Improving S5P NO$_2$ retrievals

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Introduction

Current instruments provide excellent coverage and spatial detail for NO$_2$
They will soon be followed by the TROPOMI / S5P instrument which promises even better performance and spatial resolution
S5P tropospheric NO$_2$ retrieval is state of the art – so what’s left to improve?
GOME-2A NO$_2$ above China

- Monthly GOME-2 tropospheric NO$_2$ data are missing most of the large values
- These were removed by cloud filtering as aerosol was so thick that data were classified as partially cloudy
Is it only Aerosols?

- Even without cloud screening, there are data gaps over pollution hot spots on some days
- This is due to quality checking as these fits are poor
Why are the fits poorer at strong pollution?

- There are large and clearly structured residuals in fits over pollution hot spots
- This is not random noise!

- Comparison to NO\textsubscript{2} cross-sections shows that scaling of NO\textsubscript{2} should change over fitting window
Wavelength dependence of Air Mass Factor

- For constant albedo, AMF of NO\textsubscript{2} layer close to the surface increases with wavelength in a Rayleigh atmosphere.
- For a surface layer, this can be a significant effect.
- With radiative transfer modelling and a formal inversion, this should provide information on the altitude of the NO\textsubscript{2}.

About +/- 20%
Empirical Approach for NO$_2$(λ)

- Take standard NO$_2$ x-section
- Scale to increase amplitude with wavelength
- Orthogonalise to leave NO$_2$ columns unchanged

When introduced in the fit, large residuals are fixed
Is this the only problem at large NO$_2$ columns?

- One of the main DOAS assumptions is, that the light path enhancement (AMF) for a trace gas is independent of its column amount.
- For strong absorbers (O$_3$, SO$_2$, IR gases) this approximation is not good enough and the change of sensitivity with wavelength needs to be accounted in the fit ("modified“ DOAS).
- NO$_2$ is generally considered to be a weak absorber, but is that still true for very polluted scenarios?
AMF dependence on NO$_2$ column

- Up to a vertical column of about $1\times10^{16}$ molec cm$^{-2}$, small dependence of AMF on NO$_2$ amount
- For larger columns, the AMF decreases and NO$_2$ absorption structures appear
AMF dependence on NO$_2$ column

- Effect on DOAS fit on synthetic data is larger than on AMF alone as both smaller AMF and spectral structures reduce NO$_2$ columns
- Effect increases with SZA
- Even at a column of 5x10$^{16}$ molec cm$^2$, the error is > 10%
- Effect decreases with increasing albedo
NO$_2$ saturation on real GOME-2A data

- Many measurements above China are in the saturation range
- Corrections of 5% - 40% need to be applied to individual pixels
- In monthly averages, the effect is still > 10% in January and December
- Real effect is even larger as cloud effects reduce columns but not saturation effects
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Results Empirical Approach $\text{NO}_2(\lambda)$: GOME-2A

- The empirical $\text{NO}_2$ AMF proxy is found over the pollution hotspot in China
- It is not found at other locations where the $\text{NO}_2$ slant column is large
- There is some noise in the retrieval of the proxy
Is there more than China? **GOME-2**

**GOME-2 NO$_2$ Chisq. Improvement January 2013**

- Fit is improved by AMF proxy everywhere over pollution hotspots
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Comparison to NO$_2$ columns: **GOME-2**

- Overall pattern similar to NO$_2$ map
- Differences in distributions of maxima
- Artefacts over water
- Noise
On many days in winter, very large NO$_2$ slant columns are observed over Europe and the US.

The NO$_2$ AMF proxy picks up only very few of these signals.
Impact of Clouds: GOME-2

On many days in winter, very large NO$_2$ slant columns are observed over Europe and the US.

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This is linked to the fact that most of the events are related to cloudy scenes or snow on the surface, resulting in small wavelength dependence.
Sensitivity Study for $\text{NO}_2(\lambda) / \text{NO}_2$

**Synthetic data:**
- Rayleigh atmosphere
- Constant albedo
- $\text{NO}_2$ layer in different altitudes
- DOAS fit on spectra
- $\text{NO}_2$ temperature dependence corrected by using 2 $\text{NO}_2$ x-sections
- AMF proxy included
- Ratio of AMF proxy / $\text{NO}_2$ to normalise signal

- Ratio of AMF proxy and $\text{NO}_2$ has strong dependence on $\text{NO}_2$ layer height
- Dependence on albedo is small between 3% and 7%
Sensitivity Study NO$_2$(λ) / NO$_2$: SZA

- Effect varies with SZA; larger effect at larger SZA
- At large SZA, AMF proxy also found for high NO$_2$
- Dependence on albedo is small between 3% and 7%
Sensitivity Study $\text{NO}_2(\lambda) / \text{NO}_2$: Bright Surfaces

- Increasing albedo reduces effect as expected for reduced importance of Rayleigh scattering
- For large albedo (> 50%), negative fit factors are found for AMF proxy $\Rightarrow$ wavelength dependence is inverted and only weakly dependent on altitude

$\Rightarrow$ multiple scattering over bright surfaces is stronger at shorter wavelengths
$\Rightarrow$ wavelength dependence of AMF is inverted
\( \text{NO}_2(\lambda) / \text{NO}_2: \) Case Study Highveld: GOME-2

- \( \text{NO}_2 \) plume from Highveld power plants can be tracked onto the ocean
- \( \text{NO}_2 \) SC values increase downwind of the source
- AMF Proxy also has higher values within the plume, but
  - Is more narrow
  - Has largest values at beginning of plume, not at the end of it
Summary

- At large NO$_2$ values (> 5 x 10$^{16}$ molec cm$^{-2}$), AMF becomes a clear function of NO$_2$ column which needs to be corrected (> 10% effect)
- The effect increases with large SZA and low surface albedo
- A simple correction can be applied using tabulated factors

- At large BL NO$_2$ values, the wavelength dependence of the NO$_2$ AMF becomes relevant in the fit
- A simple empirical correction can be used to account for the AMF change
- At large NO$_2$ columns, the effect can be used to derive some information on NO$_2$ layer height

- All effects of large NO$_2$ values are expected to increase in frequency for instruments having better spatial resolution (S5P, S4)

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