← cannot be measured

$$\ln\left(\frac{I(\lambda, L)}{I_0(\lambda)}\right) = -\sum_{i=1}^{N} \mathrm{SCD}_i \ldots$$

- ► Retrieved quantity ⟶ **Differential Slant Column Density (DSCD):**

$$\mathrm{DSCD} = \mathrm{SCD}_{\text{off-axis}} - \mathrm{SCD}_{\text{ref}}$$

Reference spectrum - usually taken at 90°



Taken from Seyler (2021)

For tropospheric absorbers:
lower elevation angle → longer light path → higher sensitivity to trace gas

Backup slides

Example of NO_2 fit

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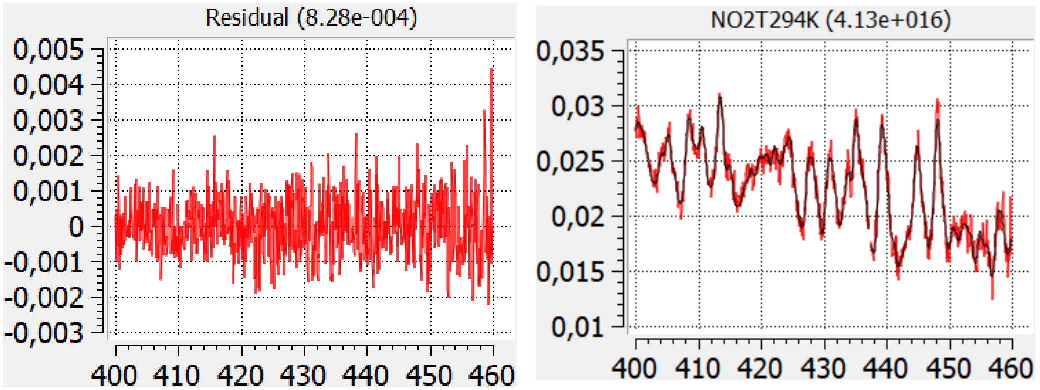
- DSCDs of NO_2 are retrieved using **QDOAS** software (Danckaert et al., 2012)
  - Absorber cross-sections, reference spectrum are fitted to the recorded spectra (offset and dark current corrected)
  - Reference spectrum for the retrieval of DSCDs → **constant reference** (spectrum taken at 90°)
    - Viewing direction 181° = 2024-03-09 at 12:49:26 (UTC +1h)
    - Viewing direction 85° = 2024-03-09 at 12:50:47 (UTC +1h)
  - **Integration time** = 5 seconds

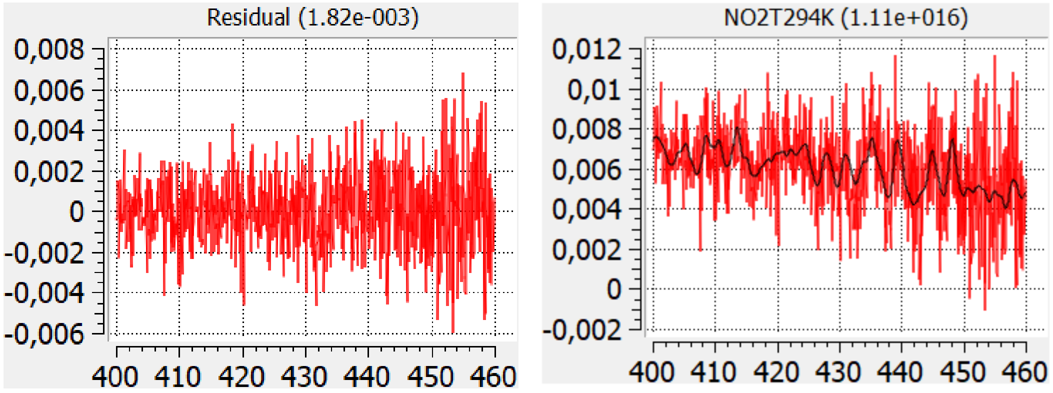
Standard MPIC fit settings for NO_2 (vis)

Parameter	Setting / Reference
NO_2 (at 294 K)	Vandaele et al. (1998)
H_2O (at 293 K)	Lampel et al. (2015)
O_3 (at 223 K)	Serdyuchenko et al. (2014)
O_4 (at 293 K)	Thalman and Volkamer (2013)
Ring effect	Two pseudo cross sections derived from reference
Fit interval	400-460
Polynomial	5th order
Intensity offset	Constant and 1st order
Shift and stretch	Spectra shifted and stretched (1st order) against reference
Reference	Constant spectrum

