About the information content of the DOAS polynomial

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1. Introduction

The DOAS-approach uses a least-square-fit of trace gas cross-sections to retrieve differential slant column densities. In addition, a polynomial is fitted to the optical depth accounting for Rayleigh and Mie scattering on molecules and aerosols, broadband absorptions, cloud offsets, spectral surface reflectance and instrumental effects.

Here, several radiative-transfer-model-simulations (RTM) were used to evaluate the impact of the different components on the polynomial. Therefore, ideal atmospheres and ground-based MAX-DOAS viewing geometries were simulated using the IUP-Bremen in-house RTM-software-package SCIATRAN. Spectral surface reflectance and instrumental effects were neglected.

The largest impact on the polynomial can be split up into scattering and cloud effects. Under clear sky conditions, we analyzed the effects of Rayleigh and Mie-scattering. Mainly, we focused on aerosols and their influence on the polynomial, which depends strongly on the aerosol optical thickness and on the wavelength and scattering angle dependency of aerosols.

The objective of this study is to investigate the feasibility of deriving aerosol information (e.g. optical thickness, phase function or Angström-exponent) from the DOAS polynomial.

2. Theoretical background

General DOAS - approach

$$\tau(\lambda) = \overbrace{\ln\left(\frac{I(\lambda)}{I_0(\lambda)}\right)}^{Measurment} = \underbrace{-\sum_i SC_i\,\sigma_i(\lambda)}_{Object\ of\ interest} + \overbrace{Poly.}^{Normally\ neglected} + \underbrace{Res.}_{Determ.fit\ quality\ (forgotten\ objetcs)}$$

Possible information content of the polynomial

- Rayleigh λ^{-4} & Mie-Scattering $\lambda^{-\alpha}$
- Broadband absorption
- ~~Cloud offset~~ → Only clear sky days
- ~~Instrumental effects~~ → First step: Only simulated spectra
- ~~Surface spectral reflectance~~ → Only groundbased measurements

Assumption for normal measurements:

$$\tau_{all}(\lambda,\theta_1,\theta_2) = \ln\left(\frac{a(\lambda,\theta_1)\cdot I_0(\lambda)\cdot \exp\left(-\sum_i SC_i\,\sigma_i(\lambda) - \tau_{Ray}(\lambda,\theta_1) - \tau_{Mie}(\lambda,\theta_1)\right)}{b(\lambda,\theta_2)\cdot I_0(\lambda)\cdot \exp\left(-\sum_i SC_i\,\sigma_i(\lambda) - \tau_{Ray}(\lambda,\theta_2) - \tau_{Mie}(\lambda,\theta_2)\right)}\right)$$

Spectrum measured in an arbitrary direction divided by a spectrum in Zenith

$$\tau_{all}(\lambda,\theta) = -\sum_i DSCD_i\,\sigma_i(\lambda) + \boxed{\ln\left(\frac{a(\lambda)}{b(\lambda)}\right) - \cancel{\delta\tau_{Ray}(\lambda,\theta)} - \delta\tau_{Mie}(\lambda,\theta)}$$

Well known

$$\tau_{all}(\lambda,\theta) = -\sum_i DSCD_i\,\sigma_i(\lambda) + \boxed{\sum_j c_j\,\lambda^j}$$

3. Current Aerosol treatment

Aerosol information is only retrieved indirectly!

Retrieval with simulated O_4 SCD's because O_4 depends only on the O_2-profile and meteorological conditions.

Simulation need an a priori Aerosol-profile in Step 1!

Every additional Aerosol-information would improve the retrieval algorithm

Can we retrieve Aerosol informations from the DOAS polynomial?

