Vertical information content of nadir measurements of tropospheric NO₂ from satellite

Motivation
- Retrievals of tropospheric NO₂ 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 NO₂ distribution.

Aim
- Investigate information content of satellite nadir NO₂ measurements.
- Proof-of-concept NO₂ profile retrieval for extremely high polluted scenes.

Information Content: Formulation
- Weighting function (vertical measurement sensitiivity): K (modelled by RTM)
- A-priori covariance:
- Measurement covariance:
- Gain matrix (uncertainty information):
- Averaging kernel
- Degrees of freedom for signal (indep. pieces of info.): DOF = trace(A)

Test Scenarios
- O₃, H₂O vap, strat. NO₂: U.S. Standard Atmosphere 1976
- Tropospheric NO₂: box profile with constant VMR: 4.4–220 ppb
- Boundary layer height 1 km / 2 km
- Simulated GOME-2/Metop-A measurements
- Channel 2: 310.0–403.6 nm
- Channel 3: 403.6–601.8 nm
- 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 0.27/0.51 nm (channels 2/3)
- Spectral sampling 0.12/0.22 nm (channels 2/3)
- Absorption: O₃ (Seryuchenko), NO₂ (Vandaele), H₂O vap (HITRAN), O₃ (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 (NO₂ > 1E17), and low measurement noise, the DOF 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 0–100 km (in vmr).
- In cases of extremely high BL pollution (NO₂ > 1E17), the retrieval correctly places almost all NO₂ 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 1 km 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 profile shapes.
- Test influence of albedo.
- Add noise to the simulated spectra.

Profile retrieval: Wavelength ranges

Conclusions
- Satellite nadir NO₂ 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.
- www.doas-bremen.de

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- O3, H₂O vap, strat. NO₂: U.S. Standard Atmosphere 1976
- SCIATRAN 3.3.2
- Retrieval method: Optimal estimation
- A-priori variance: 100%
- SNR: 1200
- Polynomial subtracted (degree 3)
- Shift & squeeze correction
- With and without Tikhonov regularization

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