Introduction into IUP Bremen's new MAX-DOAS profile retrieval algorithm BOREAS

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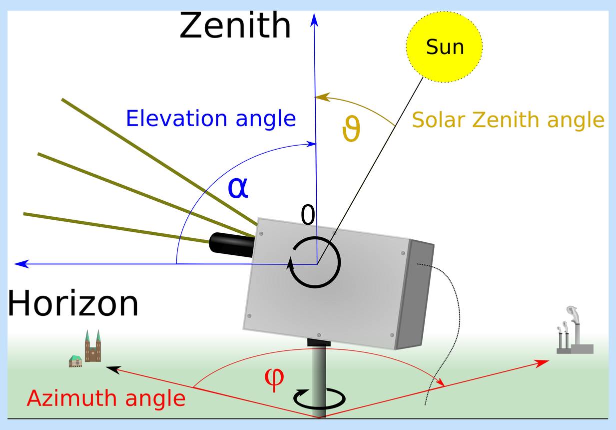
1. Introduction

Although ground based MAX-DOAS measurements at different elevation angles have been used for several years to investigate the distribution of trace gases and aerosols, the retrieval of vertical profiles is still a difficult task and results of well-established algorithms differ strongly.
Here, we introduce IUP Bremen's new profile retrieval algorithm BOREAS (**B**remen **O**ptimal estimation **RE**treival for **A**erosols and trace gase**S**) and apply it to synthetic data computed with the radiative transfer model SCIATRAN and real data from the CINDI2 camapaign (Cabauw, 2016).
The results indicate that commonly used regularization tends to give not the proper weight to the measurement which results in oscillating profiles.

2. MAX-DOAS measurement vs. retrieval

- Azimuthal scans with different elevation angles allow retrieval of trace gases.
- Inverse problem is ill-imposed! ($dSCD_{NO_2} = BAMF \cdot x$)
  → Adding of known information on the atmosphere (a priori information)
- Maximum number of **degrees of freedom (DOF)** is the number of altitude layers **($AK = I_n$)**.



3. SCIATRAN [2]

Calculations within a full-spherical atmosphere including multiple scattering.

- **Tracegas retrieval:** Calculations of box air-mass factors for all geometries and altitude layers: $BAMF_{ij} = dSCD_i / VCD_j$
- **Aerosol retrieval:** Minimization of O_4 optical depth of measurement and forward model by variation of the aerosol extinction profile via Tikhonov regularization.

4. Aerosol profile retrieval

Assumption: Variation of absorber i is equal to a scaled a-priori $N_{true,j} = N_{apri,j} \cdot f_j$

The sun-normalized intensity can be written as Taylor series: $f_j = 1 + v_j$

$$\ln(I_{meas}) = \ln(I_{apri}) + \sum_{absorber} WF_j \cdot v_j + WF_{aer} \cdot v_{aer}$$ with retrieval parameter v_i.

Subtraction of a polynomial →

$$\|\ln(I_{meas}) + WF_{O4,apri} \cdot v_{meas}\|^2 \rightarrow min \qquad \|\ln(I_{apri}) + WF_{O4,apri} \cdot v_{apri}\|^2 \rightarrow min$$

$$\|WF_{O4,apri} \cdot (v_{meas} - v_{apri}) - WF_{aer} \cdot v_{aer}\|^2 \rightarrow min$$

This minimization problem is solved iteratively within a Thikonov regularization.

$$x_{i+1} = x_0 + (K_i^T S_y^{-1} K_i + S_r)^{-1} K_i^T S_y^{-1} (y - y_i + K_i(x_i - x_0))$$

with $S_r = S_a^{-1} + \beta S_t^T S_t$

β: Tikhonov parameter
WF, K: weighting function
x_i, y_i profile and measurement vector
S_a, S_y, S_t: Covariance/Thikonov matrix

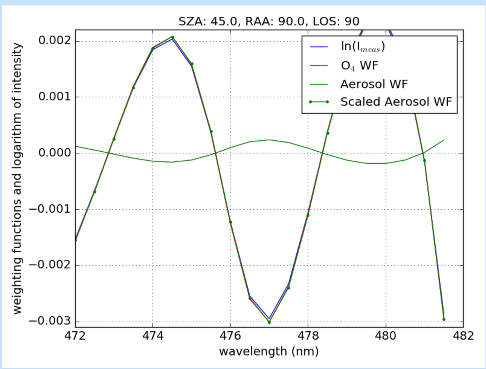


Fig. 1: Representation of the aerosol weighting function, which reproduces the spectral structures of the measurement and the O_4 WF well.