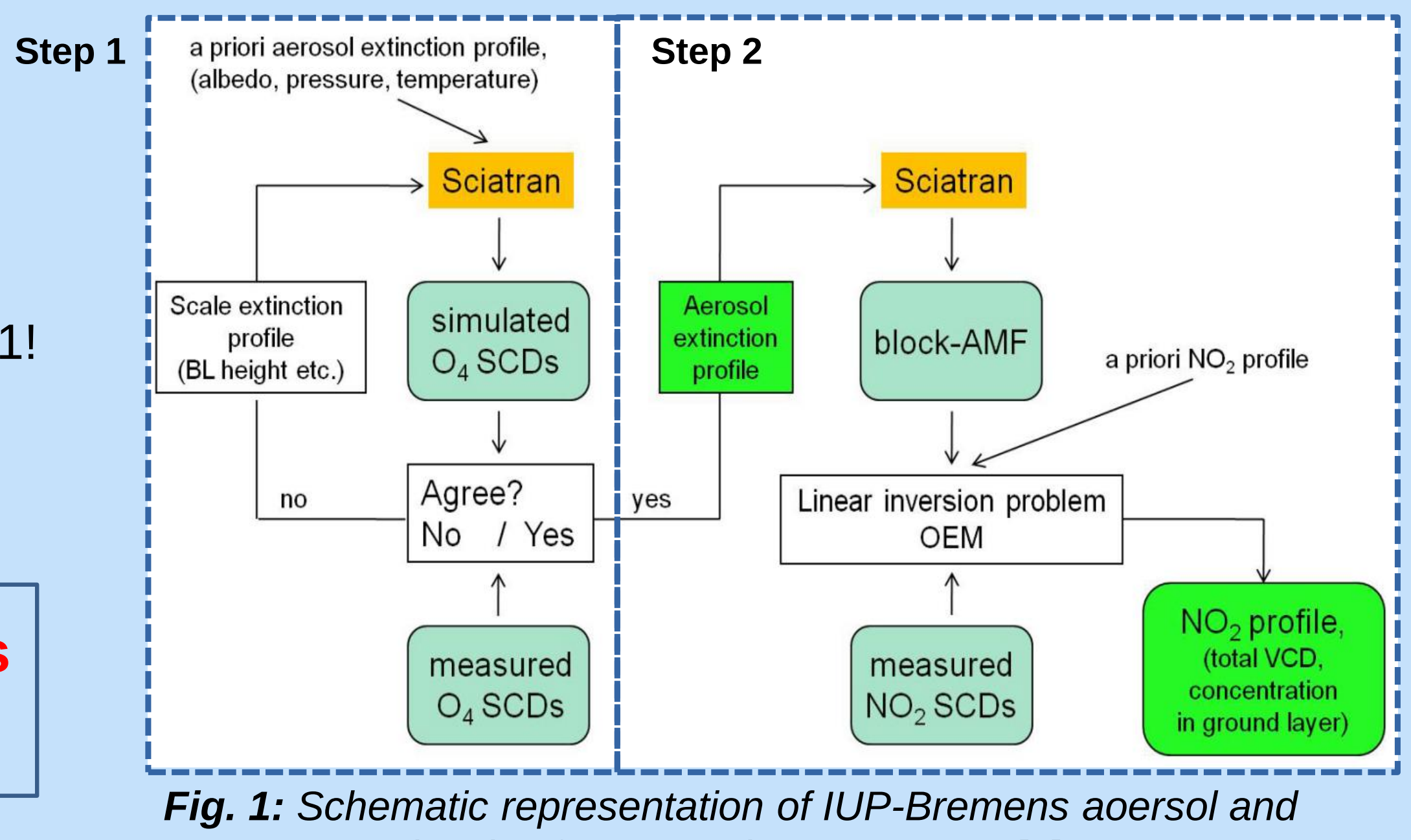
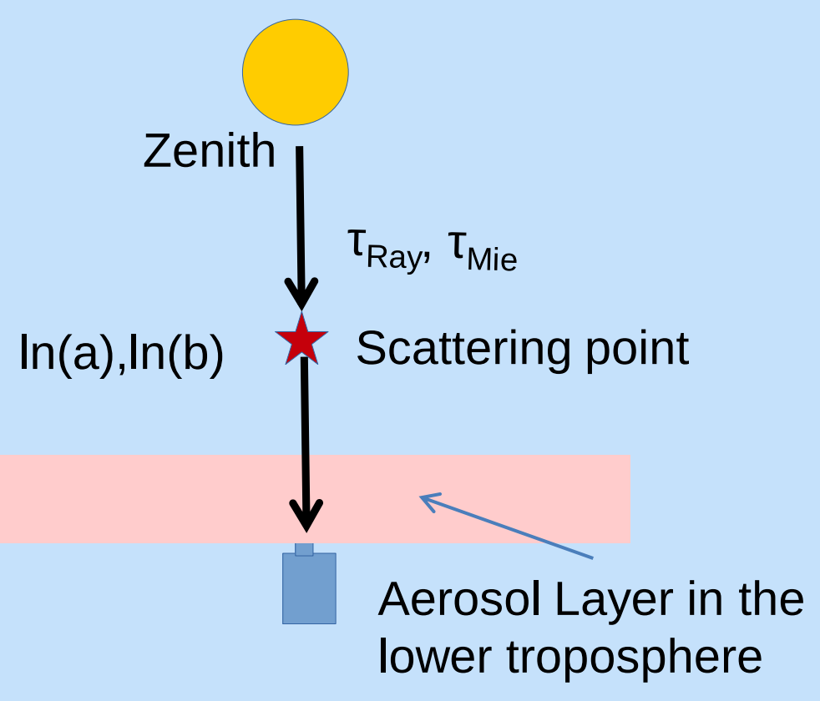


