

**Sicherstellung der SCIAMACHY-Datenqualität
in den Bereichen "Referenzspektren"
und "Red Grass"-Korrektur**

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Schlussbericht

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Zusammenfassung

Im Rahmen dieses Vorhabens wurden im Januar 2000 Referenzspektrenmessungen (Absorptionsquerschnitte von Ozon und Stickstoffdioxid, Okkultations-, Zenit- und Ringreferenzspektren) mit dem SCIAMACHY PFM Spektrometer durchgeführt und ausgewertet. Die Absorptionsquerschnitte von O₃ und NO₂ wurden dem SCIAMACHY Team zugänglich gemacht und über das WWW veröffentlicht (<http://www.iup.physik.uni-bremen.de/gruppen/molspec/index.html>).

Zudem wurde der Einfluß von erhöhten Rauschbeiträgen (sogenanntes "Red Grass") in SCIAMACHY-Spektren untersucht und Detektions- und Korrekturalgorithmen entwickelt, die im operationellen 0-1 und 1-2 Datenprozessor eingesetzt werden sollen.

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Einleitung

Die Studie gliedert sich in zwei Arbeitspakete:

- a) Messung von Referenzspektren nach der Streulichtminimierung am SCIAMACHY PFM Spektrometer,
- b) Untersuchungen zur Detektion und zur Korrektur des sogenannten „Red Grass“ Effektes.

Die Ergebnisse zu diesen Arbeitspaketen sind im Folgenden zusammengefasst. Detailliertere Ergebnisse zu a) sind in den Anhängen 1 und 2 zu finden. Zu b) enthält Anhang 3 einen ausführlichen Technischen Bericht.

Referenzspektren

Im Frühjahr 1999 wurde im Rahmen der Instrument Consent to Ship Reviews festgestellt, daß das Streulicht in Kanal 1 (240 nm - 310 nm) eine Größenordnung über der Spezifikation liegt (PO-NC-FOK-SH-300). Dies hätte zur Folge, daß Ozonprofile nur noch unzureichend aus SCIAMACHY-Messungen abgeleitet werden können. Ursache des erhöhten Streulichtes ist eine unzureichende Streulichtunterdrückung der Spektrometeroptik (Spiegelqualität, fehlende Lichtfallen, Oberflächenbeschichtungen). Es wurden daher alle erdenklichen Maßnahmen eingeleitet, um dieses Problem durch eine Anpassung der Optik zu beheben. Die Anpassungsmaßnahmen haben zur Folge, daß sich die Spaltfunktion der Kanäle 1 und 2 ändern wird. Die bisher mit dem SCIAMACHY Spektrometer gemessenen Absorptionsquerschnitte im UV (1. PI-Periode, Oktober 1998) sind daher bezüglich zweier wichtiger Parameter (Streulicht und Spaltfunktion) nicht mehr repräsentativ für die SCIAMACHY-Datenauswertung. Es war daher zwingend erforderlich, Messungen der wichtigsten UV-Absorber (Ozon, NO₂) sowie einige atmosphärische Spektren im UV (Sonnenokkultation, Zenit-, Ring-Spektren) erneut mit dem SCIAMACHY-Instrument unter operationellen Bedingungen (Vakuum, gekühltes Instrument) durchzuführen.

Durchführung der Delta2 – PI – Periode

Im Januar 2000 wurde bei Fokker Space and Systems in Schiphol/Amsterdam die Delta2–PI–Periode durchgeführt. Ziel war die Aufnahme von Referenzspektren von O₃ und NO₂ in den SCIAMACHY Kanälen 1 und 2, die durch technische Modifikationen für eine verbesserte Streulichtunterdrückung verändert worden waren (PO-NC-FOK-SH-300). Es wurden Absorptionsspektren von O₃ im Temperaturbereich von 203 – 293 K und von NO₂ im Temperaturbereich von 223 – 293 K mit für die Kanäle 1 und 2 geeigneten optischen Dichten gemessen. Ferner wurde eine Messung durchgeführt, in der das Ozon in der Zelle als UV-Filter benutzt wurde, so dass kein Licht der Lampe in Kanal 1 fallen konnte und somit alles noch auftretende Licht in Kanal 1 Streulicht war. Zur Überprüfung der Wellenlängeneichung des SCIAMACHY–Spektrometers wurden Absorptionsspektren von CO₂ und N₂O und Spektren einer CrPtNe–Linienlampe aufgenommen. Zudem wurden an einem halben Messtag Sonnenokkultationsmessungen durchgeführt.

Auswertung bzgl. Instrument-Charakterisierung

Die während der PI–Perioden gemessenen Absorptionsspektren wurden zur Charakterisierung des SCIAMACHY – Instrumentes verwendet. Anhand der Messung aus der Delta2–PI– Periode, bei der das Ozon in der Zelle als UV–Filter verwendet wurde, und einer äquivalenten Messung aus der PI–Periode wurde gezeigt, dass das Streulicht in Kanal 1 während der Delta2–PI– Periode um den Faktor 30 geringer war (siehe Abb. 1).

Durch Vergleich der Spektren einer CrPtNe-Lampe und CO₂- und N₂O-Absorptionsspektren aus der Delta2 – PI – Periode und Delta-PI-Periode wurde gezeigt, dass es zu keinen nennenswerten Verschiebungen der Wellenlängenachse in den Kanälen 3 – 8 durch den Umbau der Kanäle 1 und 2 gekommen ist. Die Bestimmung der Spaltfunktion der Kanäle 7 und 8 aus den Spektren der CrPtNe-Lampe wurde mit Absorptionsspektren überprüft und bestätigt, sofern die Druckverbreiterung in den Absorptionsspektren berücksichtigt wurde. Ferner wurden die Kanäle 1 und 2 für die Delta2-PI-Periode mit den Absorptionsspektren neu geeicht. Die Ergebnisse bzgl. der spektralen Eichung wurden in einer TN dokumentiert (Bogumil et al. 2001, siehe Anhang 1) und dem SCIAMACHY Projekt zur Verfügung gestellt. Die Ergebnisse wurden auf der Kalibrations-Untergruppensitzung der SSAG im Oktober 2000 präsentiert und diskutiert.

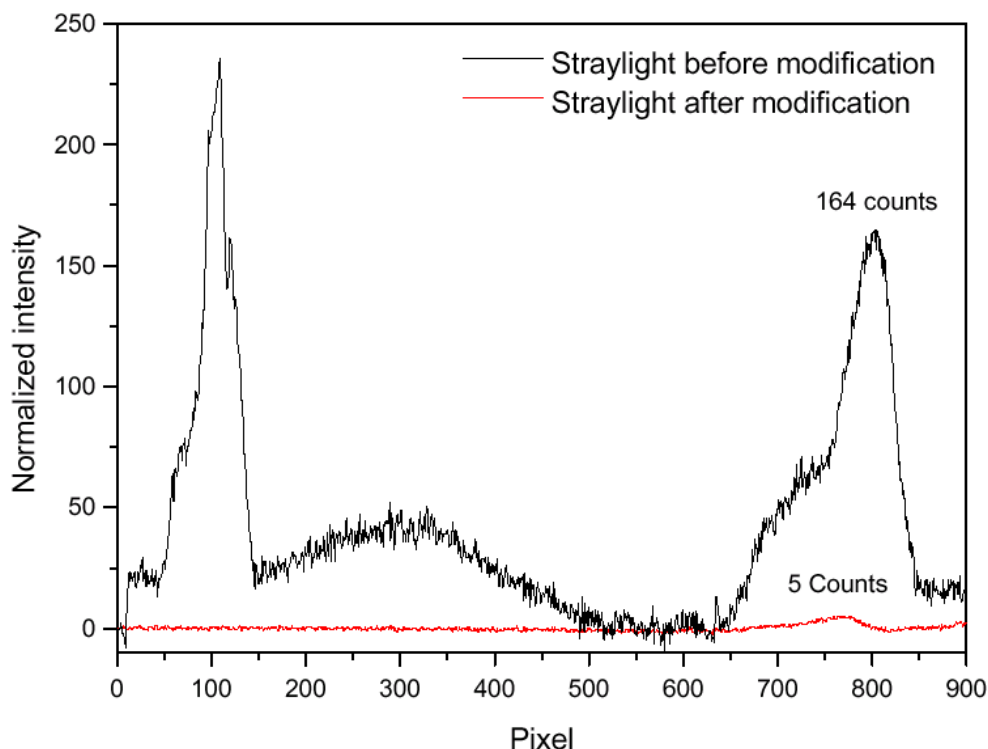


Abb. 1: Streulicht in Kanal 1 vor (PI-Periode) und nach (Delta-2 PI Periode) der Modifikation des SCIAMACHY PFM Spektrometers Delta2-PI-Periode

