Vertical information content of nadir measurements of tropospheric NO_2 from satellite

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Motivation

- Retrievals of tropospheric NO_2 from nadir satellite observations are commonly based on the application of the DOAS method to UV/visible spectra.
- Close to the surface, the measurement sensitivity changes with wavelength.
- Empirical studies suggest that in principle, the radiances measured in nadir should contain some information about the vertical NO_2 distribution.

Aim

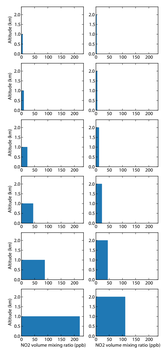
- Investigate information content of satellite nadir NO_2 measurements.
- Proof-of-concept NO_2 profile retrieval for extremely high polluted scenes.

Information Content: Formulation

- Weighting function (vertical measurement sensitivity): $\mathbf{K}$ (modelled by RTM)
- A-priori covariance: $\mathbf{S_a}$
- Measurement covariance: $\mathbf{S_e}$
- Gain matrix (uncertainty information): $\mathbf{G} = \mathbf{S_a}\,\mathbf{K}^T\,(\mathbf{K}\,\mathbf{S_a}\,\mathbf{K}^T + \mathbf{S_e})^{-1}$
- Averaging kernel: $\mathbf{A} = \mathbf{G}\,\mathbf{K}$
- Degrees of freedom for signal (indep. pieces of inf.): $DOF_s = \mathrm{trace}(\mathbf{A})$

Test Scenarios

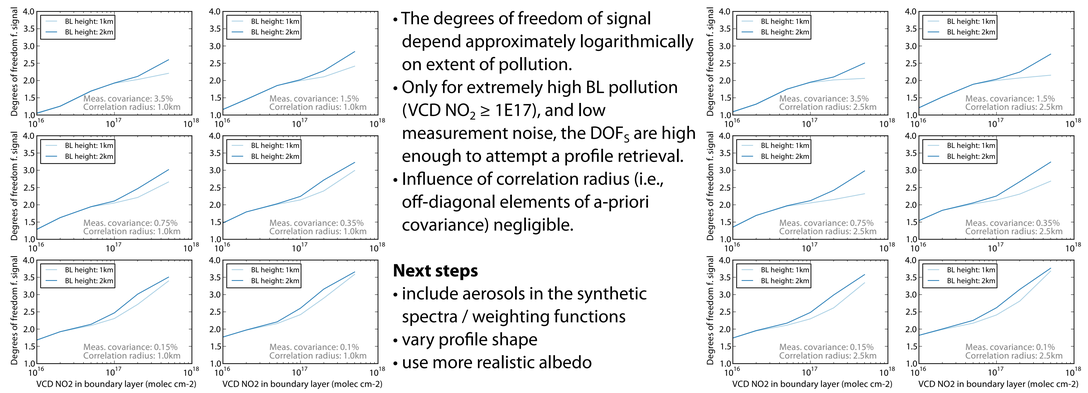
- O_3, H_2O_{vap}, strat. NO_2: U.S. Standard Atmosphere 1976
- tropospheric NO_2:
  - box profile with constant VMR: 4.4–220ppb
  - boundary layer height 1km / 2km
- Simulated GOME-2/MetopA measurements
  - channel 2: 310.0–403.6nm
  - channel 3: 403.6–601.82nm
- Nadir-viewing satellite measurement
- line-of-sight: 31.2°
- solar zenith angle: 60.2°
- Albedo: 6% (constant)
- no clouds / aerosols



Radiative Transfer Simulation

- SCIATRAN 3.3.2
- Spectral resolution 0.27/0.51nm (channels 2/3)
- spectral sampling 0.12/0.22nm (channels 2/3)
- Solar spectrum: Chance & Kurucz (2010)
- Absorption: O_3 (Serdyuchenko), NO_2 (Vandaele), H_2O_{vap} (HITRAN), O_4 (Greenblatt)

Information Content: Sensitivity to retrieval assumptions



- The degrees of freedom of signal depend approximately logarithmically on extent of pollution.
- Only for extremely high BL pollution (VCD $NO_2 \geq$ 1E17), and low measurement noise, the DOF_S are high enough to attempt a profile retrieval.
- Influence of correlation radius (i.e., off-diagonal elements of a-priori covariance) negligible.