Fig. 1: *Schematic representation of IUP-Bremens aoersol and trace-gas retrieval software-package BREAM. [1]*

4. Basic idea



DOAS approach with real spectrum and synthetic spectrum within a pure Rayleigh-Atmosphere without trace-gases as reference in the same geometry.

$$\tau_{all}(\lambda,\theta) = \ln\left(\frac{a(\lambda,\theta)\cdot I_0(\lambda)\cdot\exp\left(-\tau_{Ray}(\lambda,\theta) - \tau_{Mie}(\lambda,\theta)\right)}{b(\lambda,\theta)\cdot I_0(\lambda)\cdot\exp\left(-\tau_{Ray}(\lambda,\theta)\right)}\right) = \ln\left(\frac{a(\lambda,\theta)}{b(\lambda,\theta)}\right) - \tau_{Mie}$$

For an AOT-retrieval, we need to know the scattering-terms ln(a) and ln(b) !

5. Rayleigh - scattering term ln(b)

Atmosphere with **only Rayleigh-scattering** divided by an **simple transmission** atmosphere.

$$\ln\left(\frac{b(\lambda,\theta)I_0(\lambda)\exp^{(-\tau_{Ray})}}{I_0(\lambda)\exp^{(-\tau_{Ray})}}\right) = \ln(b(\lambda,\theta))$$

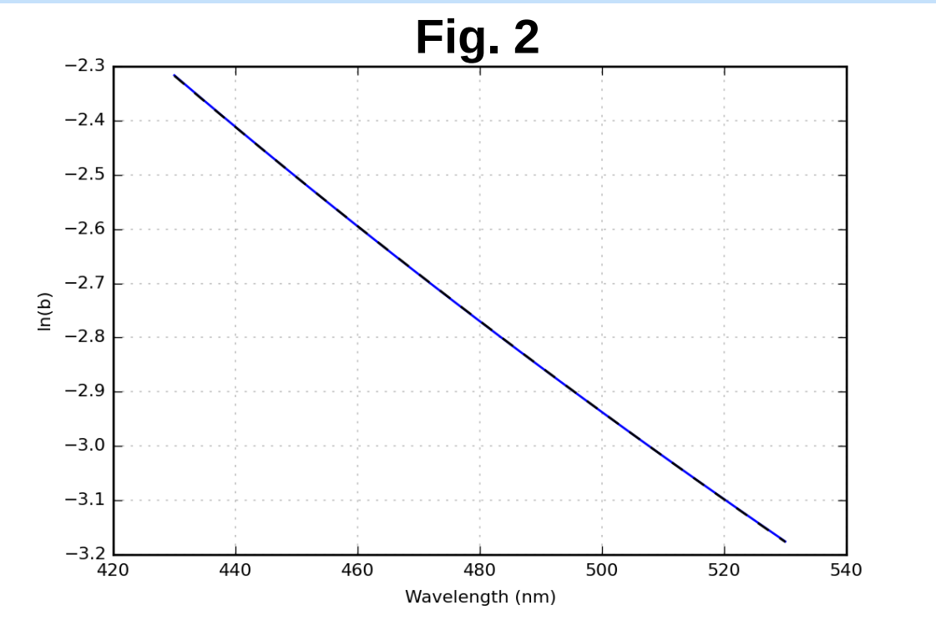
ln(b) depends only on wavelength (λ^{-4}), the Rayleigh phase-function and a constant factor c_1.