Auswertung bzgl. Absorptionsquerschnitte von O₃ und NO₂

Tabelle 1 gibt eine Übersicht über die in den verschiedenen PI-Perioden durchgeführte Messungen. In Bogumil et al. 2000 wurden Details der Auswertung beschrieben und veröffentlicht (siehe Anhang 2). Die Ergebnisse wurden auf dem ERS-ENVISAT Symposium in Göteborg präsentiert. Aus den Ozonabsorptionsmessungen aus der PI und Delta2 – PI – Periode wurden Ozonspektren im Wellenlängenbereich von 230 – 1070 nm und im Temperaturbereich von 203 – 293 K zusammengesetzt und auf absolute Absorptionsquerschnitte skaliert. Damit liegt ein Satz von Ozon-Absorptionsquerschnitten über einen so breiten Spektral- und Temperaturbereich vor, wie er bisher noch nicht existiert. Aus den NO₂ – Absorptionsmessungen aus der PI und Delta2 – PI – Periode wurden NO₂ – Spektren im Wellenlängenbereich von 230 – 930 nm und im Temperaturbereich von 203 – 293 K zusammengesetzt und auf absolute Absorptionsquerschnitte skaliert. Damit liegt ein Satz von NO₂ – Absorptionsquerschnitten über einen sehr breiten Spektral- und Temperaturbereich mit einem guten Signal-zu-Rausch – Verhältnis vor.

Molekül	PI - Periode		Delta - PI - Periode		Delta2 - PI - Periode	
	Temperatur in K	Anzahl der Partial-Drücke	Temperatur in K	Anzahl der Partial-Drücke	Temperatur in K	Anzahl der Partial-Drücke
O₃	293, 273, 243, 223, 203	5	-	-	293, 273, 243, 223, 203	2
NO₂	293, 273, 243, 223, 203	2 - 4	293	7	293, 273, 243, 223	1 - 3
SO ₂	293, 273, 243, 223, 203	2	-	-	-	-
OCIO	293	1	-	-	-	-
NO	293	1	-	-	-	-
O ₂	293, 243, 203	1	-	-	-	-
H ₂ CO	293	1	-	-	-	-
H ₂ O	293	1	293	2	-	-
CO	293	2	293, 243	2 - 3	-	-
N₂O	293	2	293, 243	1 - 2	293	1
CH ₄	293, 273, 243, 223, 203	2 - 4	293, 243	2 - 4	-	-
CO₂	293, 243, 203	2 - 4	293, 243	2 - 4	293	1

Tabelle 1: Übersicht der während der PI-Perioden durchgeführten Messungen

Bei den Ozonabsorptionsquerschnitten wurde festgestellt, daß in Kanal 1 der sogenannte Memory-Effekt die Spektren beeinflusst und zu Artefakten führt. Daraufhin wurde ein Korrekturprogramm für diesen Effekt entwickelt, die Ozonabsorptionsquerschnitte unter Berücksichtigung dieses Effektes neu ausgewertet und eine Version 2.0 der Absorptionsquerschnitte erstellt. Ungeklärt ist weiterhin, wie es zu der Stufe in den Ozonabsorptionsquerschnitten zwischen Kanal 1 und 2 kommt.

Die Dateien mit den Absorptionsquerschnitten sind unter <http://www-iup.physik.uni-bremen.de/gruppen/molspec/index.html> veröffentlicht worden und werden bereits im Rahmen der SCIAMACHY Prozessorenentwicklung am DLR-IMF genutzt.

Zusammenfassung „Referenzspektren“

Die Delta2-PI-Periode erbrachte folgende, für das Projekt SCIAMACHY wichtige Ergebnisse:

- Das Streulicht in Kanal 1 wurde durch die technischen Modifikationen deutlich verringert (siehe Abb. 1).
- Es wurde neue Referenzspektren für O₃ und NO₂ in den Kanälen 1 und 2 nach dem Umbau gemessen, ausgewertet und über das WWW zur Verfügung gestellt.
- Die spektrale Eichung wurde in den Kanälen 1 und 2 verbessert.

"Red Grass"-Rauschen

Im Frühjahr 1999 wurde im Rahmen der Störmeldung (PO-NC-FOK-SH-0277) festgestellt, daß für die SCIAMACHY Kanäle 1-5 zusätzliches Odd-Even-Rauschen zufällig und unvorhersehbar für bestimmte spektrale Bereiche auftritt. Die Ursache hierfür konnte nicht eindeutig identifiziert werden, ist aber aller Wahrscheinlichkeit nach in der Detektorelektronik zu suchen. Auf dem Material Review Board und dem Instrument Consent to Ship Board (PO-MN-DAR-SH-0137) wurde entschieden, keine Hardware-Modifikation zur Lösung dieses Problems durchzuführen sondern die Auswirkungen auf die Datenqualität durch geeignete Filterung und Mittelung der Meßdaten zu minimieren. Da das "Red-Grass"-Phänomen prinzipiell bei allen Messungen auftreten kann (atmosphärische Messungen sowie Kalibrationsmessungen) und eine Erkennung via Software schwierig ist, wurde im Rahmen dieser Studie untersucht, welche Filter- und Mittellungsstrategien zur Detektion und zur Minimierung des Einflusses auf die Datenqualität einsetzbar sind. Es wurden die folgenden Untersuchungen durchgeführt:

- Entwicklung von Detektions-, Filter- und Mittellungsstrategien für die 0-1 Prozessierung
- Auswirkungen auf die Datenqualität des Level 1 Produktes
- Einfluss der Filter- und Mittellungsstrategien auf Level-2 DOAS Datenqualität

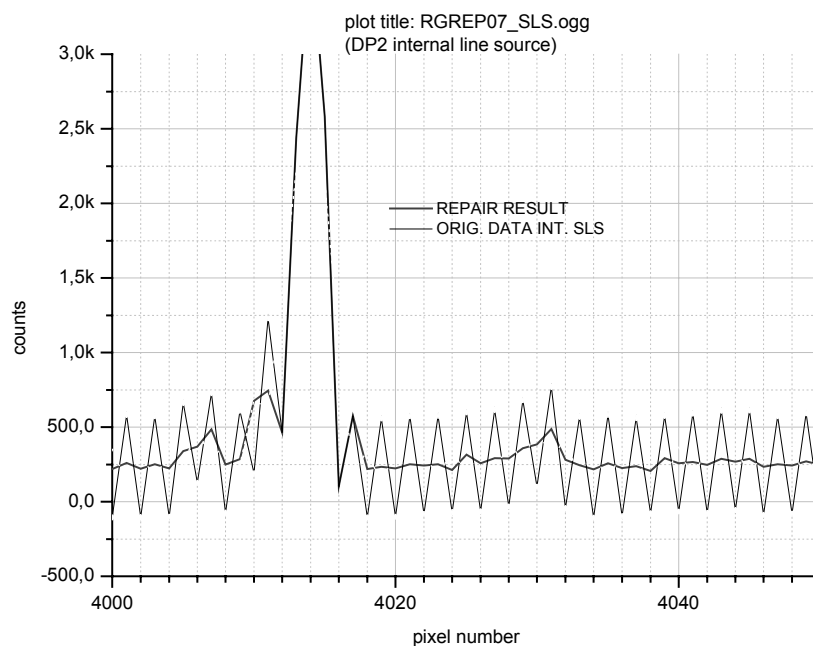


Abb. 2: Red Grass Korrektur am Beispiel eines SLS Spektrum.

Dabei wurde ein Algorithmus zur Detektion- und Minimierung des Red Grass entwickelt (vgl. Abb. 2), getestet und dem DLR-IMF zur Implementierung in den Prototyp-Prozessor zur Verfügung gestellt. Zudem wurden Abschätzungen auf den zu erwartenden Einfluss von Red Grass auf DOAS Datenprodukte durchgeführt. Details der Ergebnisse dieses Arbeitspakets wurden in einer TN zusammengefasst (Gurlit 2000, Anhang 3).

