Uncertainties of tropospheric ozone column data from OMPS limb-nadir matching

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1 Outline

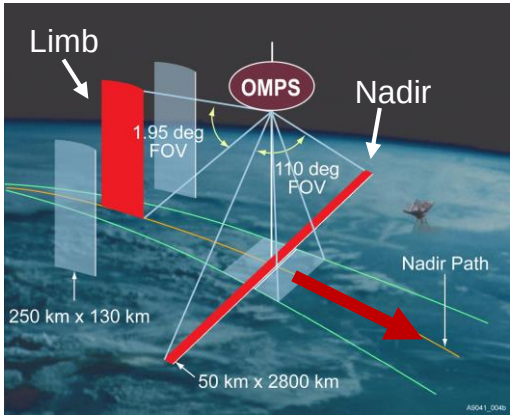
1. OMPS data sets in Bremen and the limb-nadir matching technique
2. The three sources of uncertainties for tropospheric ozone column:
    a. Limb profiles - how to go from profiles to stratospheric column errors?
    b. Tropopause altitude
    c. Total ozone column
3. Total uncertainty estimation
4. Conclusion and outlook

1 Used data and method

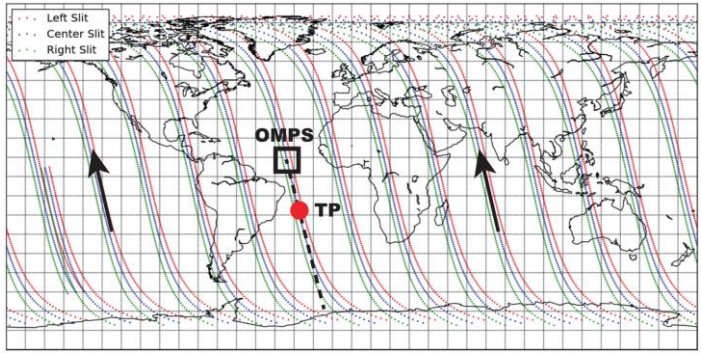
The retrieval of ozone profiles and total column from OMPS (Ozone Mapper and Profiler Suite) observations has been performed at IUP:

1. Total ozone column (**TOC**) from OMPS-NM nadir observations
   - Retrieval: WFFA (WF-DOAS modification) [Orfanoz-Cheuquelaf et al., 2021]
2. Stratospheric ozone column (**SOC**) from limb profiles from OMPS-LP observations
   - Retrieval: IUP-OMPS V3.3 (spectral fitting with Tikhonov regularization) [Arosio et al., 2018]

1. Limb - Nadir matching to obtain tropospheric column (**TrOC**):
   - **TrOC = TOC - SOC**



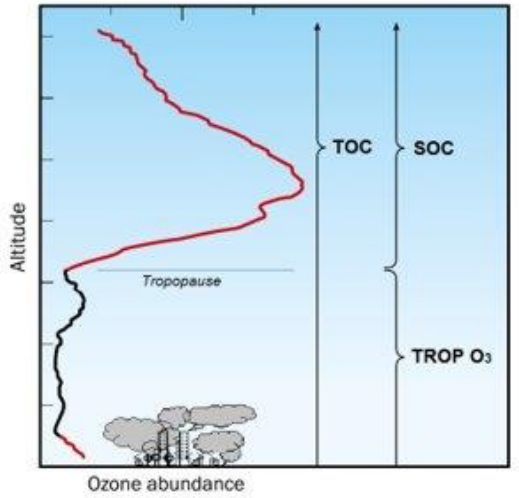
Adapted from Flynn: Extending the Records: OMPS Ozone Products. NOAA Satellite Science Week

