A method for retrieving the spatial distribution of trace gases using measurements of three ground-based MAX-DOAS instruments

Three MAX-DOAS instruments in Vienna

Site Address

BOKU Universität für Bodenkultur Peter-Jordan-Gasse 82 1190 Vienna, Austria

VETMED Veterinärmedizinische Universität Veterinärplatz 1 1210 Vienna, Austria

Arsenal A1 Avenel 24 1030 Vienna, Austria

Altitude: 267 m asl 171 m a.s.l. 333 m asl

Elevation angle of "horizontal" plane: 1° 3° 0°

Spectrum: Visible, UV Visible, Visible, Visible

Spectrum of evaluated vertical profiles: Visible, UV Visible UV

Spatial retrieval method for trace gases

2D spatial distribution of trace gases estimated using:

- multiple MAX-DOAS instruments (within range of optical lengths)
- Measured slant column densities (SCD) (see Fig. 1):
  - For various azimuthal directions
  - Within approximately the same vertical plane
  - Intersecting in 2D space

Retrieval method:

- For each "measurement line" the slant column density $S$ is:

  \[ S = \frac{1}{d} \int I(x) \, dx \] (1)

  depending on known effective optical path $d$ and the unknown number density $I(x)$ along the segment $d$.

- The finite number of measurements and intersections divide each measurement line in segments of known discrete lengths $d_i$ such that:

  \[ d = \sum d_i \] (2)

- Eq. (1) is formulated using the sparse matrix $D$ for segment lengths as:

  \[ S = D \cdot I \] (3)

- To account for different number densities in the respective mean altitude of each segment "correction factors” $F$ are introduced:

  \[ I = F \cdot S \] (4)

  The correction factor allows to translate the results to:

  - reference altitude (where $F=1$)
  - Back to each segments’ mean altitude.

Vertical NO$_2$ concentration profiles

Vertical NO$_2$ number density relative to 16th-value [%]

- 2019-06-03 12:00 UTC
- 2019-06-03 12:00 UTC

Retrieved spatial distribution of NO$_2$


Comparison: MAX-DOAS vs. In-situ

Different correction factors have been used as well as data obtained at different spectral ranges:

a) Using SCD and vertical profiles in UV (BOKU @Arsenal) in visible @VetMed (see the measurement lines for this case in Fig. 3). Interpolation between profile data points using a spline of order 5. Comparison with In-situ in Niederösterreich. 19

b) Using the very first approach of vertical profiles in comparison: linear (see black line in Fig. 2 right). Comparison with In-situ in Vienna, Austria. 19

c) As a) but using linear interpolation between profile data points. Comparison with In-situ in green. 19

d) Using SCD and vertical profiles in visible range, except the profile @Arsenal (UV as well not valid as yet). Comparison with In-situ in dark-blue. 19

e) As d) but replacing the value of vertical profiles at 100 m altitude with the In-situ value at St. Stephen’s Square. Comparison with In-situ in brown. 19

Summary & Outlook

- A method for estimating the 2D spatial distribution of trace gas concentrations above an urban environment was developed using DOAS from three MAX-DOAS instruments in Vienna, Austria.
- Vertical profiles of the concentration are used as correction factors to deal with different altitudes of measurement.
- Estimated values close to ground are systematically underestimated.
- Problem: Higher, localized emissions near-in-situ measurement stations and low mixing in deep street canyons.
- Unskewed: impact of terrain in Vienna in combination with the prevailing wind condition.
- In the future: Car-DOAS measurements will be used additionally for comparison with the estimated spatial distribution and the data is expected to improve the vertical profiles close to ground.

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Motivation

- Ground-based MAX-DOAS spectra can be used for the retrieval of tropospheric vertical column densities, horizontal path-averaged mixing ratios/concentrations and vertical profiles of different trace gases.
- Within the VINDOBONA project, three 2D MAX-DOAS instruments have been installed at three different locations in Vienna.
- Measurements in various directions covering the central area of the city of Vienna open a new way to determine the spatial distribution of trace gases above this area.
- In this study, (E) a method was developed to retrieve the spatial distribution of trace gases using MAX-DOAS measurements, (D) show the new method of the NO$_2$ concentrations and (A) assess a couple of different settings to improve results retrieved.

Vertical NO$_2$ measurements of NO$_2$ VODs via

- BOREAS – MAX-DOAS profile retrieval algorithm
- 2019-06-03 12:00 UTC
- 2019-06-03 12:00 UTC

Fig. 2: Vertical profiles of NO$_2$ concentration for the three sites and evaluated spectra (VINDOBA), with a direction Vienna city center.

- Left: number density for each case measured in situ value at St. Stephen’s Square in Vienna, Right: Correction factor for the retrieval method calculated as number density for each case normalized by each respective value in Fig. 3, and a simple linear profile "approximation" (initial method).

Fig. 3: Results: Estimation of a 2D spatial distribution of NO$_2$ over Vienna, Austria on a clear day (Fig. 03 June 2019 (Vind)). Using SCD and vertical profiles in UV (BOKU @Arsenal) in visible @VetMed and linear interpolation between profile data points. For comparison, the measured data of in-situ stations is shown as circles. Left: Vertical profile, Right: 12:00 UTC.

Fig. 4: Sentinel-2P vertical column densities of NO$_2$, over Vienna, Austria for qualitative comparison with estimated MAX-DOAS results in Fig. 3. The locations of the three MAX-DOAS instruments are shown as red dots.

Fig. 5: Estimated NO$_2$ concentration (μg m$^{-3}$) depending on reference altitude different correction factors or data from different spectral optical ranges.

- Estimation vertical profile values, using spline or linear, has no significant effect.
- Due to hilly terrain in the north west using data for UV spectral range (shorter effective optical path) is preferred.
- No mixing of data for different spectral ranges.
- Using In-situ measurement data from ground profile value for lowest altitude improves estimated values close to the ground.