Die Ergebnisse wurden zudem der Kalibrations-Untergruppensitzung der SSAG im Oktober 2000 präsentiert und diskutiert.

Veröffentlichungen

K. Bogumil, J. Orphal und J. P. Burrows, „Temperature dependent absorption cross sections of O₃, NO₂, and other atmospheric trace gases measured with the SCIAMACHY spectrometer“, Proceedings of the ERS – Envisat Symposium Gothenborg 2000, ESA-ESTEC, ISBN 92-9092-685-6, Noordwijk, 2000. (Anhang 2)

J. Orphal, K. Bogumil, A. Dehn, B. Deters, S. Dreher, O.C. Fleischmann, M. Hartmann, S. Himmelmann, T. Homann, H. Kromminga, P. Spietz, A. Türk, A. Vogel, S. Voigt and J.P. Burrows, Laboratory Spectroscopy in Support of UV-Visible Remote-Sensing of the Atmosphere", in: Recent Research Developments in Physical Chemistry, edited by S. G. Pandalai, Transworld Research; in press

Projektberichte

K. Bogumil, H. Bovensmann, J. Orphal; Improved wavelength calibration of the SCIAMACHY PFM spectrometer using molecular absorption spectra, IFE-TN-120201, Universität Bremen, 2001 (Anhang 1)

W. Gurlit, Study of the REDGRASS phenomenon, Final Report, University of Bremen, November 2000 (Anhang 3)

Tagungsbeiträge

K. Bogumil, J. Orphal und J. P. Burrows, „Temperature dependent absorption cross sections of O₃, NO₂, and other atmospheric trace gases measured with the SCIAMACHY spectrometer“, ERS – Envisat – Symposium, Göteborg, Schweden, 2000

K. Bogumil, J. Orphal and J. P. Burrows, "Spektrale Charakterisierung des SCIAMACHY-PFM - Satellitenspektrometers mit Molekülspektren"; Poster, Frühjahrstagung der Deutschen Physikalischen Gesellschaft, 21-24. März 2000, Bremen

Anhang 1

K. Bogumil, H. Bovensmann, J. Orphal; Improved wavelength calibration of the SCIAMACHY PFM spectrometer using molecular absorption spectra, IFE-TN-120201, Universität Bremen, 2001

Improved wavelength calibration of the SCIAMACHY PFM spectrometer using molecular absorption spectra

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1 Introduction

The wavelength calibration of grating spectrometers is usually performed using lines of spectral calibration lamps. For the wavelength calibration of the SCIAMACHY PFM spectrometer an external PtCrNe hollow cathode lamp, a HgAr and a low pressure Xenon lamp were used as spectral line sources during the on-ground calibration measurements in August and September 1998 (OPTEC 2) (RD 1). During the re-calibration period OPTEC 5 the external PtCrNe hollow cathode lamp was only used as spectral line sources (RD 2). However, the spectral lines of the PtCrNe hollow cathode lamp are not evenly spread over the wavelength range of the SCIAMACHY spectrometer. In some spectral regions and in the overlap regions of the channels spectral lines useful for wavelength calibration are missing. In this spectral regions the polynomials for the wavelength calibration have to be extrapolated resulting in an inaccurate absolute and relative wavelength calibration. In order to solve this problem and to improve the wavelength calibration especially in the overlap regions of the channels molecular absorptions bands of SO₂, OClO, NO₂, and O₃ and molecular absorption lines of CO, CO₂ and N₂O were used. In this technote the polynomial coefficients for the improved wavelength calibration are given, the improvement in the overlap regions of the channels is shown and the results are compared with previous wavelength calibrations.

2 Used Data

The presented wavelength calibration is based on the spectra of external spectral line sources and on molecular absorption spectra of SO₂, OClO, NO₂, O₃, CO, CO₂ and N₂O measured with the SCIAMACHY spectrometer as well as on molecular absorption spectra of the same gases measured with a Fourier transform spectrometer (RD 3–RD 6). Spectra of an external PtCrNe hollow cathode lamp and molecular absorption spectra were measured with the SCIAMACHY spectrometer using CATGAS (Calibration Apparatus for Trace Gas Absorption Spectra), a transportable set-up for absorption spectroscopy, during the PI, Delta PI and Delta2 PI period. The PI period measurements took place following the on-ground calibration measurements in August and September 1998 and are therefore representative for the OPTEC 2 calibration campaign. The Delta PI and Delta2 PI period measurements were performed subsequent to the OPTEC 3 and OPTEC

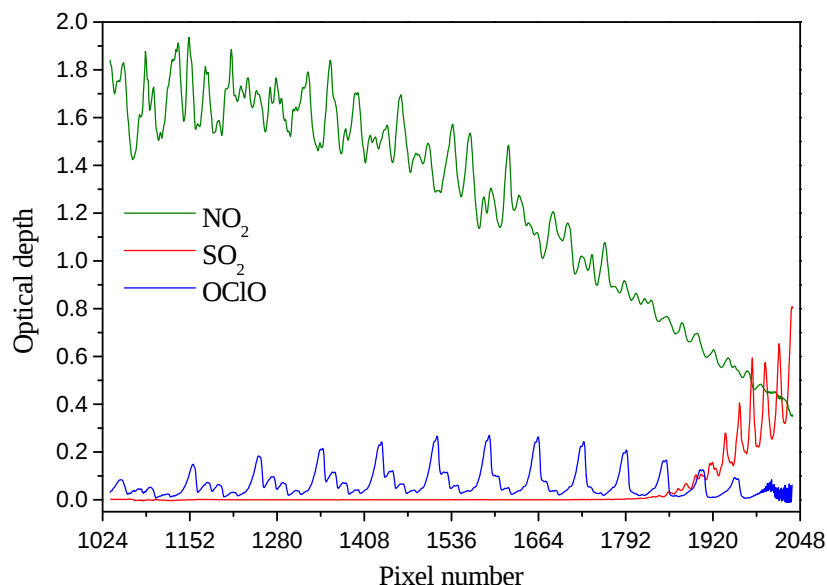


Figure 1: Optical depths of OClO, NO₂, and SO₂ in channel 2 used for wavelength calibration of the PI period measurements.

5 measurements and are representative for these calibration campaigns. The experimental set-up CATGAS, the measurement procedure and the data reduction are described in RD 7. For the wavelength calibration described in this technote, the optical depths of the different gases measured at 293 K and at appropriate pressures are used. In the channels 7 and 8 all used spectra were carefully examined for dead and bad pixel. From the spectra of the external PtCrNe hollow cathode lamp all dead pixels (RD 8) have to be excluded from the analysis. From the molecular optical depths most of the pixels labelled “dead, noise too low test” (RD 8) and some of the pixels “dead, noise too high test” (RD 8) have to be removed, but the other dead and bad pixels appear to be useful and are not excluded from the analysis. For example, the optical depths used for the wavelength calibration in channel 2 and 7 are shown in figure 1 and 2.

In order to determine the wavelength of the molecular absorption bands and lines molecular absorption spectra measured by Fourier transform spectroscopy are used. These spectra show an accurate wavelength calibration due to the internal calibration of the Fourier transform spectrometer with a HeNe laser.

Highly resolved spectra of CO₂, CO, and N₂O were recorded in Bremen before the PI period using a Fourier transform spectrometer in order to determine the experimental conditions of the PI period measurements. Therefore these optical depths are measured at the same experimental conditions as the Delta PI period measurements and were used to determine the wavelengths of the molecular absorption lines.

The molecular absorption cross sections used to determine the wavelength of the absorptions bands of SO₂, OClO, NO₂, and O₃ are described in RD 3–RD 6.

For the wavelength calibration of the PI period measurements the pixel positions of the Pt–, Cr–, Ne–, Hg–, Ar– and Xe–lines given in RD 9 are used. The wavelength of the lines are given in RD 10–RD 12. Additionally, the optical depths of SO₂ (channel 1 and 2), OClO (channel 2 and 3) and NO₂ (channel 2–4) were used for the wavelength calibration of the PI period measurements.

