Eight-component retrievals from ground-based MAX-DOAS observations

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Exploring the potential of MAX-DOAS - multi-component retrievals -

• The CINDI campaign has provided the first opportunity for an intensive MAX-DOAS intercomparison study. Most of MAX-DOAS instruments covered UV and/or VIS regions, in which significant absorptions by not only NO₂ but also other trace gases are available.

• In principle, the MAX-DOAS NO₂ vertical profile retrieval method utilizing AMFs derived through the aerosol profile retrieval can be applied to other trace gases, where O₄ absorptions are available for both UV and VIS regions.

• However, this potential has been poorly explored, as the MAX-DOAS development is at an early stage.

• It is expected that exploring this potential using CINDI data would accelerate the MAX-DOAS development over a wide research area.

• Here, we present results obtained from our multi-component retrieval applied to CINDI data.
The JAMSTEC's MAX-DOAS was installed on the roof of the porte cabin #4.
Windows chosen for the "8-component" retrievals

<table>
<thead>
<tr>
<th>Target component</th>
<th>Fitting window (nm)</th>
<th>Absorbers fitted</th>
<th>Representative wavelength (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SO₂</td>
<td>310-320</td>
<td>O₃, NO₂, HCHO, SO₂, Ring</td>
<td>315</td>
</tr>
<tr>
<td>O₃</td>
<td>310-335</td>
<td>O₃, NO₂, HCHO, SO₂, Ring</td>
<td>317</td>
</tr>
<tr>
<td>HCHO</td>
<td>336-359</td>
<td>O₃, NO₂, HCHO, BrO, O₄, Ring</td>
<td>344</td>
</tr>
<tr>
<td>AEC₃₅₇nm</td>
<td>338-370</td>
<td>O₃, NO₂, HCHO, BrO, O₄, Ring</td>
<td>357</td>
</tr>
<tr>
<td>CHOCHO</td>
<td>436-457</td>
<td>O₃, NO₂, CHOCHO, H₂O, O₄, Ring</td>
<td>448</td>
</tr>
<tr>
<td>NO₂</td>
<td>460-490</td>
<td>O₃, NO₂, H₂O, O₄, Ring</td>
<td>474</td>
</tr>
<tr>
<td>AEC₄₇₆nm</td>
<td>460-490</td>
<td>O₃, NO₂, H₂O, O₄, Ring</td>
<td>476</td>
</tr>
<tr>
<td>H₂O</td>
<td>495-515</td>
<td>O₃, NO₂, H₂O, Ring</td>
<td>506</td>
</tr>
</tbody>
</table>

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Japanese MAX-DOAS profile retrieval algorithm, version 1 (JM1)
Special parameterization of profile

- In my intensive development period 2005-2007, Frieß et al. (2006) suggested that the aerosol retrieval can strongly depend on the a priori, if the absolute value of AEC is used.

- Indeed, lidar data at Tsukuba showed large temporal variations, but most aerosols were, in general, near the surface (70% of AOD in 0-1 km).

- At that time, some groups (incl. Heidelberg group) were using a simplified profile, represented by AOD and the mixing height.

- I decided to use a parameterization consisting of:
  - AOD (total column)
  - profile shape (e.g., $F_1$ is the fraction of AOD in 0-1 km)

How do we set a-priori values?
General characteristic of the retrieval, in terms of the a priori parameters used

- **Aerosol retrieval**
  - The retrieval is not subject to the a priori of AOD, because the area* for AOD is almost unity. (*a rough measure of the fraction of the retrieval that comes from the measurements)
  - The retrieval of AEC at 0-1 km is less subject to the a priori of $F_1$, but the AECs above 1 km could be influenced to some extent.

- **NO$_2$ (and other trace gases) retrieval**
  - Profile shape factors are based on lidar aerosol data at Tsukuba for 2006-2007.
  - The a priori NO$_2$ column used is the 20% of the largest value in a set of NO$_2$ DSCDs for each retrieval. → The a priori varies with time.
  - The retrieval is not subject to the a priori of NO$_2$ column, because the area is almost unity.
  - The retrieval of NO$_2$ at 0-1 km is less subject to the a priori of $F_1$, but the NO$_2$ above 1 km could be influenced to some extent.

