Sampling error estimation in monthly mean SCIAMACHY datasets using a data assimilation system

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Abstract

As part of the ozone CCI (Climate Change Initiative) project, monthly average level-3 (L3) datasets (1°x 1° grid) have been produced from nadir measurements taken by GOME, GOME-2 (A and B) and SCIAMACHY. Due to the different sampling properties of the instruments, level-3 datasets can exhibit significant differences. This is in particular the case for SCIAMACHY which has a relatively narrow observing swath as compared to the other instruments and which has data gaps along the orbit track due to the alternating nadir and limb observation modes.
Using a data assimilation system and an orbit simulator, we present a method to estimate (and remove) the sampling error of nadir instruments, with specific focus on SCIAMACHY and the year 2008. We have simulated the geolocation of a "super" SCIAMACHY (SuperSCIA) instrument, i.e. an instrument with the same orbit as SCIAMACHY but with a larger swath and without gaps due to the limb mode. Using the observation operator of the Belgian Assimilation System for Chemical ObsErvations (BASCOE), the state of the BASCOE model (no assimilation) is saved into the spaces of SCIAMACHY and SuperSCIA in order to estimate and remove the sampling error of SCIAMACHY. This significantly reduces the differences between L3 datasets from GOME-2A and SCIAMACHY and reduces the sampling artifacts present in the merged L3 data product.

1. Belgian Assimilation System for Chemical Observations (BASCOE)

- Chemistry Transport Model (CTM) with 58 stratospheric species (Errera et al., ACP, 2008).
- Advection, Chemistry (≈200 reactions), parameterization for Polar Stratospheric Clouds (PSC), dehydration of H_2O in the stratosphere.
- Dynamics (winds and temperatures) precalculated, usually by ECMWF.
- Data Assimilation (DA) methods: **4D-Var** (Errera and Ménard, ACP, 2012) and **Ensemble Kalman Filter** (EnKF, Skachko et al., GMD, 2014, 2016).
- Observation operator recently included for O_3 total column observations in 4D-Var.

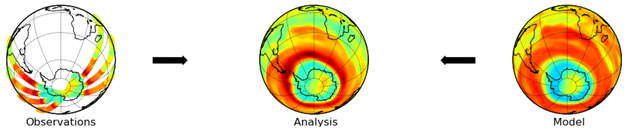
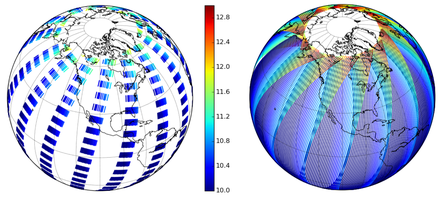


Illustration of DA principles: O_3 MLS observations around 20 km altitude (6-hour update) during the ozone hole onset in September 2008 (left), BASCOE CTM (right) and BASCOE analysis (middle). DA combines the better accuracy of the observations with the better coverage of the model: assimilated fields are not biased against observations and are filling unobserved regions.

2. Satellite nadir instrument simulator

- Python code using the PyEphem astronomical computation package.
- Computes positions of celestial bodies and artificial satellites from orbital elements and Kepler's equations. From the satellite orbit, nadir instrument observing swaths are simulated based on parameters such as time between observations, maximum swath angle, number of observations,...
- We simulated ENVISAT's orbit and a SCIAMACHY-like observing grid (SuperSCIA), but with larger swaths and no interruptions due to limb-mode observations.



SCIAMACHY O_3 nadir observation coverage and local time, 01-Jan-2008

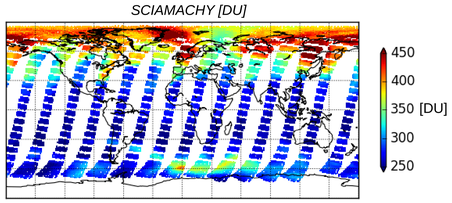
Simulated SuperSCIA nadir observation coverage and local time, 01-Jan-2008

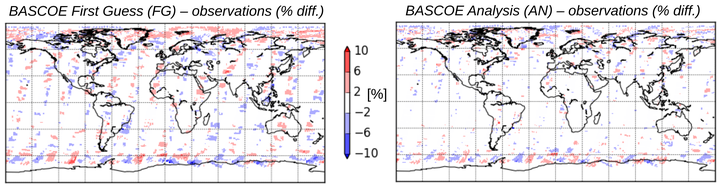
Simulated SuperSCIA observations have denser sampling compared to SCIAMACHY, no big gaps, and largely retains the spatial and temporal sampling properties of real SCIAMACHY observations.

3. SCIAMACHY data assimilation using BASCOE

- Model resolution: 2° lat x 2,5° lon x 37 vert. levels.
- Model time step: 20min.
- Dynamics provided by ERA-Interim.
- 4D-Var assimilation window: 24 hours.
- **SCIAMACHY O_3 total column L2 GODFITv3 retrieval** (Lerot et al., 2014).
- Period: Jan-Apr 2008.
- Model is saved in space of observations (assimilated and monitored) at the model time for observations available around the model time step (i.e. max. 10min difference between model and observations).