For the wavelength calibration of the Delta and Delta2 PI period spectra of the PtCrNe

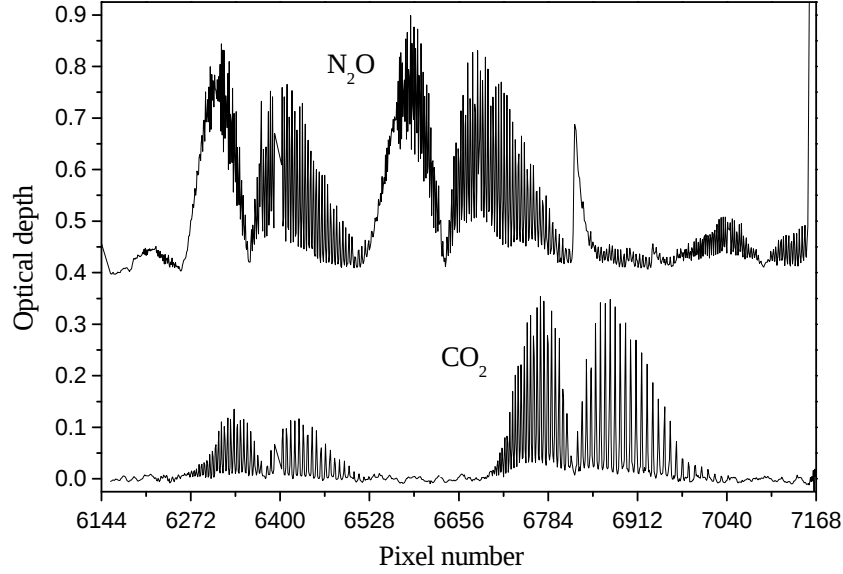


Figure 2: Optical depths of CO_2 and N_2O in channel 7 used for wavelength calibration of the Delta PI period measurements. The optical depth of N_2O is shifted for +0.4 units for a better presentation.

hollow cathode lamp on CATGAS were used together with optical depths of CO_2 , CO , and N_2O (Delta PI period) and O_3 and NO_2 (Delta2 PI period).

An overview over the spectral lines, molecular absorption bands and lines is given in table 1

3 Methodology

First the pixel positions and the wavelengths of the spectral lines, molecular absorption bands and lines have to be determined.

The pixel positions of the spectral lines determined during the on-ground calibration (RD 9) can also be used for the wavelength calibration of the PI period measurements taking place after the on-ground calibration, because the SCIAMACHY spectrometer was permanently stabilized to nominal temperatures. For the Delta PI and Delta2 PI period measurements the pixel positions of the spectral lines of the external PtCrNe hollow cathode lamp on CATGAS were determined in the channels 1, 7 and 8 by fitting the actual slit function (RD 13, RD 14) to the lines using a nonlinear least square fitting routine. In order to find the pixel position of the molecular absorption bands of SO_2 , OCIO , and NO_2 the optical depths are interpolated to a grid which is finer than the spectral stability of the SCIAMACHY spectrometer using cubic splines. Then the positions of the maxima of the molecular absorption bands are read off. For the wavelength calibration of the Delta2 PI period measurements in channel 1 differential optical depths of O_3 and NO_2 are used in order to detect the absorption peaks more easily. The pixel positions of the molecular absorption lines in channel 7 and 8 are determined by fitting Voigt line shape profiles to the lines using a nonlinear least square fitting routine.

The wavelength of the Cr-, Pt-, and Ne-lines are given in RD 10 and RD 11, the wavelength of the Hg-, Ar-, and Xe-lines in RD 12. To determine the wavelengths of the molecular absorption bands and lines the molecular absorption cross sections measured

Kanal	Number of spectral lines			Number of molecular absorption bands and lines
	PtCrNe-lamp	HgAr-lamp	Xe-lamp	
1 PI period	11	1	–	SO ₂ : 20
1 Delta2 PI period	6	–	–	O ₃ : 11, NO ₂ : 13
2 PI period	12	1	–	SO ₂ : 2, OClO: 12, NO ₂ : 12
3 PI period	21	5	5	OClO: 3, NO ₂ : 33
4 PI period	17	8	4	NO ₂ : 11
5 PI period	23	–	11	–
6 PI period	13	2	12	–
7 Delta PI period	4	–	–	CO ₂ : 43, N ₂ O: 65
8 Delta PI period	7	–	–	CO: 34, N ₂ O: 35

Table 1: Number of the spectral lines and of the molecular absorption bands and lines used for wavelength calibration in the different channels.

by Fourier transform spectroscopy are interpolated and convoluted with the actual slit function (RD 1, RD 13, RD 14). The positions of the maxima are read off.

A polynomial (function of the pixel number) is fitted to the wavelength of the different channels. Different orders of the polynomial are tested. The residuals are analyzed to identify and remove outliers. The root mean square (RMS) of the residuals is used to determine the order of the polynomial.

4 Results

For the wavelength calibration polynomials up to fifth order are used in the different channels:

$$\lambda = a_0 + a_1 \cdot p + a_2 \cdot p^2 + a_3 \cdot p^3 + a_4 \cdot p^4 + a_5 \cdot p^5. \quad (1)$$

The wavelength λ is given in nanometer for vacuum conditions. p is the pixel number. The number of the first pixel in each channel is 0.

The polynomial coefficients and the RMS of the residuals are given in the tables 2–4. The polynomial coefficient a_2 is omitted in the wavelength calibration of channel 1 for the PI period measurements because the term is not significant. Generally, the polynomial coefficients are highly correlated. Therefore they cannot mixed up with coefficients obtained in other wavelength calibrations to improve these calibrations. The RMS of the residuals is a measure for the accuracy of the wavelength calibration. In order to test the wavelength calibration absorption cross sections measured by the SCIAMACHY spectrometer were fitted to absorption cross sections measured by Fourier transform spectroscopy. The

Kanal	1	2	3
a ₀	213.914394232754 ±0.0672656	411.958173645994 ±0.0202686	383.698000870210 0.0330998
a ₁	0.135888727350164 ±0.00036668	−0.105896979345404 ±0.000356089	0.250322277175679 ±0.00056555
a ₂	0.00 ±0.00	−6.99079016079668 · 10 ^{−6} ±1.99827 · 10 ^{−6}	−2.18182814929041 · 10 ^{−5} ±0.311879 · 10 ^{−5}
a ₃	−1.00128312317065 · 10 ^{−7} ±0.0287576 · 10 ^{−7}	2.58325767068200 · 10 ^{−8} ±0.480359 · 10 ^{−8}	−5.96309192276385 · 10 ^{−9} ±7.365076 · 10 ^{−9}
a ₄	1.40887149528135 · 10 ^{−10} ±0.0529935 · 10 ^{−10}	−3.49670120591909 · 10 ^{−11} ±0.517192 · 10 ^{−11}	2.64573726186063 · 10 ^{−11} ±0.7725617 · 10 ^{−11}
a ₅	−6.00227387625200 · 10 ^{−14} ±0.282445 · 10 ^{−14}	1.32335136310812 · 10 ^{−14} ±0.204872 · 10 ^{−14}	−9.97128629485997 · 10 ^{−15} ±2.95572 · 10 ^{−15}
RMS in nm	0.008235	0.007813	0.021651

Kanal	4	5	6
a ₀	595.237059506309 0.0088	773.033256136432 ±0.0204832	971.516808682106 ±0.097107
a ₁	0.224946666200801 ±0.000126128	0.301886629357001 ±0.000207507	0.806692646645848 ±0.00107271
a ₂	−2.67918834755433 · 10 ^{−5} ±0.0519417 · 10 ^{−5}	−4.01597200857541 · 10 ^{−5} ±0.0689416 · 10 ^{−5}	−8.91423331420010 · 10 ^{−5} ±0.377291 · 10 ^{−5}
a ₃	1.25480052773764 · 10 ^{−8} ±0.0799889 · 10 ^{−8}	2.02807262530259 · 10 ^{−8} ±0.0915867 · 10 ^{−8}	5.32595829015918 · 10 ^{−8} ±0.520366 · 10 ^{−8}
a ₄	9.50033762992689 · 10 ^{−13} ±4.06455 · 10 ^{−13}	9.88749344032840 · 10 ^{−13} ±4.16722 · 10 ^{−13}	1.09062136085195 · 10 ^{−11} ±0.243546 · 10 ^{−11}
RMS in nm	0.008533	0.006469	0.031865

Table 2: Polynomial coefficients for the wavelength calibration of PI period measurements in the channels 1–6 using a fourth or fifth order polynomial. These coefficients have to be compared with OPTEC 2 data.

wavelength axis of the SCIAMACHY absorption cross sections were shifted and squeezed and the absorption cross sections measured by Fourier transform spectroscopy were scaled and a baseline polynomial was subtracted. The necessary change of the wavelength of the SCIAMACHY absorption cross sections was always smaller than the RMS of the residuals. The improvement of the wavelength calibration in the overlap regions is shown in the figures 3 – 6.

