SENSITIVITY ANALYSIS FOR SCIAMACHY OZONE LIMB RETRIEVAL

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ABSTRACT

Limb measurements performed by SCIAMACHY on the ENVISAT satellite can be used for the retrieval of stratospheric profiles of various trace gases on a global scale. The operational SCIAMACHY Level 1b-2 processor was developed at the German Aerospace Center (DLR). The more sophisticated, scientific version of the operational processor is developed in parallel and allows us to test various approaches and tools. In this paper we analyze the different inversion models and regularization methods for the ozone retrieval from SCIAMACHY limb measurements by means of the scientific processor. The difference between the DLR outcomes and the extensively validated reference algorithm of the Institute of Environmental Physics, University of Bremen (IUP-Bremen), is investigated and discussed. Also a comparison with the results from the satellite instrument SAGE-III is performed. Till now the operational ozone limb retrieval was performed up to 45 km only. Thus special attention is given to an extension to the upper stratosphere / lower mesosphere ($45 - 65$ km).

Key words: SCIAMACHY; Ozone; Limb.

1. INTRODUCTION

The SCIAMACHY Quality Working Group (SQWG) recommended to expand the operational ozone limb processing up to 65 km.

At the present time the limb ozone retrieval is performed by the means of the well-established DOAS method [2] in the visible spectral window $520 - 590$ nm, and gives reasonable results only up to 45 km due to intensive absorption of solar radiation in the Hartley and Huggins bands. To extend the altitude range up to 65 km, ozone absorption structures from the ultra-violet (UV) band have to be included in the retrieval. This can be achieved either by considering an additional spectral window ($280 - 310$ nm) or by employing a **radiance-triplet method** [5]. Before starting the technical implementation, it is crucial to analyze the above-mentioned methods using the scientific processor for the SCIAMACHY data.

Developed at the German Aerospace Center (DLR), the scientific processor is the counterpart of the offline processor and not 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 number of regularization methods can be used for a specific retrieval.

2. INVERSION MODELS

For the retrieval problems in the ultraviolet and visible (UV-Vis) spectral regions several inversion models can be considered:

1. The **radiance model** is given by

   $$R_{meas}(\lambda, h) \approx P_{scl}(\lambda, \mathbf{p}_{scl}(h)) R_{sim}(\lambda, h, \mathbf{x}), \quad (1)$$

   where λ is the wavelength and R stands for the scan-rationed radiance ratio, that is, the radiance spectrum normalized with respect to a reference tangent height,

   $$R(\lambda, h, \cdot) = \frac{I(\lambda, h, \cdot)}{I(\lambda, h_{ref}, \cdot)}. \quad (2)$$

   The normalization procedure minimizes the influence of the solar Fraunhofer structure and avoids the need of the absolute radiometric calibration of the instrument. In addition, there is a reduction in the effect of surface reflectance and clouds that can influence the diffuse radiation even at high altitudes. The scale polynomial P_{scl} is intended to account on the contribution of aerosols with smooth spectral signature.

2. The **triplet model** [5] exploits the differential absorption structure between the center and the

wings of the Chappuis absorption band of ozone, centered at 600 nm. The main idea of the triplet model is to combine the scan-rationed radiance averaged over 2 nm spectral intervals centered around $\lambda_1 = 525$ nm, $\lambda_2 = 600$ nm and $\lambda_3 = 675$ nm into the so-called Chappuis vector

$$C(h, \cdot) = \ln \left[\frac{R(\lambda_2, h, \cdot)}{\sqrt{R(\lambda_1, h, \cdot) R(\lambda_3, h, \cdot)}} \right]; \quad (3)$$

the inversion model then takes the form $C_{meas}(h) \approx C_{sim}(h, \mathbf{x})$.

3. The **differential radiance model** reads as $\ln \bar{R}_{meas}(\lambda, h) \approx \ln \bar{R}_{sim}(\lambda, h, \mathbf{x})$, with

$$\ln \bar{R}_{sim}(\lambda, h, \mathbf{x}) = \ln R_{sim}(\lambda, h, \mathbf{x}) - P_{sim}\left(\lambda, \mathbf{p}_{sim}(h, \mathbf{x})\right) \quad (4)$$

and

$$\ln \bar{R}_{meas}(\lambda, h) = \ln R_{meas}(\lambda, h) - P_{meas}\left(\lambda, \mathbf{p}_{meas}(h)\right). \quad (5)$$

For any state $\mathbf{x}$ and tangent height h, the coefficients of the smoothing polynomials P_{sim} and P_{meas} are computed as

$$P_{sim}(h, \mathbf{x}) = \arg\min_{p} \| \ln R_{sim}(\cdot, h, \mathbf{x}) - P_{sim}(\cdot, p) \|^2, \quad (6)$$

and

$$P_{meas}(h) = \arg\min_{p} \| \ln R_{meas}(\cdot, h) - P_{meas}(\cdot, p) \|^2, \quad (7)$$

respectively.