5. Tikhonov regularization

Known problems

- Profiles are underestimated when the a-priori profile is too small → scaling needed
- Weaker regularization leads to oscillations for scenarios close to the a-priori.
- Chosen settings might be good for the retrieval of AOD's but bad for bottom values (or vice versa)

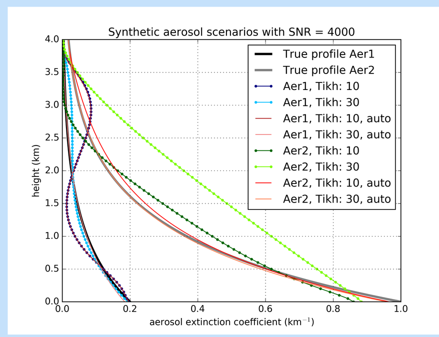


Fig. 2: Synthetic aerosol profiles and retrieved profiles for different parameters with and without a-priori scaling.

Why is a-priori scaling important?

50m grid, a-priori profile: exponential (1km SH, 0.18 AOD, σ: 4.0)

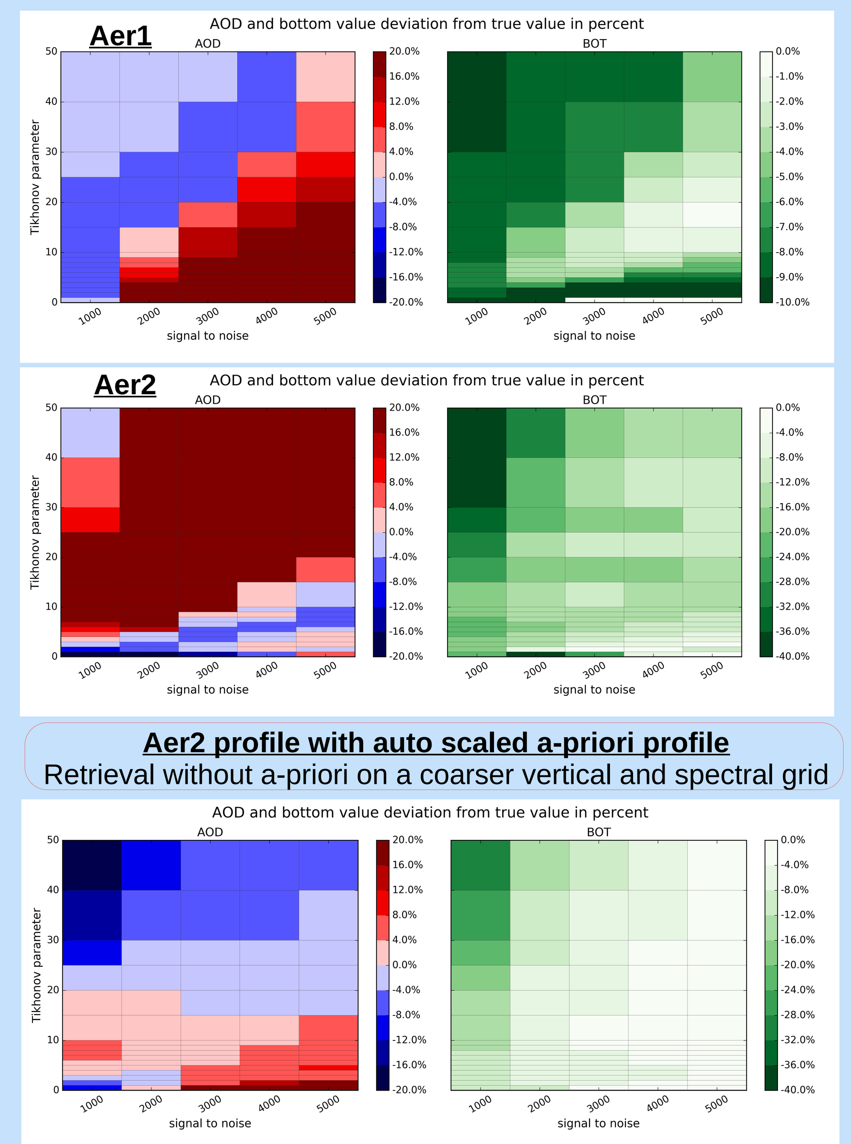
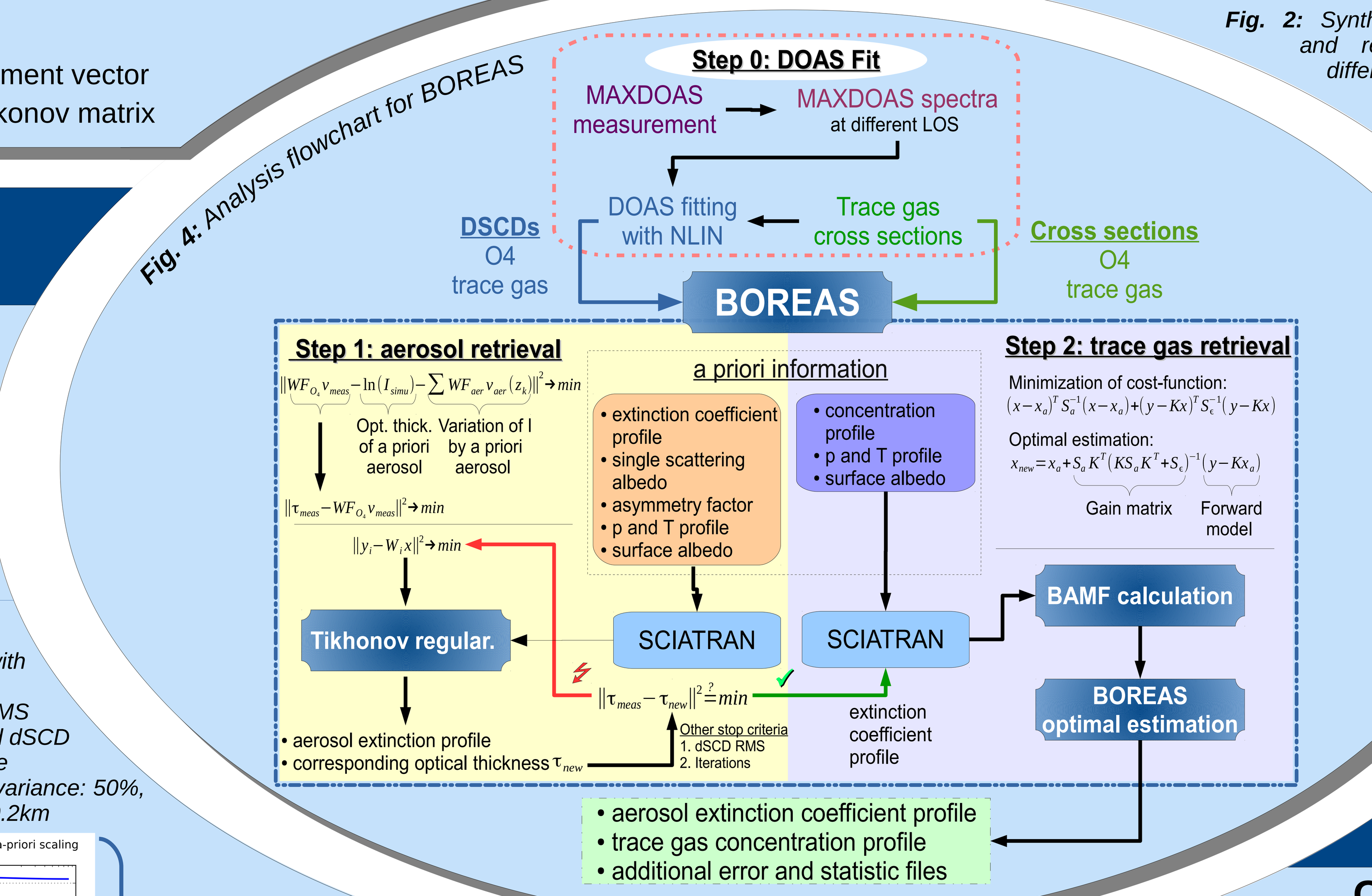


Fig. 3: Comparison of AOD (left) and bottom values (right) of retrieved profiles for different SNR and Tikhonov parameter values for aerosol scenarios without (top plots) and with prescaling of a-priori (bottom).



