OPERATIONAL AND SCIENTIFIC LIMB RETRIEVAL FOR THE SCIAMACHY INSTRUMENT

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ABSTRACT

A comparison between limb retrieval results obtained by the operational and the scientific processor for the SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY) instrument is presented. The scientific processor is based on the same retrieval method as the operational processor, but without the strict requirements for computation speed. It uses as a forward model, the Picard iteration model, and as an inversion model, direct and iterative regularization methods. In contrast, the operational processor uses an approximate forward model with a multiple scattering correction and the Tikhonov regularization with a constant value of the regularization parameter. Both processors were developed at DLR-IMF.

1. INTRODUCTION

Due to the strict requirements regarding the computation time, the off-line processor of the SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY) instrument operates with several approximations. These approximations are incorporated in both the forward and the inversion models. Here we would like to investigate the impact of these approximations.

The main simplification which is done in the forward model concerns the treatment of the multiple scattering. At the a priori state $X_{\mathtt{a}}$ in essence we compute the signal measured by the detector $I\left(X_{\mathtt{a}}\right)$ with a radiative transfer model for a pseudo-spherical atmosphere and in the independent pixel approximation. Then, we define the correction factor for the multiple scattering effect by

$$c_{\mathtt{ms}}\left(X_{\mathtt{a}}\right)=\frac{I\left(X_{\mathtt{a}}\right)-I_{\mathtt{ss}}\left(X_{\mathtt{a}}\right)}{I\left(X_{\mathtt{a}}\right)}, \qquad (1)$$

where $I_{\mathtt{ss}}\left(X_{\mathtt{a}}\right)$ is the single scattering term, and in the inversion process we use the representation

$$I\left(X\right)=I_{\mathtt{ss}}\left(X\right)\left[1+c_{\mathtt{ms}}\left(X_{\mathtt{a}}\right)\right], \qquad (2)$$

where X is the actual atmospheric state. Thus, 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. Note that not only the forward model but also the Jacobian are affected by the multiple scattering approximation.

The regularization method which is used in the inversion process is the Tikhonov regularization [4] with an a priori regularization parameter. This means that the regularization parameter, which should 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.

The scientific processor developed at the German Aerospace Center is the counterpart of the off-line processor, which is not, however, limited by any time constraints. This brings the opportunity to employ more time-consuming approaches and study their impact. The processor uses the Picard iteration method to simulate the radiance field in a full spherical atmosphere and includes polarization as well as Ring effects. A large class of regularization methods as for instance, the Tikhonov regularization, the iteratively regularized Gauss-Newton method, the regularizing Levenberg-Marquardt method, the asymptotical regularization approach and the regularized total least-squares method can be used for a specific application.

2. POINTING ERROR CORRECTION

The SCIAMACHY O_3 profiles retrieved both by the scientific and the off-line processors are shown in Fig. 1 together with the corresponding ground-based LIDAR profile measured during the satellite overpass at Tsukuba, Japan. Comparing the measured profile and the profile retrieved by the off-line processor one can recognize the pointing error causing an altitude shift of the retrieved profile. In the scientific processor the altitude shift is treated by using the quasi-optimality principle introduced in [2, 3]. Namely, if $\mathbf{x}_{\triangle h}^{\delta}$ is the retrieved profile corresponding to the altitude shift $\triangle h$, then the optimal value