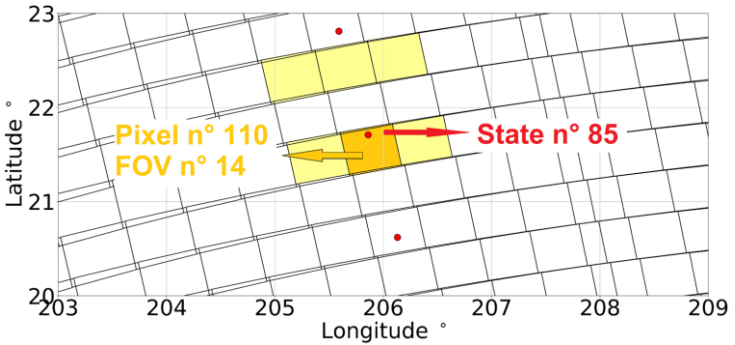


1 Used data and method

The limb-nadir matching technique:

- Tropopause height (TPH) from ERA5, definition changing as a function of latitude (thermal or dynamical);
- If TPH lower than limb profile bottom:
  use a climatology to complete the limb profile and compute SOC;
- SOC interpolated between the neighboring limb observations along track;
- Cloud fraction < 0.1 threshold for nadir pixels;
- TOC averaged over 3 ground pixels across track around the limb observation;
- **TrOC = TOC - SOC**





2 TrOC uncertainties

Three are the main contributions to the **TrOC** uncertainty

- **TOC** - several contributions and some estimations from another study:
- **SOC** - how to compute its uncertainty from errors on limb profiles?
- **TPH** - related to errors in ERA5 and TPH definition

Those are considered to be independent and are summed up in a root mean square fashion. However compensation are possible, so that the final values shall be taken as an upper limit of the uncertainty value.

$$X_{\mathrm{TrOC}} = \sqrt{X_{\mathrm{TOC}}^2 + X_{\mathrm{SOC}}^2 + X_{\mathrm{TPH}}^2}\,,$$

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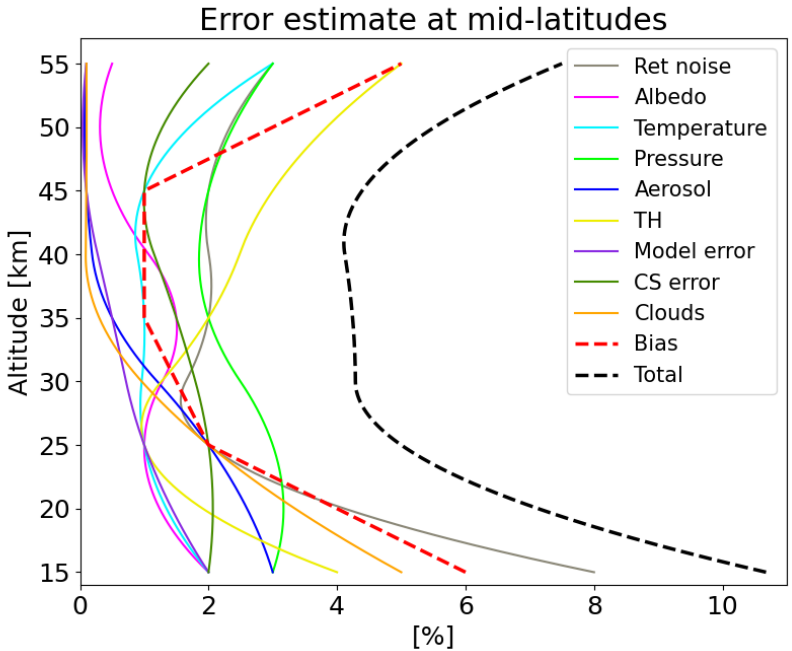
Limb uncertainties

An error budget for OMPS-LP profiles was performed at IUP (Arosio et al. 2022).
A set of OMPS-LP geometries was used to assess the error budget as a function of season and latitude.
The uncertainties were also validated by using MLS collocated observations.



Random contributions:

- retrieval noise and pre-processing;
- parameter uncertainties;

Systematic contributions:

- retrieval bias
- cloud influence (lower stratosphere)
- model errors;
- cross section uncertainties.

From synthetic simulations, contributions were assessed to be multiplicative.

