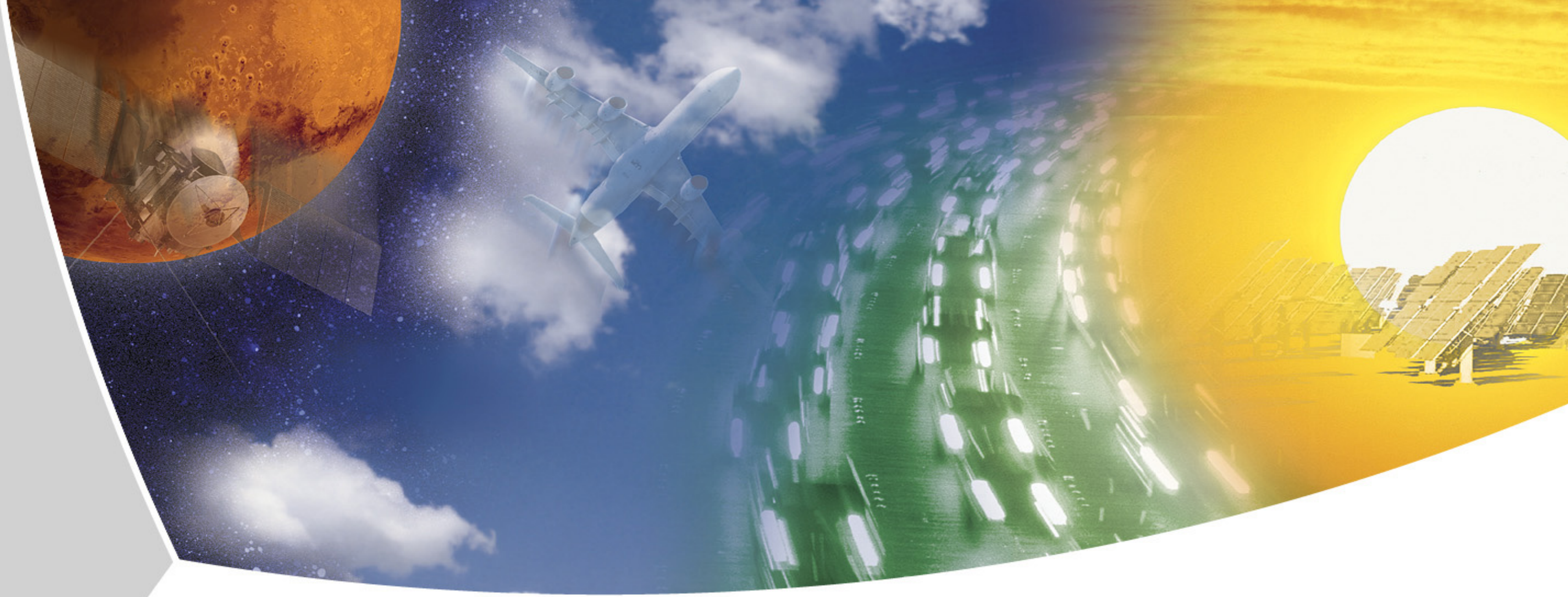

Ozone limb retrieval for the SCIAMACHY instrument

Deutsches Zentrum für Luft- und Raumfahrt e.V.
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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