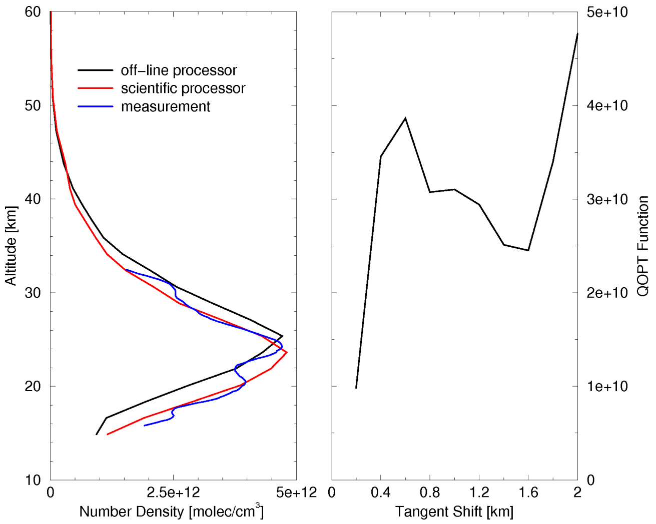

Figure 1. Left: SCIAMACHY ozone profile compared with the profile measured by groundbased LIDAR at Tsukuba on 20061211. Right: the discrete quasi-optimality function.

of $\triangle h$ is given by

$$(\triangle h)_{\mathtt{opt}} = \arg\min_{\triangle h} \left\| \triangle h \frac{\mathrm{d}\mathbf{x}^{\delta}_{\triangle h}}{\mathrm{d}\triangle h} \right\|^2 . \quad (3)$$

Fig. 2 explains graphically the idea expressed in Eq. 3.

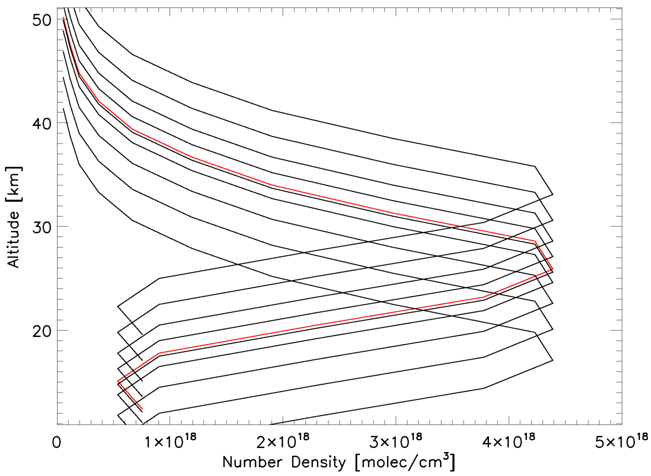

Figure 2. Set of profiles retrieved assuming different $\triangle h$. The profile corresponding to the local minimum of the quasi-optimality function is shown in red.

For a set of $\triangle h$ values a set of profiles is retrieved. Every next profile is shifted relative to a previous one by $\mathrm{d}\mathbf{x}^{\delta}_{\triangle h}$. For the profile retrieved with optimal $\triangle h$ its shift relative to the previous becomes smaller than for other ones. This corresponds to local minimum of the quasi-optimality function expressed as

$$QOPT\ Function = \arg\min_{\triangle h} \left\| \triangle h \frac{\mathrm{d}\mathbf{x}^{\delta}_{\triangle h}}{\mathrm{d}\triangle h} \right\|^2 . \quad (4)$$

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.

3. ADDRESSING THE UNDERREGULARIZATION PROBLEM

3.1. The Nonlinear Discrepancy Principle

The plots in Fig. 3 illustrate that the profile retrieved

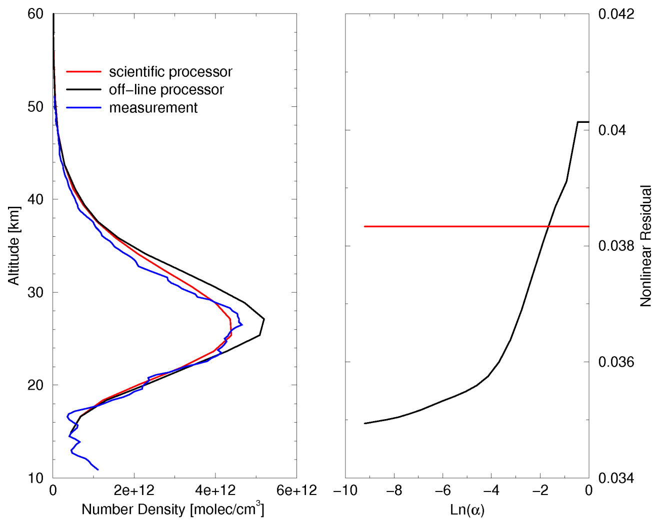

Figure 3. Left: same as left panel on Fig. 1, but for Mauna Loa on 20061013. Right: nonlinear residual together with the noise level.