Next steps

- include aerosols in the synthetic spectra / weighting functions
- vary profile shape
- use more realistic albedo

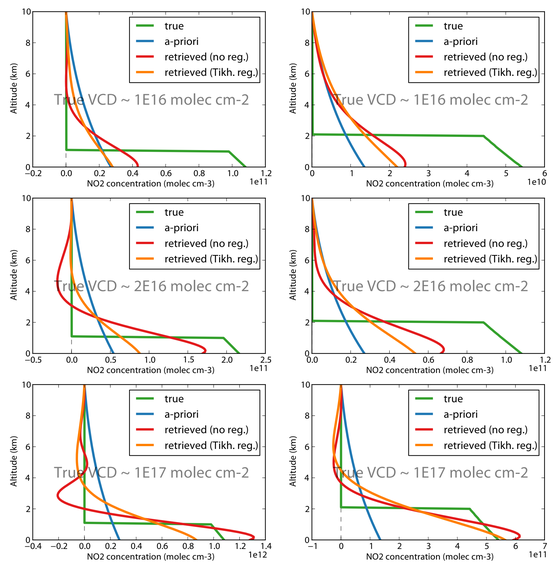
Profile retrieval: First Results

- An optimal estimation profile retrieval has been performed on the synthetic box profile scenarios (settings: see top right).
- No noise has been added to the simulated spectra.
- The a-priori has been constructed by linear interpolation (in vmr) between 0–10km (in vmr).

- In cases of extremely high BL pollution (VCD $NO_2 \geq$ 1E17), the retrieval correctly places almost all NO_2 into the boundary layer.
- At lower pollution levels, the retrieval currently fails to capture the box profile shape.
- Without regularization, the extremely steep gradients in the 1km BL cases lead to overshoots into the negative above the pollution layer.
- The current retrieval setup considers 828 wavelengths
  - ↪ retrieval is computationally very expensive
  - ↪ inverse problem largely over-determined

Next steps

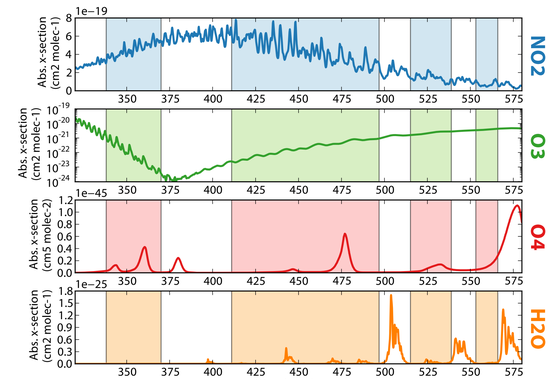
- Select retrieval wavelengths according to individual information content.
- Fine-tune retrieval parameters.
- Test more proflie shapes.
- Test influence of albedo.
- Add noise to the simulated spectra.



Profile retrieval: Setup

- Retrieval method: Optimal estimation
- A-priori variance: 100%
- SNR: 1200
- polynomial subtracted (degree 3)
- shift & squeeze correction
- With and without Tikhonov regularization
- Four selected wavelength windows
- Retrieval windows chosen to avoid main H_2O_{vap} absorption bands

Profile retrieval: Wavelength ranges



Conclusions

- Satellite nadir NO_2 measurements of extremely high polluted scenes contain enough information to retrieve general tropospheric profile shape.
- First optimal estimation retrievals on synthetic data are able to reproduce the general profile shape.
- Fine tuning of retrieval parameters necessary ...

References

- Poster EGU2014-11669 by Richter et al.
- Rodgers, C.: Inverse Methods for Atmospheric Sounding : Theory and Practice. World Scientific, 2000.
- Rozanov, V., et al.: Radiative Transfer through Terrestrial Atmosphere and Ocean: Software Package SCIATRAN. *J. Quant. Spectrosc. Rad. Transfer*, 133, 13–71, doi:10.1016/j.jqsrt.2013.07.004, 2014.

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