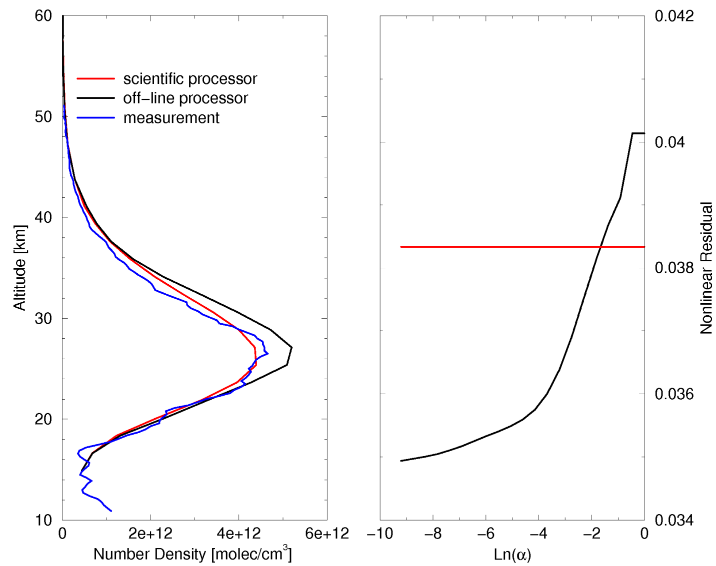
- at the a priori state X_{a} we compute the measured signal $I\left(X_{\mathrm{a}}\right)$ with a RTM for a pseudo-spherical atmosphere and in the independent pixel approximation
- then, we define the correction factor for the multiple scattering by $c_{\mathrm{ms}}\left(X_{\mathrm{a}}\right) = \frac{I(X_{\mathrm{a}})-I_{\mathrm{ss}}(X_{\mathrm{a}})}{I(X_{\mathrm{a}})}$, where $I_{\mathrm{ss}}\left(X_{\mathrm{a}}\right)$ is the single scattering term, and in the inversion process we use $I\left(X\right) = I_{\mathrm{ss}}\left(X\right)\left[1 + c_{\mathrm{ms}}\left(X_{\mathrm{a}}\right)\right]$, 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 $\Longrightarrow$ 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 $\triangle$ as the nonlinear residual at the last iteration
  - solve the inverse problem for several discrete values of the regularization parameter α_k and store the corresponding nonlinear residuals

$$\left\| \mathbf{y}^{\delta} - \mathbf{F}\left(\mathbf{x}_{\alpha_k}^{\delta}\right) \right\|$$

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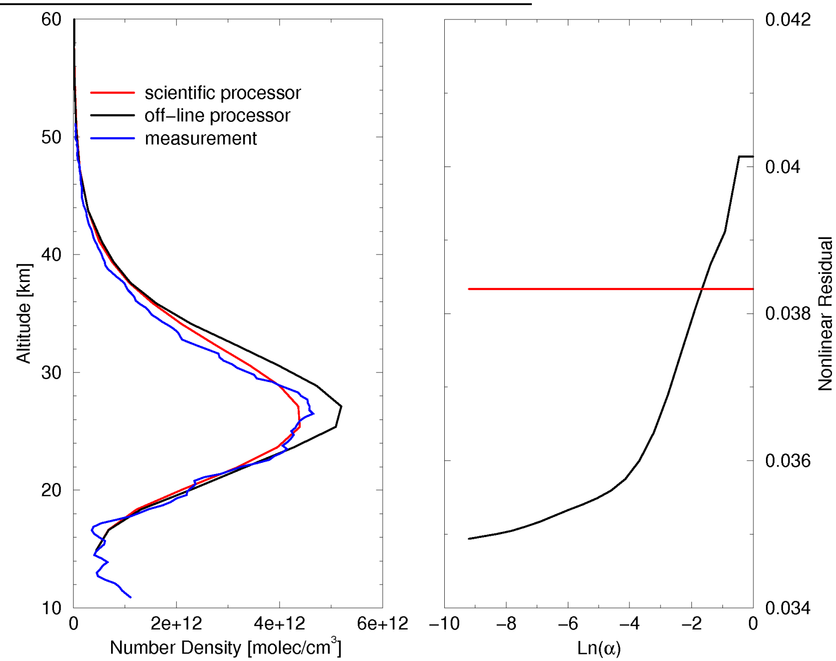
Treating an underregularization with *the nonlinear discrepancy principle*

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

$$\left\|\mathbf{y}^{\delta} - \mathbf{F}\left(\mathbf{x}_{\alpha_{k^*}}^{\delta}\right)\right\| \leq \tau\Delta,$$