How to go from profile to SOC uncertainties?

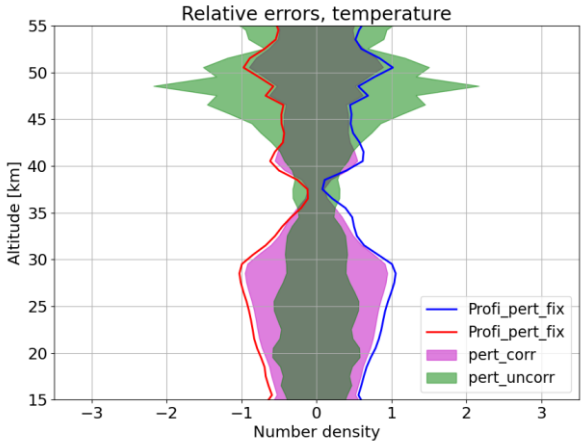
Limb uncertainties

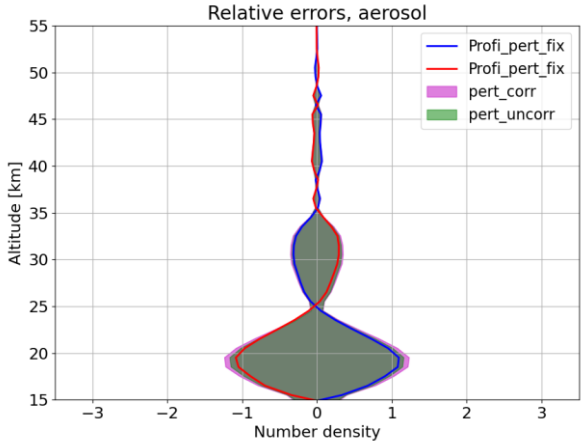
How to go from uncertainties on profiles to SOC?
Parameter errors on aerosol extinction, temperature and pressure can vary over altitude.

- Are error on parameters correlated or not in altitude?
  We assumed all errors on parameters to be correlated in the altitude domain. E.g. errors affecting temperature and pressure from reanalysis mostly scale the whole profile.
- The difference between the two assumptions are generally not very significant, except at high altitudes.

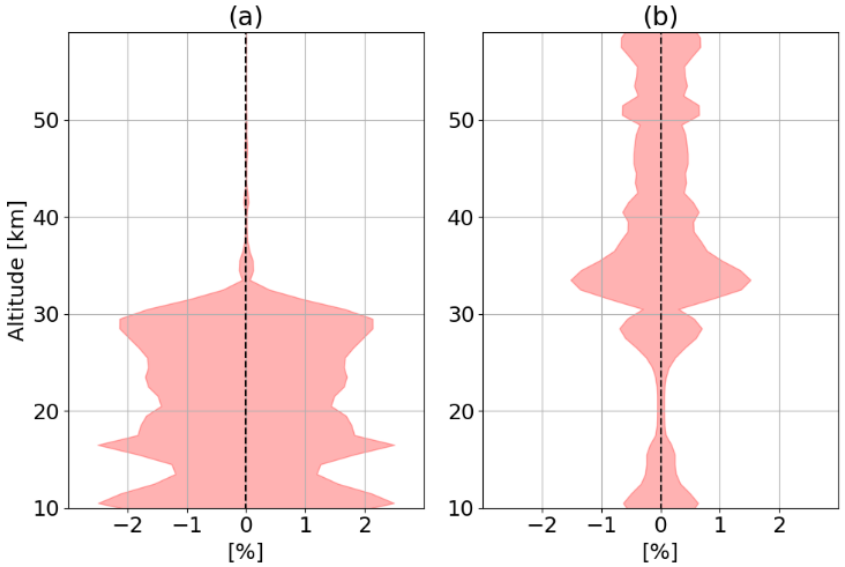
Errors on other parameters are scalar quantities, e.g. surface albedo. Their respective uncertainty profiles are then correlated with altitude.