Comparisons with previous wavelength calibrations (RD 1, RD 2, RD 15) are shown in figures 7–9 and tables 5–refComp5.

The differences shown in figure 7 and 9 arise in spectral regions in which the polynomials are extrapolated in the wavelength calibrations described in RD 1 and RD 2. In the other regions the differences are within ±0.02 nm.

In RD 15 it was suggested that the line 1 in channel 8 is misidentified. This was confirmed

Kanal	7	8
a ₀	1934.32631406374 0.00262732	2259.29502296346 0.00218264
a ₁	0.117512578934991 ±0.0000115206	0.135289190153202 0.000013531
a ₂	$-1.04610104754033 \cdot 10^{-5}$ $\pm 0.00106533 \cdot 10^{-5}$	$-1.20108305047519 \cdot 10^{-5}$ $\pm 0.00149204 \cdot 10^{-5}$
RMS in nm	0.006631	0.008794

Table 3: Polynomial coefficients for the wavelength calibration of Delta PI period measurements in the channels 7–8 using a second order polynomial. These coefficients have to be compared with OPTEC 3 data.

Kanal	1
a ₀	213.099447591191 ±0.483095
a ₁	0.143881564790716 ±0.00571214
a ₂	$-3.10384021925274 \cdot 10^{-5}$ $\pm 2.551095 \cdot 10^{-5}$
a ₃	$-4.37796094005753 \cdot 10^{-8}$ $\pm 5.41139 \cdot 10^{-8}$
a ₄	$9.14160944934119 \cdot 10^{-11}$ $\pm 5.47786 \cdot 10^{-11}$
a ₅	$-4.28238889932400 \cdot 10^{-14}$ $\pm 2.12661 \cdot 10^{-14}$
RMS in nm	0.015393

Table 4: Polynomial coefficients for the wavelength calibration of Delta2 PI period measurements in channel 1 using a fifth order polynomial. These coefficients have to be compared with OPTEC 5 data.

by the presented wavelength calibration. The wavelength of this line is 2269.414 nm. Four new lines are identified for the presented calibration. They are listed in table 7.

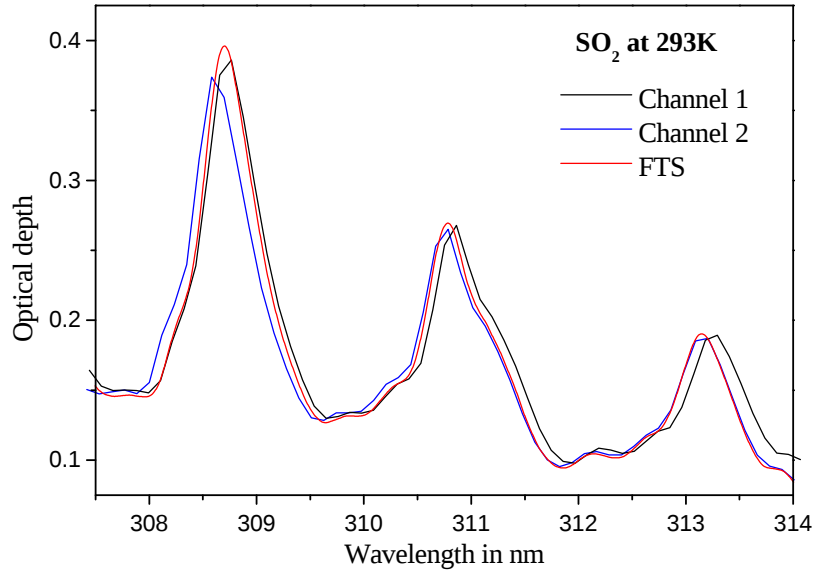


Figure 3: Optical depth of SO₂ in the overlap region of channel 1 (black line) and 2 (blue line) measured with the SCIAMACHY spectrometer during the PI period. For the wavelength calibration the polynomial coefficients given in RD 1 are used. Red line: Optical depth of SO₂ measured by Fourier transform spectroscopy (RD 3). This line shows the accurate wavelength calibration.

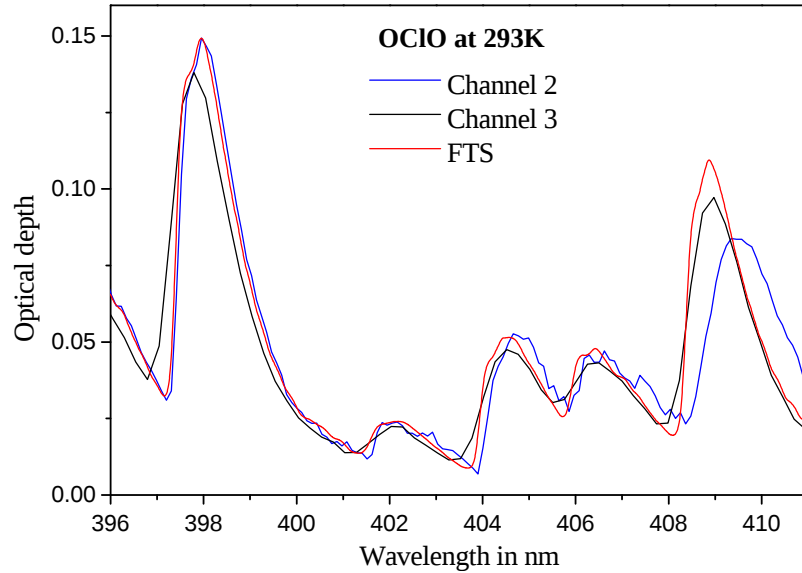


Figure 4: Optical depth of OCIO in the overlap region of channel 2 (blue line) and 3 (black line) measured with the SCIAMACHY spectrometer during the PI period. For the wavelength calibration the polynomial coefficients given in RD 1 are used. Red line: Optical depth of OCIO measured by Fourier transform spectroscopy (RD 4). This line shows the accurate wavelength calibration.

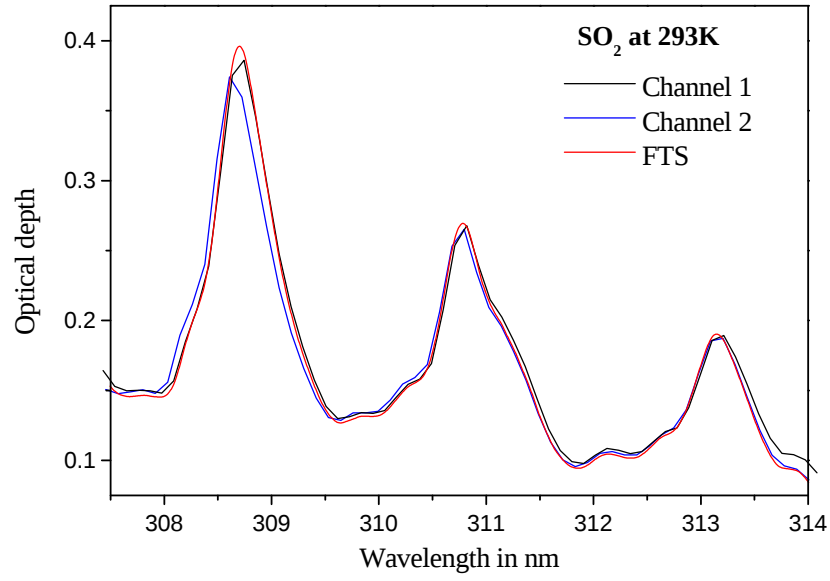


Figure 5: Optical depth of SO₂ in the overlap region of channel 1 (black line) and 2 (blue line) measured with the SCIAMACHY spectrometer during the PI period. For the wavelength calibration the polynomial coefficients given in table 2 are used. Red line: Optical depth of SO₂ measured by Fourier transform spectroscopy (RD 3). This line shows the accurate wavelength calibration.