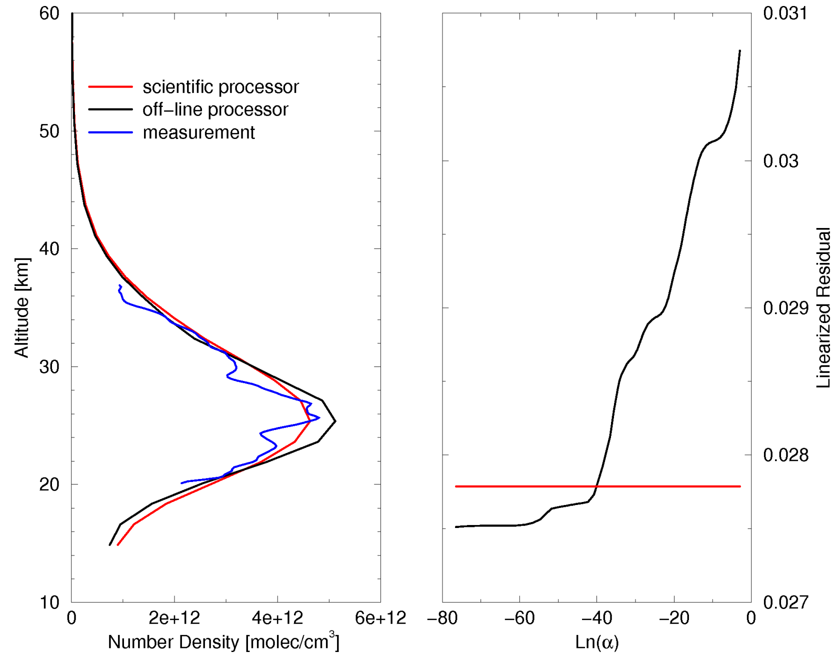
  where $\tau = (1.1..1.2)$ is a control parameter

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

$$\mathbf{K}_k (\mathbf{x} - \mathbf{x}_{\mathrm{a}}) = \mathbf{y}_k^\delta$$

and use an analytical representation of the regularized solution of parameter α, $\mathbf{x}_{k+1,\alpha}^\delta$

Treating an underregularization with *the discrepancy principle for the linearized equation*

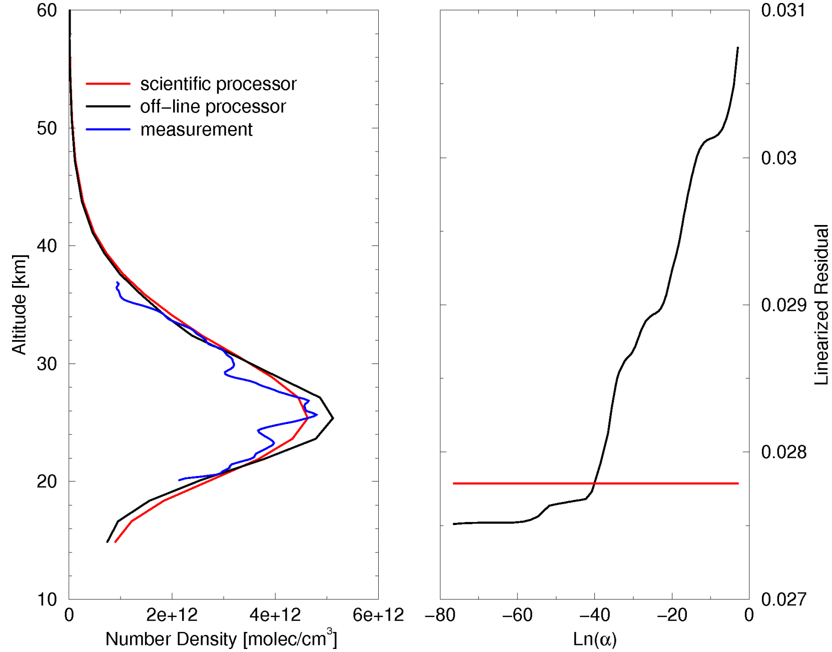
- **for $\alpha = 0$, compute the noise level as**

$$\triangle_k = \left\| \mathbf{y}_k^\delta - \mathbf{K}_k \left(\mathbf{x}_{k+1,0}^\delta - \mathbf{x}_\mathrm{a} \right) \right\|$$

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

$$\left\| \mathbf{y}_k^\delta - \mathbf{K}_k \left(\mathbf{x}_{k+1,\alpha}^\delta - \mathbf{x}_\mathrm{a} \right) \right\| = \tau \Delta_k$$