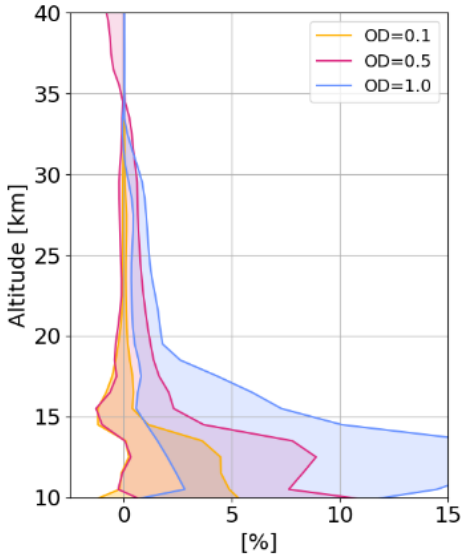
All parameter uncertainties on the profiles are correlated in the altitude domain.





Limb uncertainties





Cross section errors

- Bias-like in the Vis (a)
- Noise-like in the UV (b)

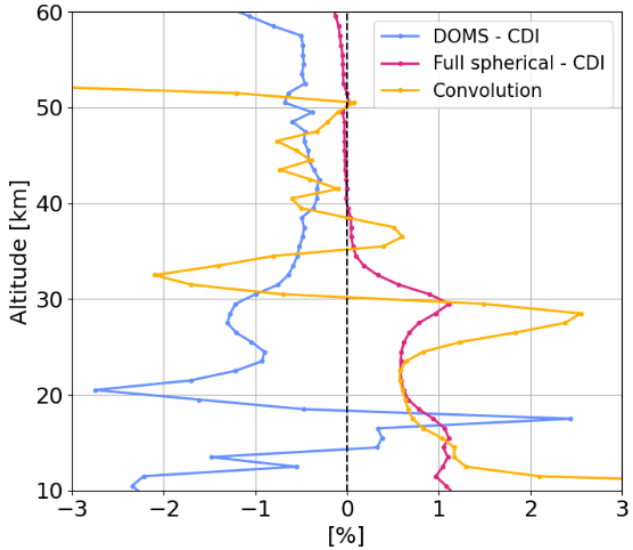
The relevant contribution for SOC comes from the Vis spectral range, so that the CS contribution is considered correlated with altitude. The resulting uncertainty is systematic.

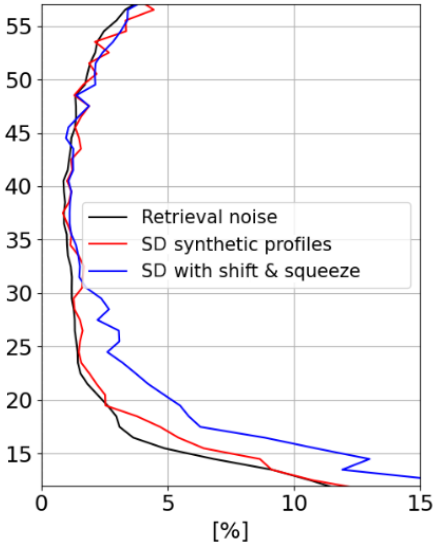
Cloud errors

Possible cloud contamination, related to this low level clouds that can pass the filter imposed on TOC pixels.

The contribution is estimated to be about 1% in SOC, correlated in altitude and systematic in nature.

Limb uncertainties





Model errors

The main contribution is related to the approximation in the RTM: choice of the radiative transfer solver and geometrical approximation (the full spherical solution is too computationally expensive)

Correlated in altitude and systematic in nature

Shift and squeeze

In the Vis spectral range a “shift and squeeze” pre-processing was applied in the retrieval, this was found to increase the variance below 30 km. Random in nature but considered correlated with altitude (applied at each TH separately but consistent results).