O_3 total column SCIAMACHY observations [DU] on 15 Apr. 2008



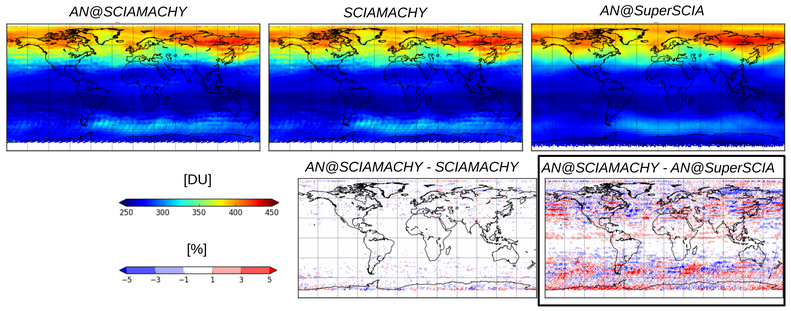


O_3 total column differences [%] evaluated at SCIAMACHY observing locations on 15 Apr. 2008, for BASCOE First Guess (left), and BASCOE Analysis (right).

Abbreviated notation: e.g. AN@SCIAMACHY refers to the BASCOE analysis evaluated at the SCIAMACHY observing locations.

4. SCIAMACHY L3 product comparison and sampling error estimation

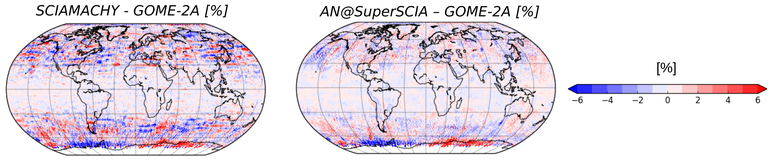
Results shown on the L3 grid (1°x 1°), April 2008 monthly mean:



Sampling error estimate of SCIAMACHY

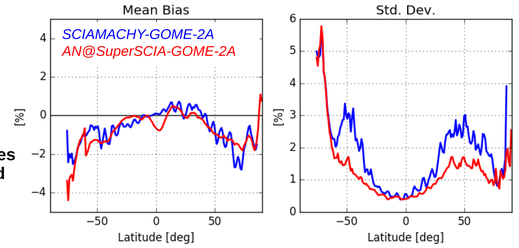
5. Comparison of SCIAMACHY and GOME-2A L3 data

SCIAMACHY - GOME-2A (left) and AN@SuperSCIA - GOME-2A (right), on L3 grid, April 2008 monthly mean:



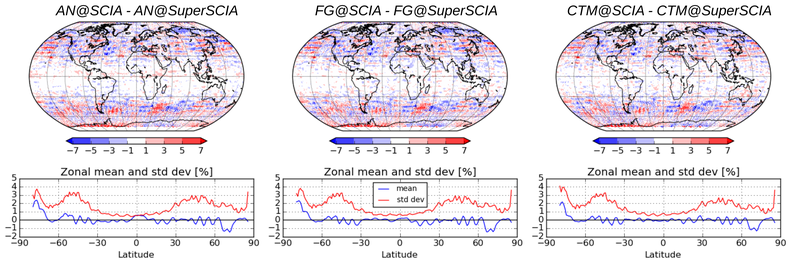
Mean bias similar, but standard deviation of difference is lower with AN@SuperSCIA

Errors due to sampling differences between instruments are reduced through the use of a SuperSCIA intermediate product



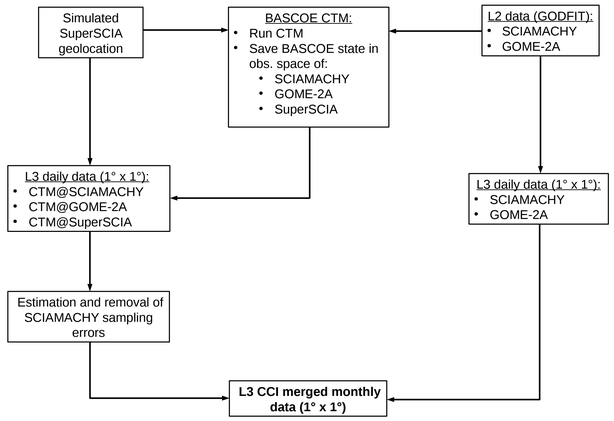
6. Sampling error estimation using a CTM only?

Sampling errors [%] on L3 grid (April 2008 monthly mean), estimated using the BASCOE Analysis (left), First Guess (middle) and CTM (right):



Very similar results: no need to do data assimilation to estimate the sampling error of SCIAMACHY, this saves CPU time that could in stead be used to increase the model resolution

7. Suggested L3 production chain with sampling correction



Conclusions

- The use of a data assimilation method and simulated instrument geolocations allows one to estimate the sampling errors of nadir (and limb) sounders.
- It seems to be sufficient to only use a chemical transport model and an observation operator to estimate the sampling errors, so no need for a complete data assimilation. This saves CPU time and the model resolution could be increased as a consequence.
- This method can be used to reduce artifacts in the monthly Ozone L3 datasets caused by the spatial and temporal sampling differences between SCIAMACHY and GOME-2A.

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