6. Trace gas retrieval

$$x_{new} = x_{apri} + S_a K^T (K S_a K^T + g \cdot S_e)^{-1} (y - K x_{apri})$$

a-priori scaling for NO_2:

A-priori pre scaling with the VCD derived from the 30° DSCD under the assumption of AMF = 1

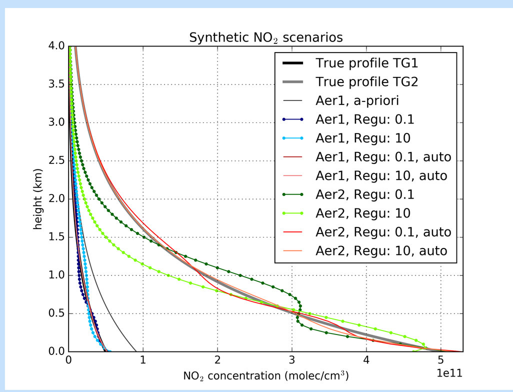
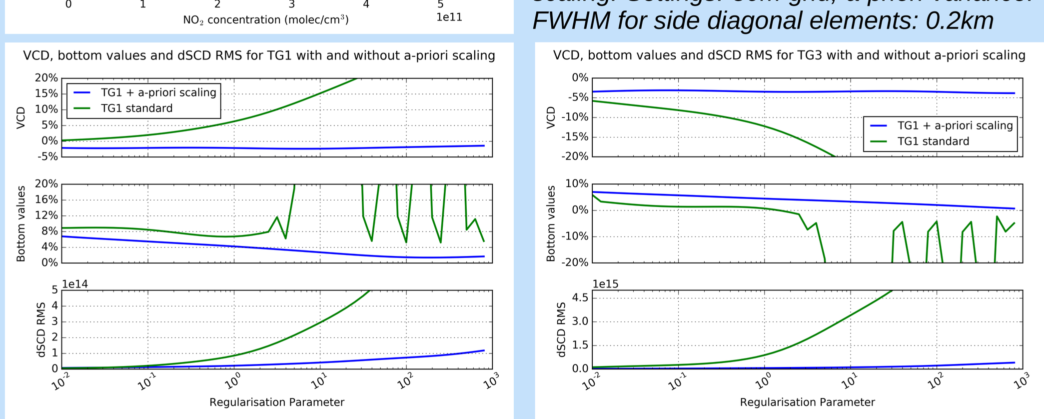


*Fig. 4: **Left:** Two NO_2 scenarios with different regularization factors with and without a-priori pre scaling. **Bottom:** VCD, bottom values and RMS between measurement and retrieved dSCD for both scenarios without a-priori pre scaling. Settings: 50m grid, a priori variance: 50%, FWHM for side diagonal elements: 0.2km*



Retrieved profiles are more stable for changes in regularization factors with prescaling.

What is the perfect regu. factor?

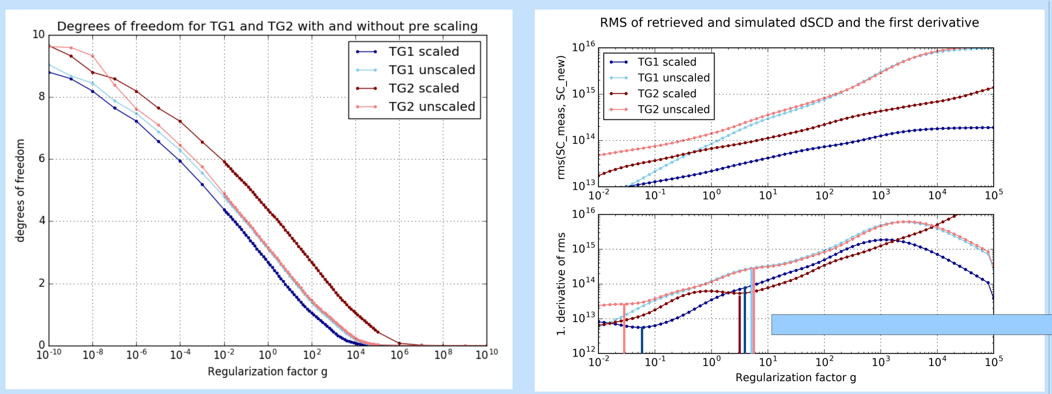


*Fig. 5: **Left:** DOF. **Right:** RMS between dSCD of measurement and retrieved profiles the derivative.*