Time: 2024-03-09 12:59:27 (UTC +1h)
Elevation angle: 2°
SZA: 55°



Time: 2024-03-09 13:03:53 (UTC +1h)
Elevation angle: 3°
SZA: 55°

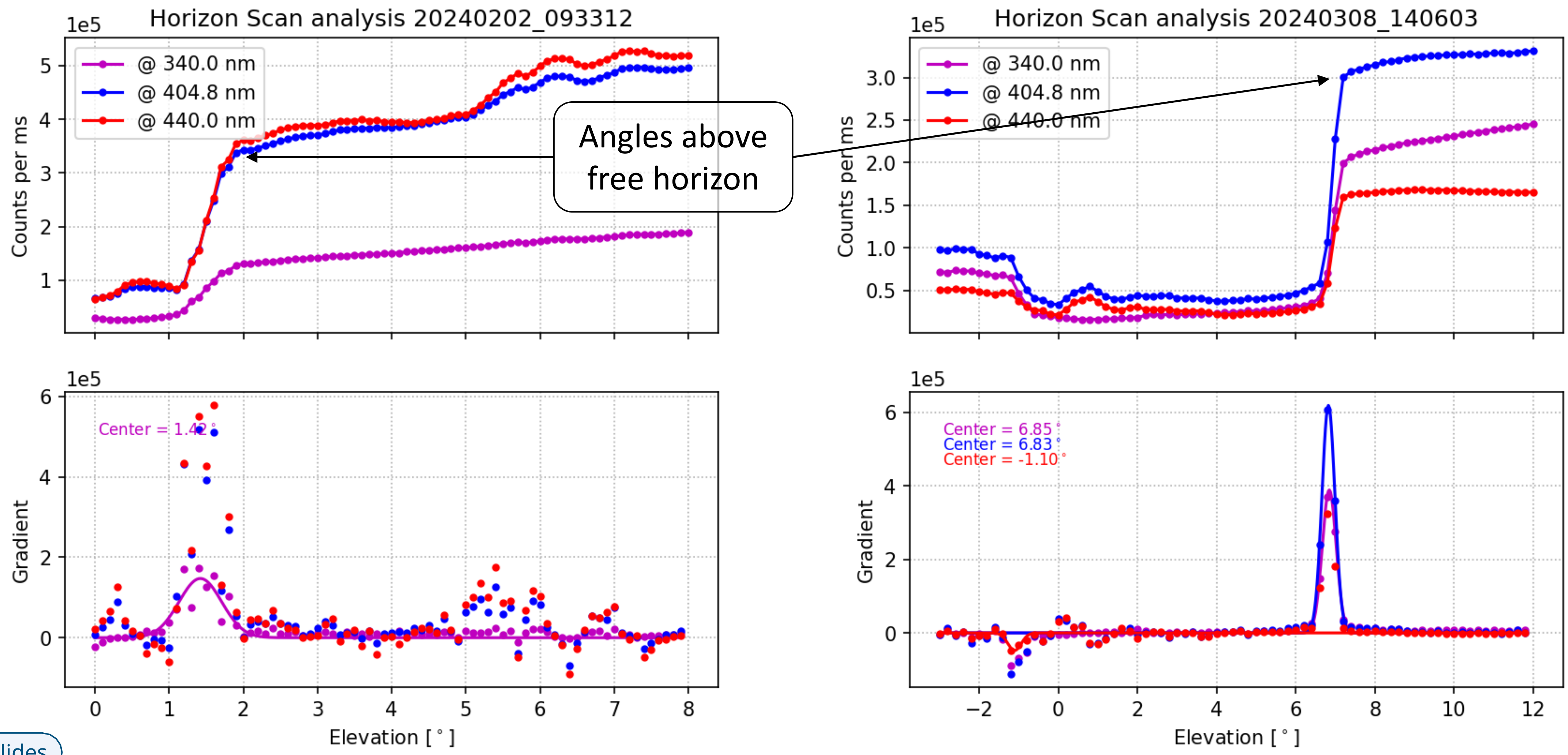


Backup slides

Horizon scans

Viewing direction = 181°

Viewing direction = 85°



Backup slides