$$\boxed{\ln(b(\lambda,\theta)) = \ln(c_1(\lambda^{-4})\cdot P_{Ray})}$$

with

$$P_{Ray}(\theta) = \frac{3}{4}(1+\cos(\theta)^2)$$

Fig. 2



6. Scattering term ln(a)

Atmosphere with **Rayleigh- and Mie-scattering** divided by a **pure Rayleigh-atmosphere** with only single scattering !

$$\tau_{all}(\lambda,\theta) = \ln\left(\frac{a(\lambda,\theta)\cdot I_0(\lambda)\cdot\exp\left(-\tau_{Ray}(\lambda,\theta) - \tau_{Mie}(\lambda,\theta)\right)}{b(\lambda,\theta)\cdot I_0(\lambda)\cdot\exp\left(-\tau_{Ray}(\lambda,\theta)\right)}\right)$$

ln(a) depends only on wavelength with dependency of the dominant factor ($\lambda^{-\alpha}$ with Ansgtröm Exp. α), the Aerosol phase-function and two constant factors.

$$\boxed{\ln(a(\lambda,\theta)) = \ln(c_1(\lambda^{-\alpha})\cdot(P_{HG} + c_{off}))}$$

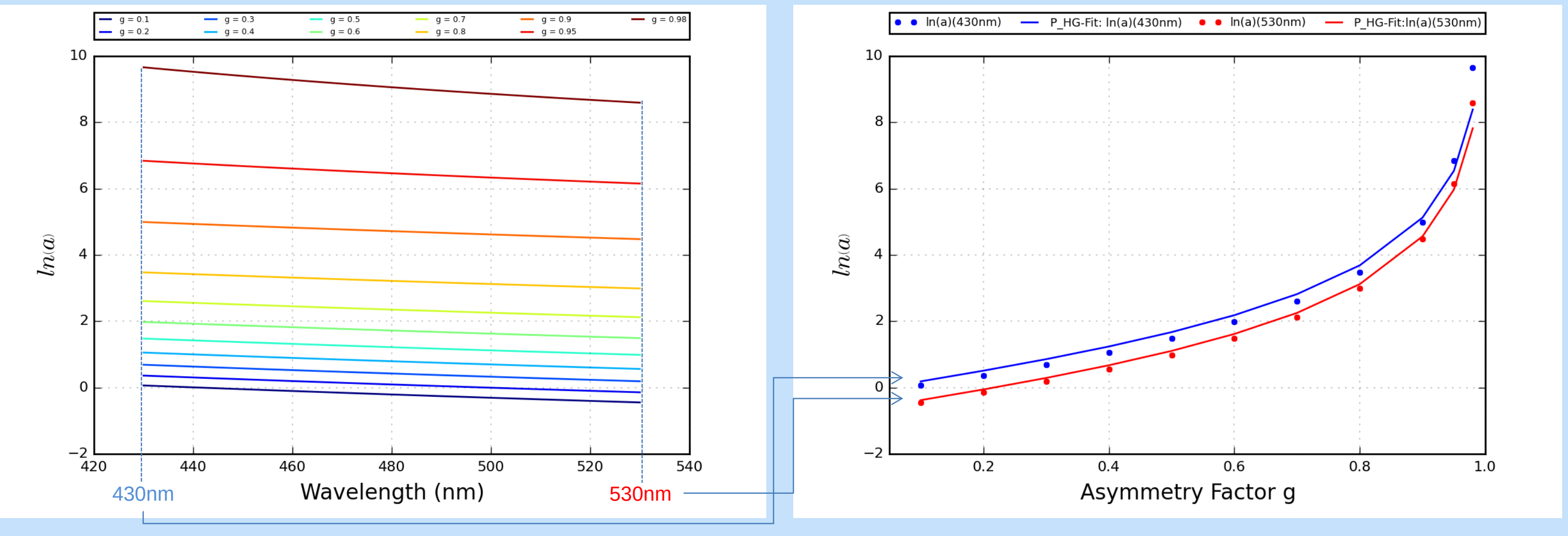


Fig. 3: Left: *ln(a) (T_{all} - ln(b) - AOT) for 11 different Aerosol-scenarios (AOT: 3, SSA: 0.99, α: -2.4, g: colorcoded).* ***Right:*** *Fit with Henyey-Greenstein phase function over all Scenarios for 430nm & 530nm.*

7. Other geometries

The scattering term ln(a) strongly depends on the geometry of the lightpath through the atmosphere.

The aerosol phase function depends on the angle between the incident path and the scattering path of a photon and should be the dominant geometry-factor for the scattering term ln(a).