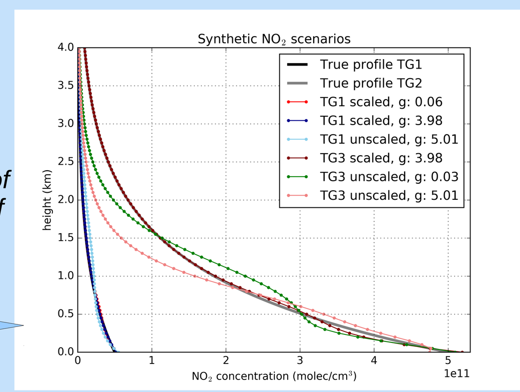
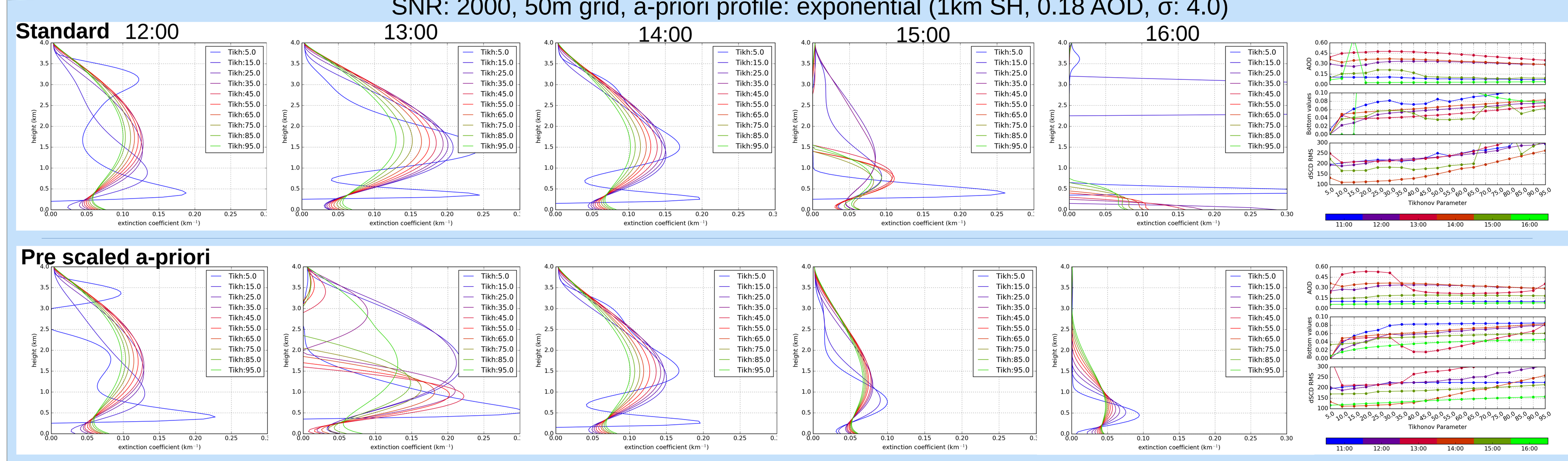


Fig. 6: Profiles chosen from local minimum of first derivative of rms between simulation and retrieved dSCD.

7. CINDI2 aerosol study

Case study on the example of the elevated aerosol layer on the 12th of September 2016 in Cabauw.

SNR: 2000, 50m grid, a-priori profile: exponential (1km SH, 0.18 AOD, σ: 4.0)



- Standard settings find a reasonable elevated layer only from 12:00 – 14:00. No convergence for 15:00 and 16:00
- Pre scaled settings converge with an decreasing layer for 15:00 and 16:00h.
- Bottom values and AOD are mostly more stable for Tikhonov variation with pre scaling.
- RMS between measured and retrieved dSCD is smaller or similar for pre scaling compared to standard settings.

8. Summary

- The best regularization between a-priori and measurement weighting differs strongly for individual szenarios
- A-priori pre scaling improves the profiling results for days with a large variability in aerosol and trace gas concentrations.
- Even with best settings there might be stable solutions which improve either the bottom concentration or the integrated concentration but not both
- An automatic regularisation via derivative of rms might be a solution for optimized weighting.
- Different minima introduce a need for regularisation factor limitations by the user.

Outlook

- A better assumption of the a-priori shape would improve the results a lot.
- Improvement of the automatic RMS-based regularisation.
- Enhanced studies for "best settings" will be performed (e.g. test of settings for Gaussian profiles with variation of height, width and maximum value)
- BOREAS will be tested for several years of measurements in Bremen to investigate the versatility of the algorithm for different atmospheric conditions with and without the presented pre scaling and automatization attempts.

9. Acknowledgement & Selected References

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[1] F. Wittrock, PhD thesis, University of Bremen, May 2006
[2] Rozanov, V. V., Rozanov, A. V., Kokhanovsky, A. A., and Burrows, J. P.: Radiative Transfer through Terrestrial Atmosphere and Ocean: Software Package SCIATRAN, J. Quant. Spectrosc. Ra., 133, 13–71, doi:10.1016/j.jqsrt.2013.07.004, 2014

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