Limb uncertainties

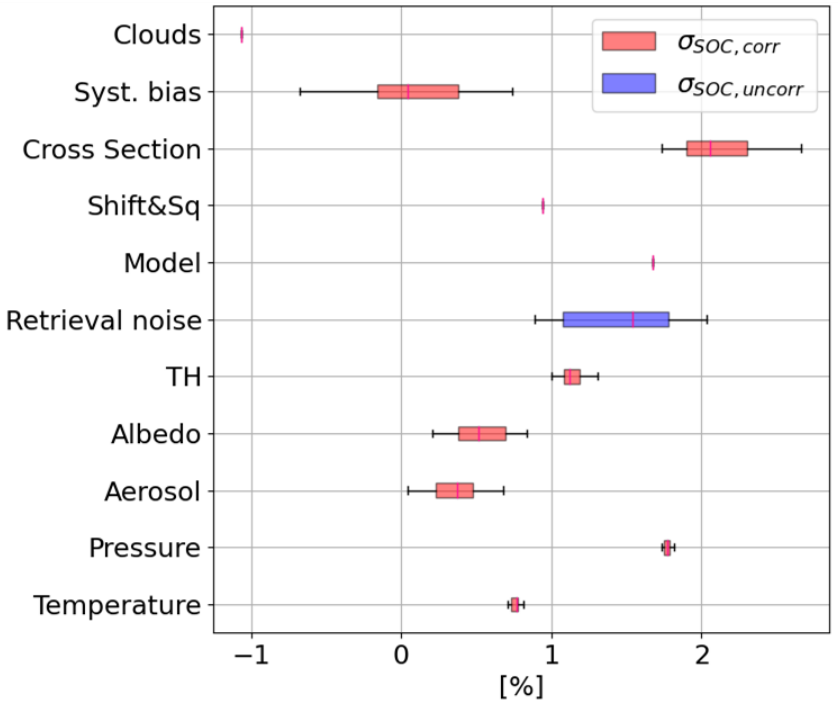
We use the following two formulas to compute SOC uncertainties. All contributions are assumed to be correlated with altitude (independently from their nature) except for the retrieval noise.

$$\sigma_{SOC,correlated} = \sum_z \sigma_{O_3}(z) / \sum_z O_3(z)$$

$$\sigma_{SOC,uncorrelated} = \sqrt{\sum_z (\sigma_{O_3}(z))^2} / \sum_z O_3(z)\,,$$

The statics over a sample of OMPS geometries is available only for parameter errors, retrieval noise, systematic bias and cross section related uncertainty. For the others a single estimation is provided.

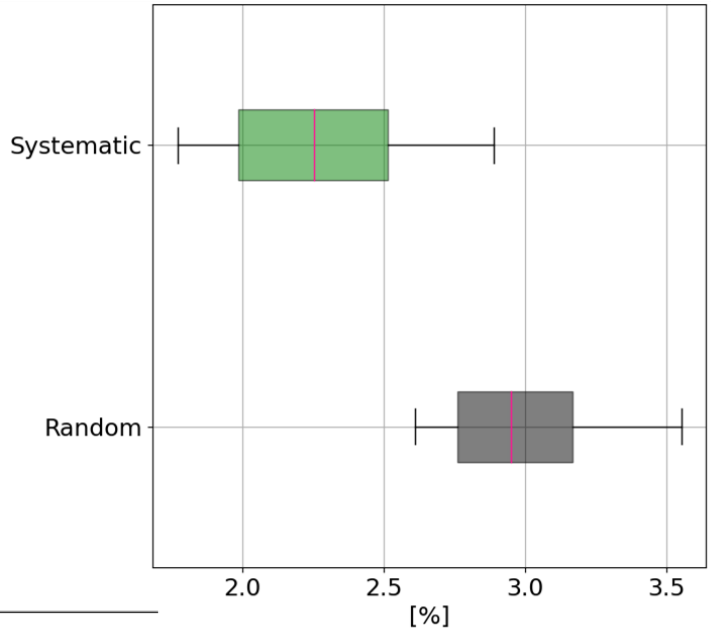
SOC uncertainties statistics



Limb uncertainties

Once the SOC contributions are obtained, it is finally possible to provide a total estimate for random and systematic uncertainties for SOC.
Using the formulas on the bottom (Arosio et al 2022).