The following model combinations were analyzed:

- the **differential radiance model** in the spectral window $520-590$ nm for the altitude range $13-45$ km (as it is now employed in the SCIAMACHY processor);
- the **differential radiance model** using two spectral windows: the spectral window $280-310$ nm for the altitude range $40-65$ km, and the spectral window $520-590$ nm for the altitude range $13-45$ km;
- a **radiance-triplet model** using 11 wavelengths (Table 1), each wavelength being appropriate for a specific altitude range.

Ozone profiles retrieved from the SCIAMACHY limb measurements at the Institute of Environmental Physics, University of Bremen (IUP-Bremen) as well as profiles measured by the SAGE-III instrument [1] have been taken as a reference. The retrieved profiles corresponding to different inversion models together with the relative errors in the solutions are shown in Figs. 1 (for the altitude range $16-60$ km) and 2 ($30-55$ km).

The best agreement with the IUP-Bremen results is obtained by using the **radiance-triplet model**. Besides, it is the best choice in terms of processing speed ($2.4-2.5$ times faster than the actual implementation). Its implementation, however, will require considerable changes in the operational processor code, which could be considered for the future versions of the SCIAMACHY processor.

For the very next version the **differential radiance model with two spectral windows** is chosen. Although it is $1.4-1.6$ times slower than that currently used in the operational environment (with one spectral window), the **differential radiance model with two spectral windows** gives better agreement with the validated IUP-Bremen algorithm and the processing time is still within the constraints set up by the European Space Agency (ESA).

3. INVERSION ALGORITHMS

A number of regularization methods can be used to solve the inverse problem $\mathbf{F}(\mathbf{x}) = \mathbf{y}^\delta$. Here, $\mathbf{F}$ is the forward model, $\mathbf{x}$ is the state vector and $\mathbf{y}^\delta$ is the noisy data vector. Two main classes of regularization methods can be distinguished:

1. *Methods with a priori information.* At the k-th iteration step the forward model is linearized about the a priori, i.e. $\mathbf{K}_{\alpha k}(\mathbf{x}-\mathbf{x}_a) = \mathbf{y}_k^\delta$, where $\mathbf{K}_{\alpha k}$ is the Jacobian matrix at the actual iteration $\mathbf{x}_{\alpha k}^\delta$, $\mathbf{x}_a$ is the a priori state vector, and $\mathbf{y}_k^\delta = \mathbf{y}^\delta - \mathbf{F}(\mathbf{x}_{\alpha k}^\delta) + \mathbf{K}_{\alpha k}(\mathbf{x}_{\alpha k}^\delta - \mathbf{x}_a)$ is the linearized residual. In **Tikhonov regularization** [4] the penalty term depends on the a priori and has to be minimized taking the form of the objective function

$$\mathcal{F}_{1\alpha k}(\mathbf{x}) = \| \mathbf{y}_k^\delta - \mathbf{K}_{\alpha k}(\mathbf{x} - \mathbf{x}_a) \|^2 + \alpha \| \mathbf{L}(\mathbf{x} - \mathbf{x}_a) \|^2. \quad (8)$$

Note that the regularization parameter, which should balance the residual and the constraint, is computed in advance and remains **constant** during the iterative process.