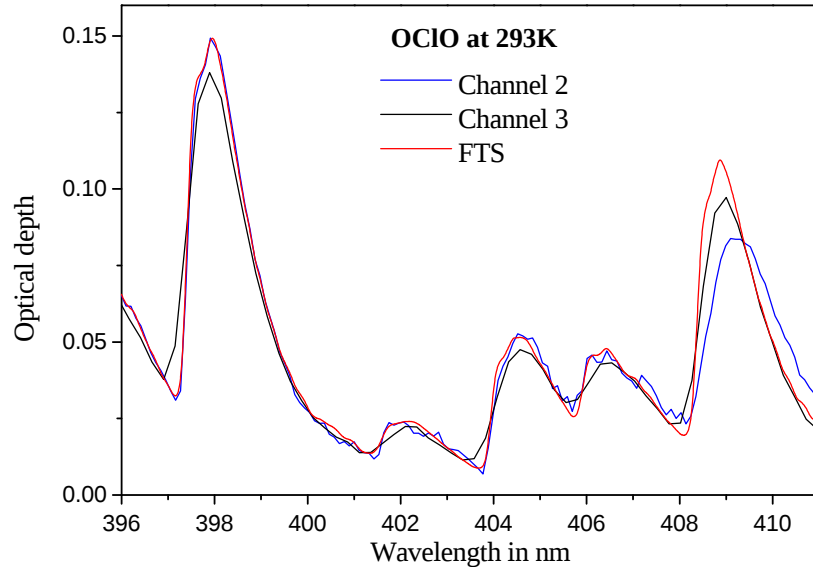


Figure 6: Optical depth of OCIO in the overlap region of channel 2 (blue line) and 3 (black line) measured with the SCIAMACHY spectrometer during the PI period. For the wavelength calibration the polynomial coefficients given in table 2 are used. Red line: Optical depth of OCIO measured by Fourier transform spectroscopy (RD 4). This line shows the accurate wavelength calibration.

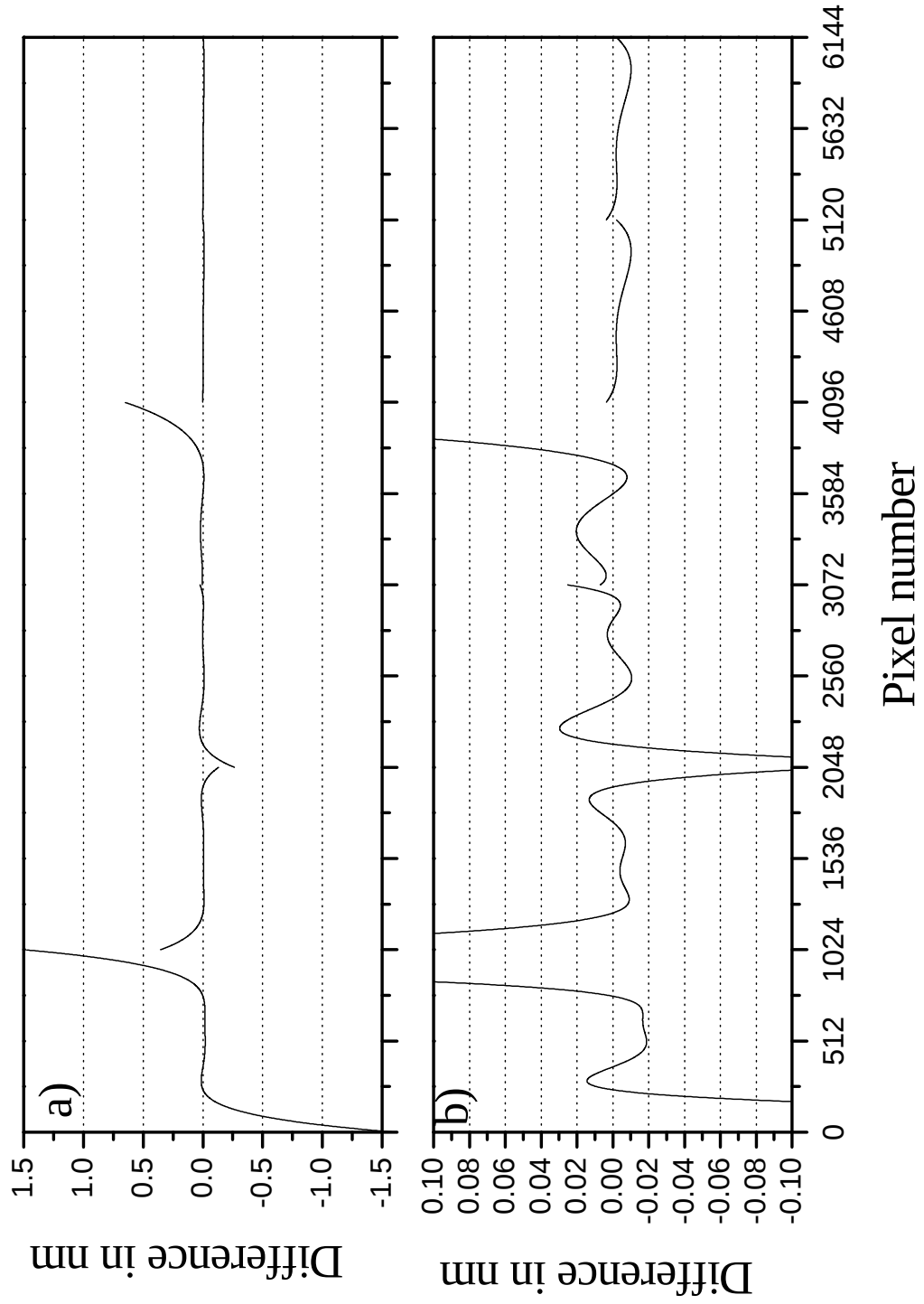


Figure 7: Differences in nanometer between the wavelength calibration given in RD 1 and the wavelength calibration using the polynomial coefficients in table 2. a) Overview. b) Enlarged view.

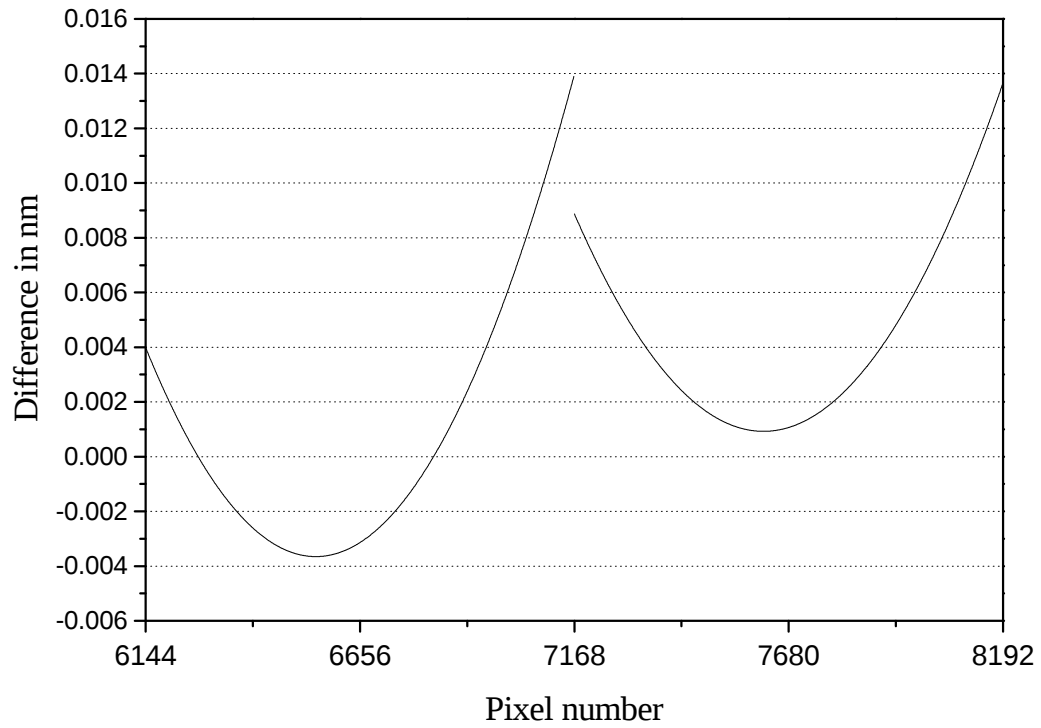


Figure 8: Differences in nanometer between the wavelength calibration given in RD 15 and the wavelength calibration using the polynomial coefficients in table 3.