Treating an underregularization with *the discrepancy principle for the linearized equation*



again the agreement is improved

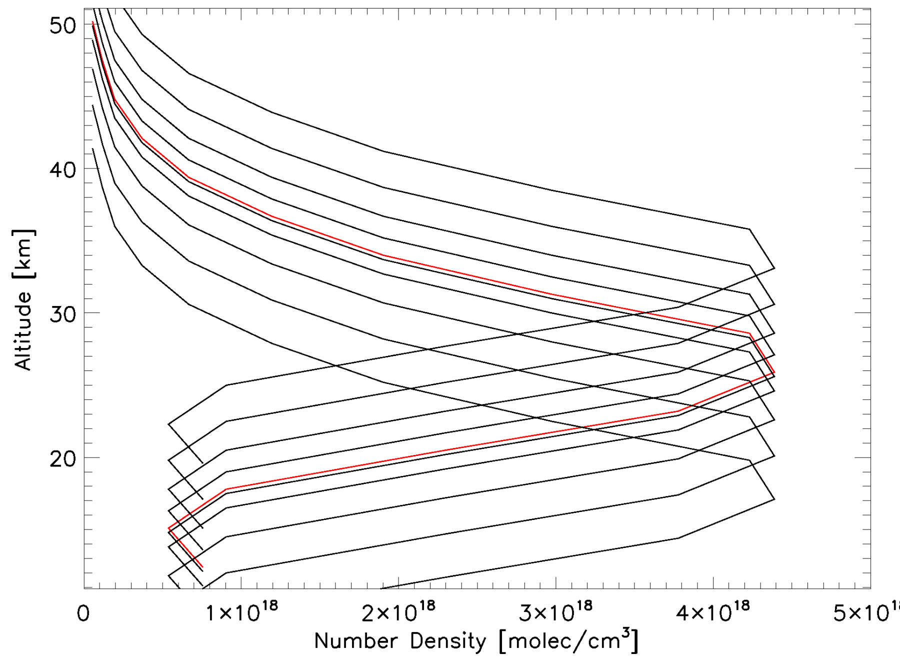
Treating a pointing error

- the quasi-optimality criterion is used
- if $\mathbf{x}^{\delta}_{\triangle h}$ is the retrieved profile corresponding to the altitude shift $\triangle h$, then the optimal value of $\triangle h$ is given by

$$(\triangle h)_{\mathtt{opt}} = \arg\min_{\triangle h} \left\| \triangle h \frac{d\mathbf{x}^{\delta}_{\triangle h}}{d\triangle h} \right\|^2$$

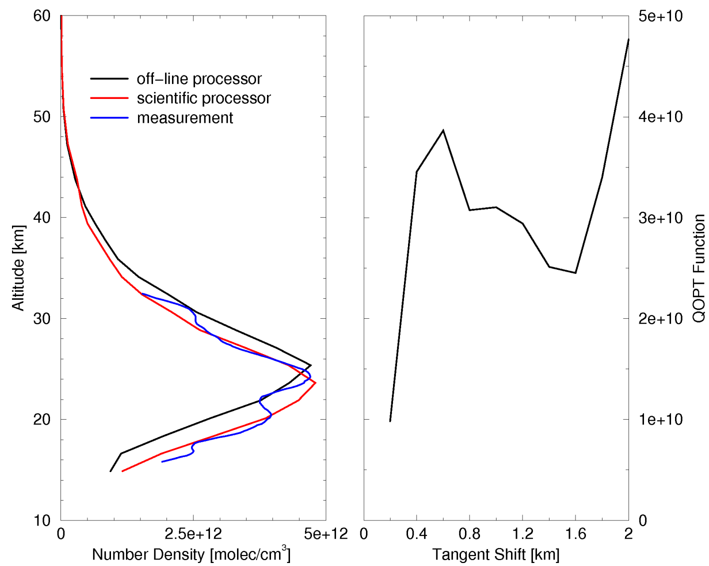
- in practice, a discrete version of the quasi-optimality criterion is used, where we compute the regularized solutions for a discrete set of $\triangle h$ values and calculate the derivatives by using finite-differences