In the **iteratively regularized Gauss-Newton method**, the regularization parameters are the terms of a geometric sequence, i.e.,

Table 1. Radiance-triplet model

λ[nm]	264	267.5	273.5	283	286	288	290	305	525	602	675
h_{min}[km]	52	52	52	45	45	45	45	35	13	13	13
h_{ref}[km]	71	71	71	68	65	65	61	55	41	41	41

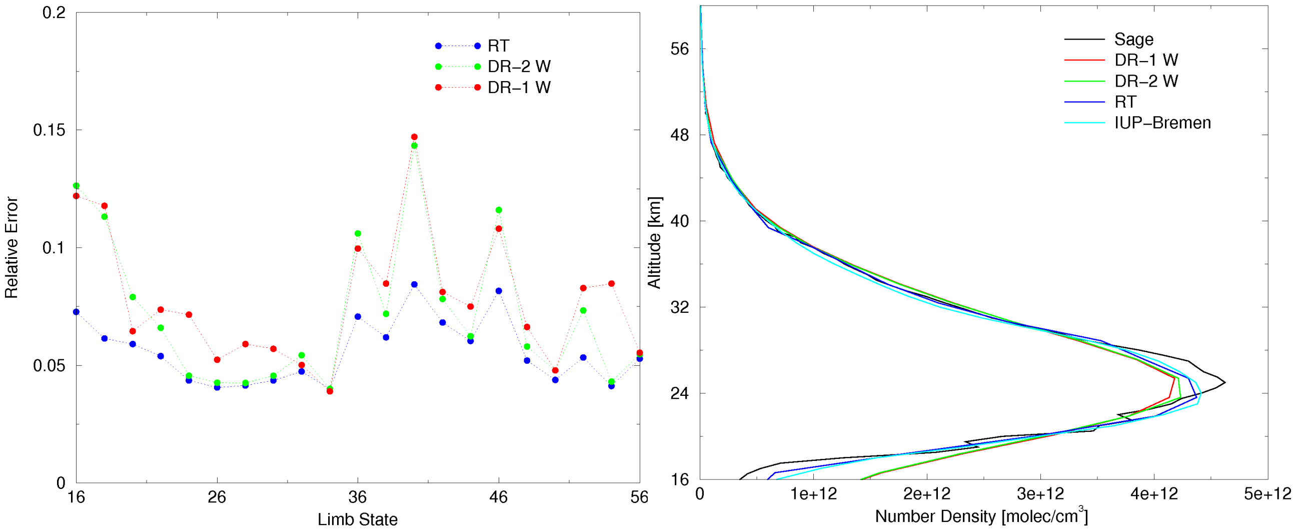

Figure 1. Ozone profiles (right panel) for the altitude range 16 − 60 km from SAGE-III (black line), IUP-Bremen (cyan), and DLR together with relative errors in the DLR solutions with respect to the IUP-Bremen solutions. The DLR results correspond to the ***differential radiance model with one spectral window*** *(DR-1W, red line),* ***two windows*** *(DR-2W, green line), and the* ***radiance triplet model*** *(RT, blue line) (left panel)*