1. Step: Different SZA

2. Step: Different LOS

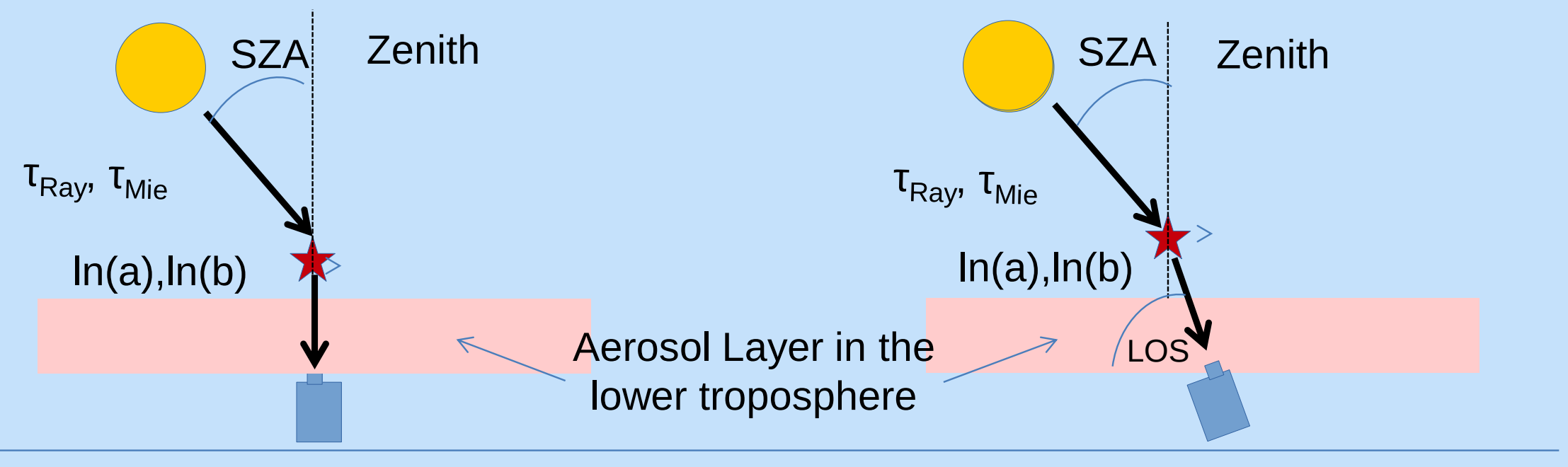
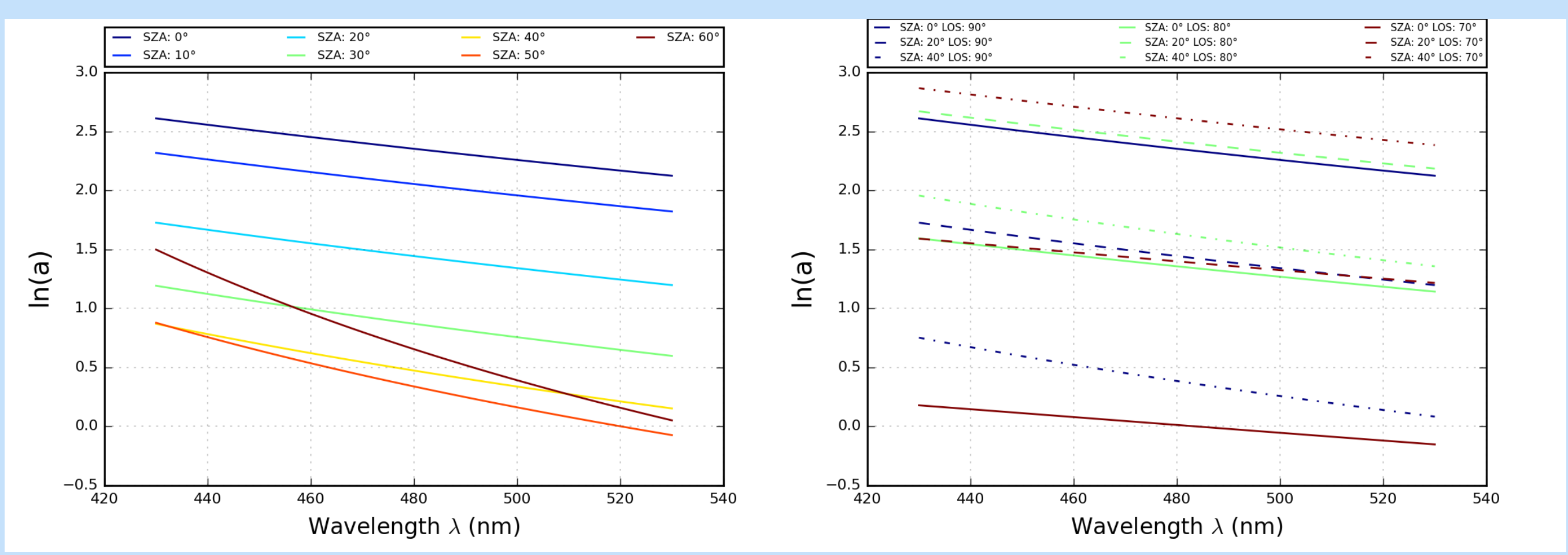


Fig. 4:
Left: *ln(a) (T_{all} - ln(b) - AOT) for 1 Aerosol-scenario with LOS: Zenith and different SZA colorcoded*

Right: *ln(a) (T_{all} - ln(b) - AOT) for 1 Aerosol-scenario with different LOS (linestyle) and different SZA colorcoded.*



8. Multiple scattering

It is well known that the Henyey-Greenstein-phase-fct. is not accurate enough for more realistic scenarios and leads to an unsatisfying fit within multiple scattering atmospheres. This problem can be solved when using more accurate phase-functions which might depend on more than one parameter. However, for these phase functions the fit is still not good enough and should be improved.