...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

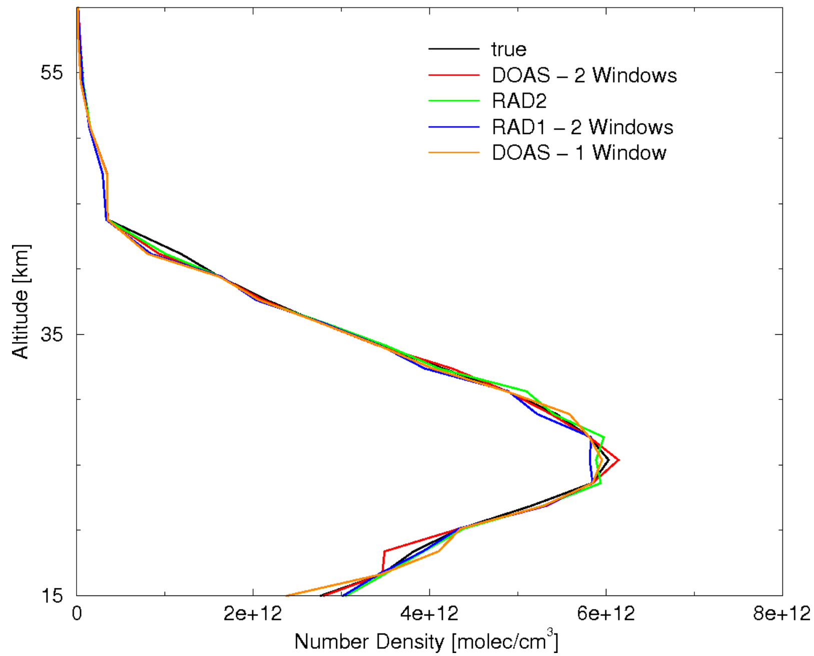
till now the retrieval was performed up to 45 km only
four different methods have been tested to extend retrieval up to 65 km:

- 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

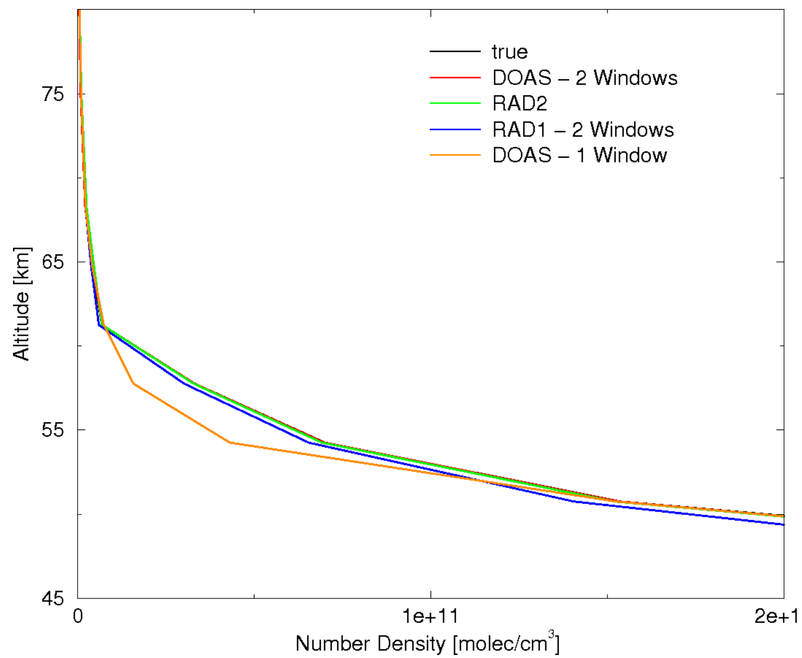
The ways to extend ozone retrieval up to 65 km

- 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



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 $\Longrightarrow$ unacceptable for the operational processor. Waiting for faster computers
- four different approaches for an extention of the ozone retrieval were tested
- the fastest one is the Radiance-Chappuis model, however, it's implementation will require complete rebuild of the processor architecture

Conclusions