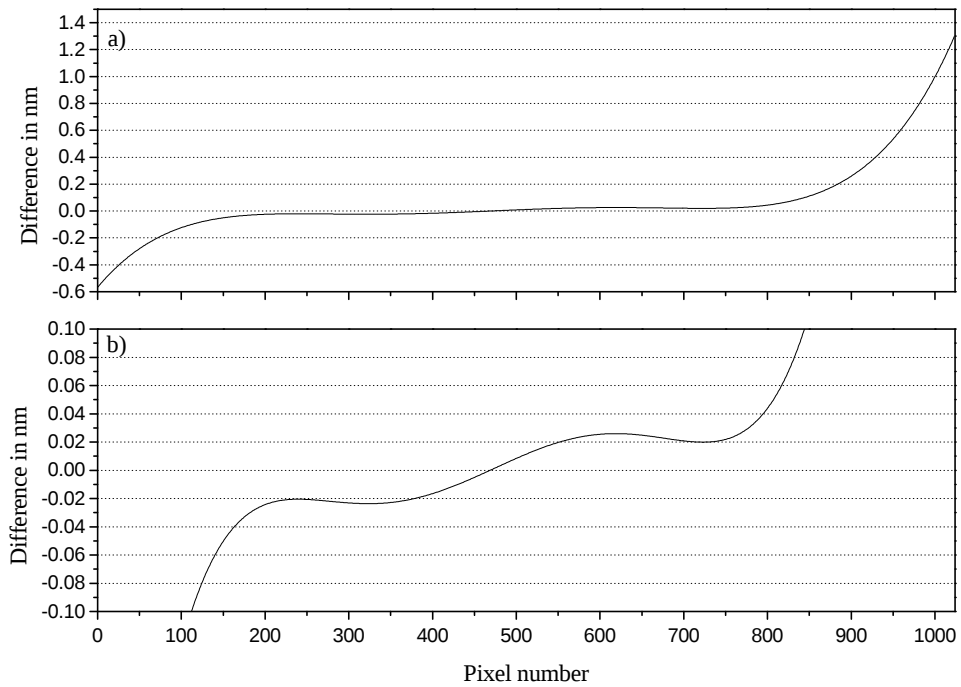


Figure 9: Differences in nanometer between the wavelength calibration given in RD 13 and the wavelength calibration using the polynomial coefficients in table 4. a) Overview. b) Enlarged view.

Channel 1:

	Presented wavelength calibration without quadratic term	with quadratic term	Wavelength calibration given in RD 1
a_0	213.914394232754	214.381008393909722	212.305115340045
a_1	0.135888727350164	0.13077353955625588	0.154092109708927
a_2	0.00	$2.11108698770985947 \cdot 10^{-5}$	$-7.77876073407846 \cdot 10^{-5}$
a_3	$-1.00128312317065 \cdot 10^{-7}$	$-1.41579333554254827 \cdot 10^{-7}$	$5.85241556829872 \cdot 10^{-8}$
a_4	$1.40887149528135 \cdot 10^{-10}$	$1.79916539892088644 \cdot 10^{-10}$	$-1.54585714063459 \cdot 10^{-11}$
a_5	$-6.00227387625200 \cdot 10^{-14}$	$-7.42076616714184567 \cdot 10^{-14}$	0.00

Channel 2:

	Presented wavelength calibration	Wavelength calibration given in RD 1
a_0	411.958173645994	412.313025392126
a_1	-0.105896979345404	-0.110055031474417
a_2	$-6.99079016079668 \cdot 10^{-6}$	$1.10217831398168 \cdot 10^{-5}$
a_3	$2.58325767068200 \cdot 10^{-8}$	$-1.10306253045083 \cdot 10^{-8}$
a_4	$-3.49670120591909 \cdot 10^{-11}$	$8.34879053480501 \cdot 10^{-13}$
a_5	$1.32335136310812 \cdot 10^{-14}$	0.00

Channel 3:

	Presented wavelength calibration	Wavelength calibration given in RD 1
a_0	383.698000870210	383.435671699233
a_1	0.250322277175679	0.254013554923858
a_2	$-2.18182814929041 \cdot 10^{-5}$	$-3.84605768788959 \cdot 10^{-5}$
a_3	$-5.96309192276385 \cdot 10^{-9}$	$2.68645733013547 \cdot 10^{-8}$
a_4	$2.64573726186063 \cdot 10^{-11}$	$-3.11589013358386 \cdot 10^{-12}$
a_5	$-9.97128629485997 \cdot 10^{-15}$	0.00

Channel 4:

	Presented wavelength calibration	Wavelength calibration given in RD 1
a_0	595.237059506309	595.244024479762
a_1	0.224946666200801	0.224806777007188
a_2	$-2.67918834755433 \cdot 10^{-5}$	$-2.50731002363058 \cdot 10^{-5}$
a_3	$1.25480052773764 \cdot 10^{-8}$	$7.73648054496758 \cdot 10^{-9}$
a_4	$9.50033762992689 \cdot 10^{-13}$	$4.72789997665034 \cdot 10^{-12}$

Table 5: Comparison of the polynomial coefficients in the channel 1 – 3 of the presented wavelength calibration and of the wavelength calibration given in RD 1.

Channel 5:

	Presented wavelength calibration	Wavelength calibration given in RD 1
a_0	773.033256136432	773.036897761747
a_1	0.301886629357001	0.301811374131375
a_2	$-4.01597200857541 \cdot 10^{-5}$	$-3.98346385575010 \cdot 10^{-5}$
a_3	$2.02807262530259 \cdot 10^{-8}$	$1.97362645337979 \cdot 10^{-8}$
a_4	$9.88749344032840 \cdot 10^{-13}$	$1.27541246592409 \cdot 10^{-12}$

Channel 6:

	Presented wavelength calibration	Wavelength calibration given in RD 1
a_0	971.516808682106	971.364644577727
a_1	0.806692646645848	0.808872132313809
a_2	$-8.91423331420010 \cdot 10^{-5}$	$-9.74672414595368 \cdot 10^{-5}$
a_3	$5.32595829015918 \cdot 10^{-8}$	$6.49151762251990 \cdot 10^{-8}$
a_4	$1.09062136085195 \cdot 10^{-11}$	$5.57065681724853 \cdot 10^{-12}$

Channel 7:

	Presented wavelength calibration	Wavelength calibration given in RD 15
a_0	1934.32631406374	1934.3303
a_1	0.117512578934991	0.117475
a_2	$-1.04610104754033 \cdot 10^{-5}$	$-1.04148 \cdot 10^{-5}$

Channel 8:

	Presented wavelength calibration	Wavelength calibration given in RD 15
a_0	2259.29502296346	2259.3039
a_1	0.135289190153202	0.135254
a_2	$-1.20108305047519 \cdot 10^{-5}$	$-1.19719 \cdot 10^{-5}$

Channel 1:

	Presented wavelength calibration	Wavelength calibration given in RD 2
a_0	213.099447591191	212.532675877075
a_1	0.143881564790716	0.151306521751326
a_2	$-3.10384021925274 \cdot 10^{-5}$	$-6.91445037505473 \cdot 10^{-5}$
a_3	$-4.37796094005753 \cdot 10^{-8}$	$4.76139988457908 \cdot 10^{-8}$
a_4	$9.14160944934119 \cdot 10^{-11}$	$-1.05552859203415 \cdot 10^{-11}$
a_5	$-4.28238889932400 \cdot 10^{-14}$	0.00

Table 6: Comparison of the polynomial coefficients in channel 1 in the channels 5–8 of the presented wavelength calibration and of the wavelength calibration given in RD 1, RD 2, and RD 15, respectively.

Kanal	Pixel position of the maximal signal	Fitting window	Fitted pixel position	Wavelength in nm	Element
1	796	793–798	796,0009 $\pm 0,0117$	308,9061	Ne II
1	831	828–835	830,6753 $\pm 0,0241$	312,7103	Ne II
5	908	893–926 ¹	907,7008 $\pm 0,0039$	1029,8204	Ne I
5	975	967–981	975,0847 $\pm 0,0111$	1048,9075	

Table 7: New identified lines in the spectrum of PtCrNe hollow cathode lamp used for the wavelength calibration.