➢ Profile is retrieved by scaling the given a-priori profile first, followed by changing the profile shape if enough information is contained.
➢ Identical a priori setups have been used for all the sites of our observations.
Results
Vertical profiles retrieved with JM1 and time series of the data for the 0-1 km layer
Our MAX-DOAS aerosol retrieval seems reasonable, when compared with CIMEL AOD data.

The systematic difference from surface AEC data can be explained by vertical (and potentially horizontal) inhomogeneity of the aerosol distributions in the lower troposphere at Cabauw.
Both in-situ and MAX-DOAS data show diurnal variations with high concentration in early morning. Minimum concentrations are found in early afternoon (around 2 pm).

When the boundary layer is well mixed, excellent agreement is found. In early morning, MAX-DOAS data is deviated from the surface value, but the same tendency occurs in in situ data at 200 m → the observed differences were likely caused by vertical inhomogeneity in NO₂ below 1 km.
HCHO & CHOCHO (0-1 km)

HCHO
- Positive correlation
- $R = 0.80$
- CHIMERE smaller by a factor of 2.5 (60%)
- Suggests the production of HCHO from isoprene

CHOCHO
- Positive correlation
- CHIMERE smaller by a factor of 4.5 (~80%)

CHOCHO/HCHO ratio
- Usually less than 0.05
- Mean
  - 0.036 (MAX-DOAS)
  - 0.013 (CHIMERE)

These results may suggest that there is the need of improvement for emissions and chemistry in CHIMERE.
H$_2$O (0-1 km)
SO$_2$ & O$_3$ (0-1 km)

SO$_2$
- Positive correlation
- Very high values seen only from MAX-DOAS

- Back trajectory analysis suggests that SO$_2$ emission from ships may have led to the observed enhancement in SO$_2$.

O$_3$
- Positive correlation
Spatial representativeness for the lowest layer in profiles retrieved by JM1

\[ D = \sqrt{A_{\text{box}, \text{max}}^2 - 1} \]

The MAX-DOAS spatial representativeness for the lowest-layer data in JM1 can be regarded as roughly **10 km (horizontal) x 1 km (vertical)**, which is comparable to or better than satellite observations and model calculations.

MAX-DOAS can provide multi-component data useful for the evaluation of satellite observation and model calculations, playing an important role by bridging different data sets having different spatial resolutions.
Summary

- We have developed a method of retrieving lower-tropospheric vertical profile information for the 8 components: AEC\textsubscript{357nm}, AEC\textsubscript{476nm}, NO\textsubscript{2}, H\textsubscript{2}O, HCHO, CHOCHO, SO\textsubscript{2}, O\textsubscript{3}.
- The developed algorithm (JM1) has been applied to CINDI data.

- AEC data showed good correspondence with CIMEL AOD data, indicating that the retrieval has been done reasonably.

- In the early morning, NO\textsubscript{2} data showed smaller values than surface in situ observations, but this can be explained by the vertical inhomogeneity of NO\textsubscript{2}.

- For NO\textsubscript{2}, H\textsubscript{2}O, HCHO, CHOCHO, SO\textsubscript{2}, O\textsubscript{3}, positive correlations with CHIMERE data (NCEP-based data for H\textsubscript{2}O) were found, although there may have been systematic differences by factors of 0.6 (NO\textsubscript{2}), 2.5 (HCHO), and 4.5 (CHOCHO), potentially due to insufficient treatment of emissions and chemistry in CHIMERE.

- For SO\textsubscript{2}, better treatment of ship emissions is expected to bring better agreement.

- The MAX-DOAS spatial representativeness is comparable to or better than satellite observations and model calculations. Thus, MAX-DOAS can provide multi-component data useful for the evaluation of satellite observation and model calculations, playing an important role by bridging different data sets having different spatial resolutions.