Ozone limb retrieval for the SCIAMACHY instrument
Content

- differences in the operational and scientific ozone retrievals from the SCIAMACHY limb measurements

- SCIAMACHY Quality Working Group recommended to extend the operational ozone limb processing up to 65 km (instead of 45 km as it was before). First results are presented how it could be done
Motivation

- the strict requirements for computation speed are applied to the operational SCIAMACHY processor
- consequently some approximations have to be used in the operational processor
- here we would like to investigate the impact of these approximations
The operational processor uses:

- an approximate forward model with a multiple scattering correction
- the Tikhonov regularization with a constant value of the regularization parameter

Whereas the scientific processor uses:

- as a forward model, the Picard iteration model
- as an inversion model, direct and iterative regularization methods
Treatment of the multiple scattering in the operational processor - the main simplification

- at the a priori state $X_a$ we compute the measured signal $I(X_a)$ with a RTM for a pseudo-spherical atmosphere and in the independent pixel approximation

- then, we define the correction factor for the multiple scattering by $c_{ms}(X_a) = \frac{I(X_a) - I_{ss}(X_a)}{I(X_a)}$, where $I_{ss}(X_a)$ is the single scattering term, and in the inversion process we use $I(X) = I_{ss}(X) \left[1 + c_{ms}(X_a)\right]$, where $X$ is the actual atmospheric state

- only the single scattering term accounts on the actual atmospheric state and it is apparent that this approximation is valid if the a priori state is sufficiently close to the true atmospheric state
Problematic of the regularization method

- the method which is used in the inversion process of the operational processor is the Tikhonov regularization with an a priori regularization parameter

- that means, the regularization parameter (which balance the residual and the constraint) is chosen in advance and is not correlated with the true measurement

- the a priori selection of the regularization parameter is performed for synthetic data and, therefore, the method appears to be dangerous especially when the measurement is affected by large systematic errors
What can we do better if the operational requirements softened?
Treating an underregularization with the nonlinear discrepancy principle

the “operational” profile (black line) is underregularized $\implies$ the value of the regularization parameter is too small
Treating an underregularization with the **nonlinear discrepancy principle**

- to deal with, an a posteriori parameter choice method is used, namely, the nonlinear discrepancy principle

- the following steps are made:

  - solve the inverse problem without regularization and estimate the noise level $\Delta$ as the nonlinear residual at the last iteration
  - solve the inverse problem for several discrete values of the regularization parameter $\alpha_k$ and store the corresponding nonlinear residuals

\[ \| y^\delta - F(x_{\alpha_k}^\delta) \| \]
Treating an underregularization with the nonlinear discrepancy principle

- select the optimal solution \( x^{\delta}_{\alpha k^*} \) corresponding to the first index \( k^* \) for which it holds true that

\[
\| y^{\delta} - F(x^{\delta}_{\alpha k^*}) \| \leq \tau \Delta,
\]

where \( \tau = (1.1..1.2) \) is a control parameter.
Treating an underregularization with the nonlinear discrepancy principle

an agreement between the retrieved and true profiles gets much better
Treating an underregularization with the discrepancy principle for the linearized equation

the "operational" profile (black line) is again underregularized
Treating an underregularization with 
the discrepancy principle for the linearized equation

- the Tikhonov regularization can be used but with the discrepancy principle for
  the linearized equation as parameter choice method
- the method is similar to its nonlinear version and involves the following steps:
  
  • at the iteration step \( k \) consider the linearized equation

\[
K_k (x - x_a) = y^\delta_k
\]

and use an analytical representation of the regularized solution of parameter \( \alpha \), \( x^\delta_{k+1, \alpha} \)
Treating an underregularization with the discrepancy principle for the linearized equation

- for $\alpha = 0$, compute the noise level as

$$\Delta_k = \| y_k^\delta - K_k (x_{k+1,0}^\delta - x_a) \|$$

- compute the optimal value of the regularization parameter $\alpha_{opt}$ as the solution of the discrepancy principle equation

$$\| y_k^\delta - K_k (x_{k+1,0}^\delta - x_a) \| = \tau \Delta_k$$
Treating an underregularization with the **discrepancy principle for the linearized equation**

again the agreement is improved
Treating a pointing error

► the quasi-optimality criterion is used

► if $x_{\Delta h}^{\delta}$ is the retrieved profile corresponding to the altitude shift $\Delta h$, then the optimal value of $\Delta h$ is given by

$$ (\Delta h)_{\text{opt}} = \arg \min_{\Delta h} \left\| \Delta h \frac{dx_{\Delta h}^{\delta}}{d\Delta h} \right\|^2 $$

► in practice, a discrete version of the quasi-optimality criterion is used, where we compute the regularized solutions for a discrete set of $\Delta h$ values and calculate the derivatives by using finite-differences
...that graphically means

the profile corresponding to the local minimum of the quasi-optimality function is shown in red
Result of the pointing error correction

Left: Ozone profile compared with the profile measured by groundbased LIDAR at Tsukuba on 20061211. Right: the discrete quasi-optimality function
The ways to extend ozone retrieval up to 65 km

till now the retrieval was performed up to 45 km only
four different methods have been tested to extend retrieval up to 65 km:

► DOAS-type model using the spectral window 520 - 590 nm with the altitude range 13 - 45 km (as it is used in the operational processor)

► DOAS-type model using two spectral windows:
  • spectral window 280 - 310 nm with the altitude range 40 - 65 km
  • spectral window 520 - 590 nm with the altitude range 13 - 45 km
The ways to extend ozone retrieval up to 65 km

- radiance together with Chappuis triplet model using 11 wavelengths, each wavelength being characterized by a specific altitude range (developed by C. von Savigny, IUP-Bremen)

- Radiance model using two spectral windows
Comparison of the four different approaches
Comparison of the four different approaches: high altitudes

![Graph showing comparison of different approaches at high altitudes]
How about performance?

- **DOAS with two spectral windows** is by a factor of 1.4...1.6 slower than the actual version.
- **Radiance-Chappuis model** is by a factor of 2.4...2.5 faster than the actual version.
Conclusions

- the abilities of the scientific version of the processor:
  - mathematical solution of the pointing error
  - solution of the underregularization problem

- were shown. However, it worsens a performance by a factor of \( \sim 10 \Rightarrow \) unacceptable for the operational processor. Waiting for faster computers

- four different approaches for an extension of the ozone retrieval were tested

- the fastest one is the Radiance-Chappuis model, however, its implementation will require complete rebuild of the processor architecture
Conclusions