$$P_{HG}(\theta,g) = \frac{1-g^2}{(1-2g\cos(\theta)+g^2)^{1.5}}$$

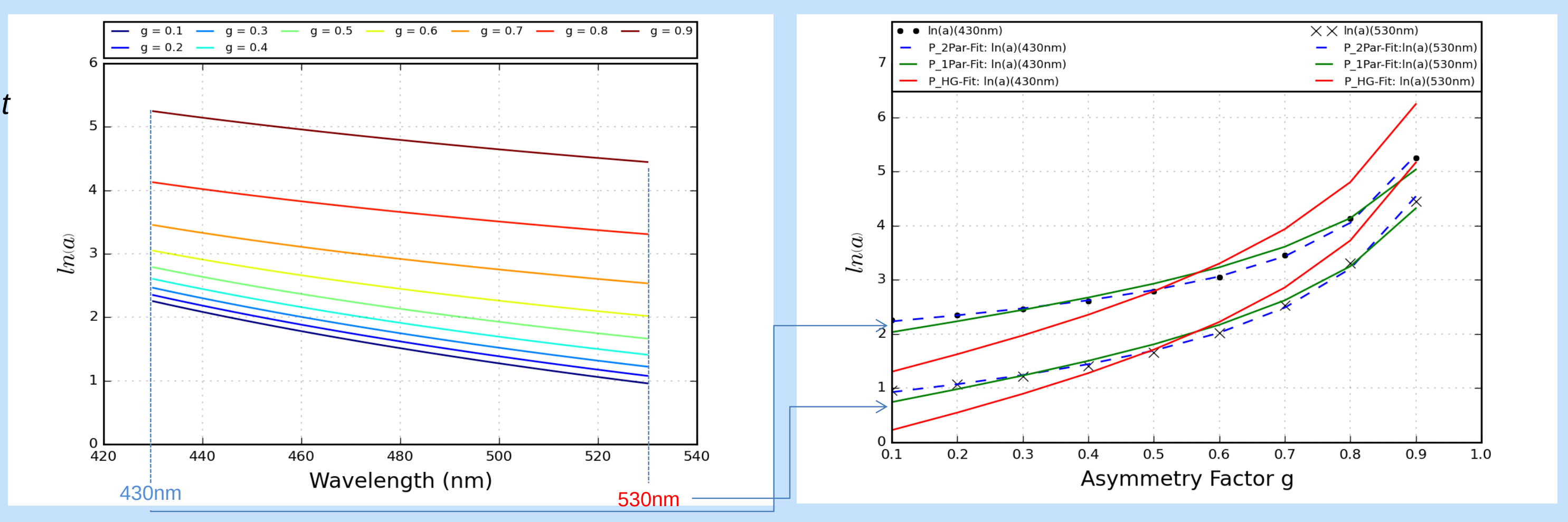
(see [2] & [3])

$$P_{2HG}(\theta,g_1,g_2) = aP_{HG}(\theta,g_1) + (1-a)\,P_{HG}(\theta,g_2)$$

$$P_{1Par}(\theta,g) = \frac{3}{2}\frac{1-\cos(\theta)^2}{2+g^2}\frac{1-g^2}{(1-2g\cos(\theta)+g^2)^{1.5}}$$

Fig. 5:
Left: *ln(a) (T_{all} - ln(b) - AOT) for 11 different Aerosol- scenarios (see above).*

Right: *Fit with different phase-fcts (Henyey- Greenstein & Two-Parameter-Henyey-Greenstein and One-Parameter-phase fct. [2,3]).*



9. Summary / Outlook

With the above formulation of the DOAS approach (see section 2), one could retrieve Aerosol information by using a synthetic spectrum for a pure Rayleigh atmosphere in the same geometry. This means, that there is a need for a fully calibrated spectroscope, since instrumental effects do not cancel any more. With knowledge of the Rayleigh-scattering-term ln(b) the remaining information in the optical depth contains only aerosol information. Then, it should be in principle possible to derive the asymmetry-factor by consideration of different geometries and to use this additional information to retrieve the AOT.

Nevertheless, several assumptions were made which complicate the problem (e.g. no instrument effects, no polarization, deviations for multiple scattering…) and might lead to an underdetermined system which solution will be a challenging task. Since this study shows only preliminary analyses a lot of work has to be done.

10. Acknowledgement & Selected References

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[1] E. Peters, PhD thesis, University of Bremen, 2013
[2] L.G. Henyey and J.L. Greenstein, Diffuse Radiation in the galaxy, 1941
[3] D. Toublanc, Henyey-Greenstein and Mie phase functions in Monte Carlo radiative transfer computations, APPLIED OPTICS Vol. 35, No. 18, 1996

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