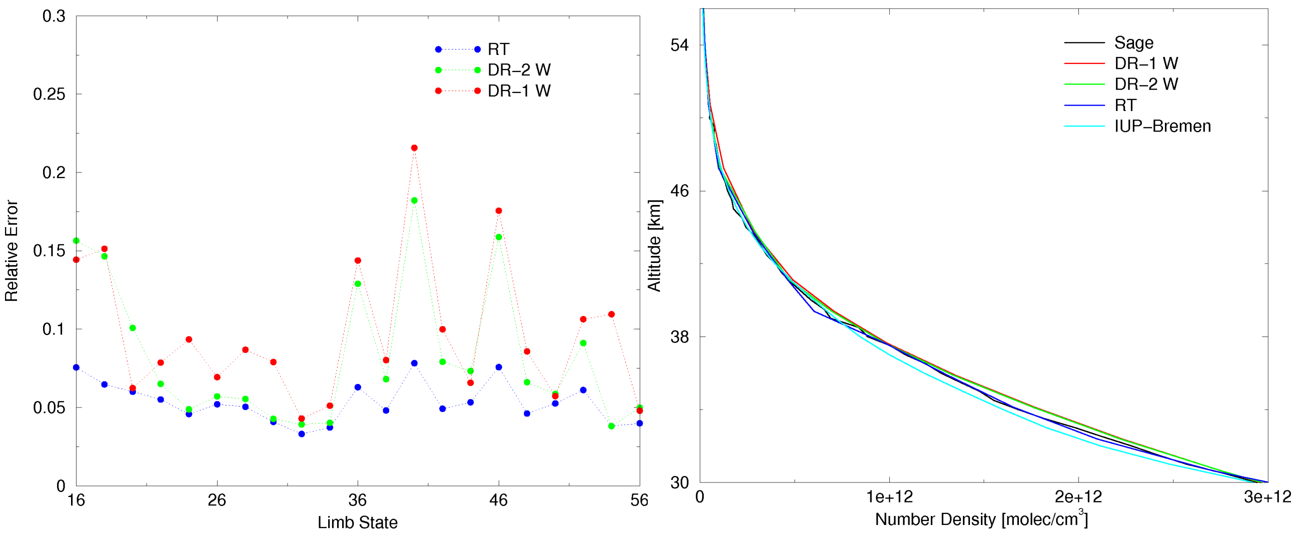

Figure 2. Same as for Fig. 1 but for the altitude range 30 − 55 km

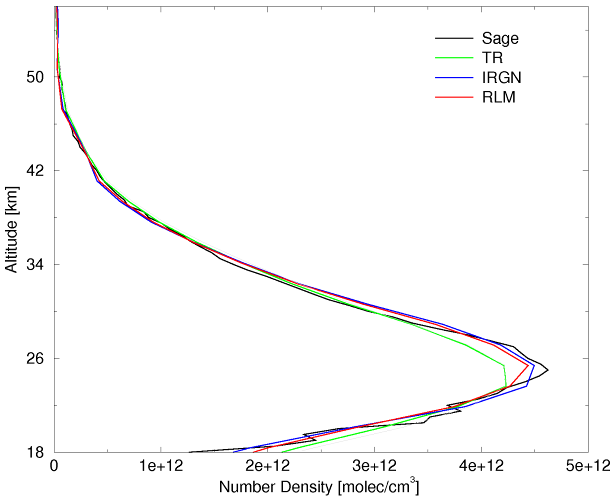

Figure 3. Retrieval results computed by using Tikhonov regularization (TR), the iteratively regularized Gauss-Newton method (IRGN) and the regularizing Levenberg-Marquardt method (RLM).

$\alpha_k = q\alpha_{k+1},\ 0 < q \leqslant 1$, and the objective function reads as

$$\mathcal{F}_{1k}(\mathbf{x}) = \|\mathbf{y}_k^\delta - \mathbf{K}_k(\mathbf{x} - \mathbf{x}_a)\|^2 + \alpha_k\|\mathbf{L}(\mathbf{x} - \mathbf{x}_a)\|^2. \quad (9)$$

2. *Methods without a priori information.* At the k-th iteration step the forward model is linearized about the actual iteration, i.e. $\mathbf{K}_k(\mathbf{x}-\mathbf{x}_k^\alpha) = \mathbf{r}_k^\delta$, where $\mathbf{K}_k$ is the Jacobian matrix at the actual iteration $\mathbf{x}_k^\delta$ and $\mathbf{r}_k^\delta = \mathbf{y}^\delta - \mathbf{F}(\mathbf{x}_k^\delta)$ is the nonlinear residual.

   In the **regularizing Levenberg-Marquardt method** the penalty term depends on the actual iteration and the objective function is given by

$$\mathcal{F}_{1k}(\mathbf{x}) = \|\mathbf{r}_k^\delta - \mathbf{K}_k(\mathbf{x} - \mathbf{x}_k^\delta)\|^2 + \alpha_k\|\mathbf{L}(\mathbf{x} - \mathbf{x}_k^\delta)\|^2. \quad (10)$$

   As in the case of the iteratively regularized Gauss-Newton method, the regularization parameters are the terms of a geometric sequence.

The ozone profiles retrieved by using different regularization methods are shown in Fig. 3.

4. CONCLUSIONS

Different inversion models suitable for the ozone retrieval from SCIAMACHY limb measurements were analyzed by means of the scientific processor. The outcomes were compared with the extensively validated algorithm of IUP-Bremen as well as with those of the SAGE-III instrument. The best agreement with the reference algorithm was obtained by using the **radiance-triplet model**. However, its implementation into the operational environment would require substantial effort and can be, therefore, considered rather for the distant future. Currently it is compromised by the SQWG to implement the **differential radiance model with two spectral windows**. It is already capable to retrieve ozone in the upper stratosphere / lower mesosphere ($45-65\ km$).

A number of regularization methods can be used in the scientific processor. Their efficiency was tested and the results are presented. The iteratively regularized Gauss-Newton method proves to be the best in terms of agreement with the SAGE-III profiles. However, this method is more time consuming than the Tikhonov regularization (by a factor of 1.6), because the use of the discrepancy principle as stopping rule requires the estimation of the noise level during an additional computational step.

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