Typical values: 8 DU random, 6 DU systematic.



$$\sigma_{SOC,systematic} = \sqrt{(\sigma_{SOC,bias} + \sigma_{SOC,clouds} + \sigma_{SOC,model})^2 + \sigma^2_{SOC,cross\ section}},$$

$$\sigma_{SOC,random} = \sqrt{\sigma^2_{SOC,P} + \sigma^2_{SOC,T} + \sigma^2_{SOC,alb} + + \sigma^2_{SOC,aer} + \sigma^2_{SOC,TH} + \sigma^2_{SOC,ret.noise} + \sigma^2_{SOC,S\&S}}$$

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$$X_{\mathrm{TrOC}} = \sqrt{X_{\mathrm{TOC}}^2 + X_{\mathrm{SOC}}^2 + X_{\mathrm{TPH}}^2},$$

Uncertainties related to the TPH are due to the natural variability of the TPH itself, to errors affecting ERA5 profiles and to the specific TPH definition used.
For the moment only the uncertainty related to the vertical resolution of the reanalysis are taken into account.

By assuming that the error on TPH is equal to the altitude span of the ERA5 level where the TPH is found (~0.3 km), it was possible to estimate the impact on TrOC of this uncertainty.

- Typical values in the 0.8 - 2.0 DU range;
- Small dependence on latitude and time;
- Random in nature.

Of course, the definition used to compute the TPH itself plays and important role, but it has more to do with a systematic bias, which shall be taken into account when comparing different TrOC products, if the TPH definitions are different.

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2c TOC uncertainties

Several contributions to TOC uncertainty:

- Aerosol and cross section - related terms are relevant and computed for the present data sets;

Source	TOC uncertainty, %
[1] Tropospheric ozone increase	<0.01%
[1] Ozone absoption cross-section	<1% below 70° SZA
	1-2% beyond 70° SZA
[1] Enhanced non-absorbing aerosols	1-2% below 50° SZA
	~0.5% beyond 50° SZA
[1] Enhanced absorbing aerosols	<1% below 50° SZA
	2-3% beyond 50° SZA
[2] O_3 and T a-priori profiles	1% below 80° SZA
	5% beyond 80° SZA
[2] Pseudo-spherical approximation	0.3%

(1) Orfanoz-Cheuquelaf et al. (2021), (2) Coldewey-Egbers et al. (2005).

TOC uncertainties

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The only systematic component is here the one related to the cross section error.

The random component ranges from 2% to 4%, its variation mostly influenced by aerosol scenarios, particularly in extreme cases.
Typical random uncertainty is estimated ~2.8 %.

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3 Final uncertainties

$$X_{\mathrm{TrOC}} = \sqrt{X_{\mathrm{TOC}}^2 + X_{\mathrm{SOC}}^2 + X_{\mathrm{TPH}}^2},$$

Component	TOC uncertainty [DU]	SOC uncertainty [DU]	TPH uncertainty [DU]	**TrOC uncertainty** [DU]
Systematic	3.0	5.9	-	**6.5**
Random	8.4	8.0	0.6 - 2.0	**12**

- Random and systematic components are kept separated;
- No relevant variations as a function of latitude or time.

Conclusion and outlook

A first estimation of the error budget for TrOC from OMPS-LP was carried out, with a focus on the computation of SOC uncertainties from limb profiles.
Contributions from SOC, TOC and TPH were added up to obtain the TrOC uncertainty estimation.

Outlook:

- Investigate other sources of uncertainties for TPH, e.g. errors in T and P profiles from ERA5;
- Are uncertainties multiplicative or additive?
- Validation of the uncertainties as done for the limb profiles, i.e. chi square method;
- Results are going to be published soon in AMT, *Orfanoz-Cheuquelaf et al. 2023*