by the off-line processor is underregularized, that is, the value of the regularization parameter is too small. To deal with this problem we use the scientific processor with an a posteriori parameter choice method, namely the nonlinear discrepancy principle. The steps of this parameter selection criterion can be summarized as follows:

1. solve the inverse problem without regularization and estimate the noise level Δ as the nonlinear residual at the last iteration;
2. solve the inverse problem for several discrete values of the regularization parameter α_k and store the corresponding nonlinear residuals $\left\| \mathbf{y}^{\delta} - \mathbf{F}\left(\mathbf{x}^{\delta}_{\alpha_k}\right) \right\|$;
3. select the optimal solution $\mathbf{x}^{\delta}_{\alpha_{k^*}}$ corresponding to the first index k^* for which it holds true that

$$\left\| \mathbf{y}^{\delta} - \mathbf{F}\left(\mathbf{x}^{\delta}_{\alpha_{k^*}}\right) \right\| \le \tau \Delta , \quad (5)$$

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

3.2. The Discrepancy Principle for the Linearized Equation

In Fig. 4 the profile retrived by the off-line processor is

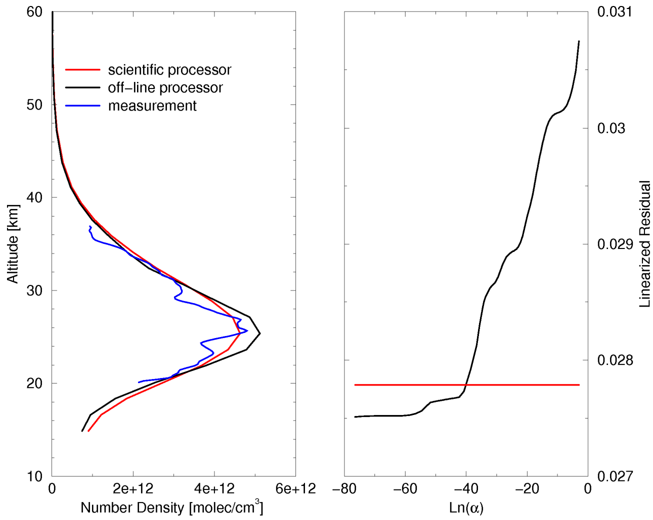

Figure 4. Left: same as left panel on Fig.1, but for Reunion on 20061211. Right: residual for the linearized equation together with the noise level.

also underregularized. To solve this inversion problem we also apply the Tikhonov regularization but use 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, $\mathbf{x}_{k+1,\alpha}^\delta$. Then,

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

$$\triangle_k = \left\| \mathbf{y}_k^\delta - \mathbf{K}_k \left(\mathbf{x}_{k+1,0}^\delta - \mathbf{x}_\mathrm{a} \right) \right\| ; \qquad (6)$$

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

$$\left\| \mathbf{y}_k^\delta - \mathbf{K}_k \left(\mathbf{x}_{k+1,\alpha}^\delta - \mathbf{x}_\mathrm{a} \right) \right\| = \tau \Delta_k . \qquad (7)$$

Note that the solution of the discrepancy principle equation requires the use of the GSVD (Generalized Singular Value Decomposition) of the Jacobian matrix and of the regularization matrix, in contrast to the off-line processor, which uses the SVD (Singular Value Decomposition) [1] of the standard form transformed Jacobian matrix. Since the SVD is much faster than the GSVD, the computation effort of the off-line processor is substantially smaller than that of the scientific processor.

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