5 Conclusions

New polynomial coefficients are given for the wavelength calibration of the SCIAMACHY spectrometer. Based on SLS and molecular absorption spectra this calibration yield a more reliable wavelength calibration in the overlap regions.

For channel 8 the misidentification of the first line in channel 8 suggested in RD 15 is confirmed and the right wavelength is given.

Four lines of the PtCrNe hollow cathode lamp are identified for an improved calibration in the channels 1 and 5.

¹In this fitting window a weak line also have to be fitted.

6 Reference Documents

- RD 1 TN-SCIA-1000TP/189, *Wavelength and slitfunction calibration of the SCIAMACHY PFM*
- RD 2 RP-SCIA-1000TP/266, *OPTEC 5: Wavelength calibration of the SCIAMACHY PFM*
- RD 3 A. C. Vandaele, P. C. Simon, J. M. Guilmot, M. Carleer, and R. Colin, *SO₂ absorption cross section measurement in the UV using a Fourier transform spectrometer*, J. Geophys. Res. **99** (D12), 25599–25605 (1994)
- RD 4 H. Kromminga, J. Orphal and J. P. Burrows, *New temperature-dependent absorption cross-sections of OClO in the 325–435 nm region measured with Fourier transform spectroscopy*, J. Phys. Chem. Chem. Phys., in preparation
- RD 5 S. Voigt, J. Orphal, and J. P. Burrows, *Absorption cross-sections of NO₂ at atmospheric temperatures (203–293 K) and pressures (100–1000 mbar) in the 12500–40000 cm⁻¹ spectral range measured using Fourier transform spectroscopy*, J. Phys. Chem. Chem. Phys., submitted
- RD 6 S. Voigt, J. Orphal, K. Bogumil and J. P. Burrows, *Absorption cross-sections of O₃ at atmospheric temperatures (203–293 K) and pressures (100–1000 mbar) in the 12500–40000 cm⁻¹ spectral range measured using Fourier transform spectroscopy*, J. Phys. Chem. Chem. Phys., submitted
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- RD 13 RP-SCIA-1000TP/267, *OPTEC 5: Slit function calibration of the SCIAMACHY PFM*
- RD 14 K. Bogumil, H. Bovensmann, *Slit Function Calibration SCIAMACHY Channel 7 and 8*, Issue 1, 10.03.2000
- RD 15 H. Schrijver, *Spectral calibration of SCIAMACHY channels 7 and 8 using gas cell absorption spectra*, SRON-EOS-HS-99001, Issue 1, 30th March 1999

Anhang 2

K. Bogumil, J. Orphal und J. P. Burrows, „Temperature dependent absorption cross sections of O₃, NO₂, and other atmospheric trace gases measured with the SCIAMACHY spectrometer“, Proceedings of the ERS – Envisat Symposium Gothenborg 2000, ESA-ESTEC, ISBN 92-9092-685-6, Noordwijk, 2000.

TEMPERATURE DEPENDENT ABSORPTION CROSS SECTIONS OF O₃, NO₂, AND OTHER ATMOSPHERIC TRACE GASES MEASURED WITH THE SCIAMACHY SPECTROMETER

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INTRODUCTION

The detection of O₃, NO₂ and other atmospheric trace gases by means of absorption spectroscopy requires accurate knowledge of their absorption cross sections at atmospheric temperatures and pressures. Using the SCIAMACHY (SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY) PFM satellite spectrometer [1], [2] a new data set of temperature dependent absorption cross sections was measured in 1998–2000 prior to the launch of SCIAMACHY on board of Envisat-1 in 2001. The data set comprises absorption cross sections of O₃, NO₂, SO₂, O₂, OClO, H₂CO, H₂O, CO, CO₂, CH₄, and N₂O measured over the whole spectral range of the SCIAMACHY spectrometer (230–2380 nm) and in broad temperature range (203–293 K). The absorption cross sections will be used in the SCIAMACHY data processing for the retrieval of column densities and vertical distributions of atmospheric trace gases from the satellite measurements. In order to obtain absorption cross sections at intermediate temperatures if necessary a temperature parametrization is applied to the O₃, NO₂ and SO₂ absorption cross sections using an exponential function. The molecular absorption cross sections were already used for improving the wavelength calibration of the SCIAMACHY spectrometer and for characterizing the slit function and the straylight properties of the instrument.

EXPERIMENTAL SET-UP

The SCIAMACHY Spectrometer

The SCIAMACHY spectrometer is a multichannel grating spectrometer operating in the ultraviolet, visible and near infrared wavelength region at medium resolution. It measures continuously from 230 to 1760 nm with a resolution of 0.21–1.44 nm (full width at half maximum FWHM of the slit function) and in two optical windows between 1940 and 2040 nm and 2265 and 2380 nm (resolution 0.20 nm and 0.17 nm, respectively). A double spectrometer design with a predisperser prism and gratings in the eight channels is used to cover this large wavelength range and to suppress straylight inside the spectrometer. The light is detected by cooled diode arrays detectors with 1024 pixels consisting of silicon for wavelengths ≤ 1000 nm and of InGaAs for the near infrared wavelength region. The pixel exposure times can independently be chosen for each channel. The spectrometer shows a high stability and can measure small absorptions due to its high dynamic range. A CrPtNe-lamp and a white light source are integrated for spectral and radiometric calibration and instrument monitoring during flight. During the measurements of the absorption cross sections the SCIAMACHY spectrometer

was controlled by a dedicated on-ground electronics made by Dornier, cooled to operational temperatures and kept in a vacuum tank at Fokker Space. Therefore all wavelengths mentioned in this paper are given for vacuum conditions. Prior to the measurements presented in this paper the SCIAMACHY spectrometer was characterized and calibrated by industry (consortium of Fokker Space, Dornier, TPD-TNO, SRON and others) providing data concerning the pixel-to-pixel gain, stray light properties, the slit function in each channel, the wavelength calibration and the polarization properties [3]. A detailed description of the SCIAMACHY instrument is given in [1], [2].

CATGAS

The acronym CATGAS means „Calibration Apparatus for Trace Gas Absorption Spectra“. CATGAS is a transportable set-up for absorption spectroscopy consisting of two coolable quartz glass cells, different light sources and a gas system for static and flow gas measurements. It may be operated at temperatures and pressures relevant to the stratosphere and troposphere: $180\text{ K} \leq T \leq 300\text{ K}$ and $1\text{ mbar} \leq p \leq 1000\text{ mbar}$.

The main components of CATGAS are two double jacketed quartz glass cells (volume 3 l). The inner jacket of the cells are floated by a circulating cooling fluid (ethanol), while the outer jackets are evacuated for thermal isolation. For this purpose, the cells are additionally wrapped by an isolating foam. The cooling fluid is pumped through the inner jackets by a two-stage cryocooler (Haake KT90) for the one cell and a cooling thermostat (Haake F6-C40) for the other cell. Temperatures between 293 K and 203 K were adjusted in the cells during the measurements with a stability and an absolute accuracy better than $\pm 1\text{ K}$ calibrated before the measurements using a Pt100 temperature element in the cell. The cells contain a White optics [4] with a baselength of 120 cm and a f-number of 60. Pathlengths of 505 cm and 985 cm were used for the measurements.

The light of either a Xenon-lamp (ILC Technology, 300 W) for the ultraviolet and visible wavelength region or a Quartz-Tungsten-Halogen-lamp (Osram, 250 W) for the visible and near infrared wavelength region is focused into one of the cells using an off-axis parabolic mirror, a spherical and a flip mirror. After having passed the cell the light is focused on the entrance of quartz glass fibre bundle (diameter 6.2 mm) consisting of about 8000 single fibres (75% UV-enhanced and 25% IR-enhanced). The other end of the fibre bundle is formed as a slit and imaged on the entrance slit of the SCIAMACHY spectrometer so that the slit is fully illuminated. For wavelength calibration using an external source the light of a CrPtNe-lamp (LOT Oriel) can also be focused on the entrance of the glass fibre bundle.

Measurements are performed while the gas mixtures flow through the cell as well as under static condition. Absorption measurements in a gas flow are used for gases which are photolyzed by the analyzing light in order to maintain a constant column density in the cell. The cells are flushed with different gas mixtures controlled by calibrated gas flow controllers (MKS). The following mixtures are used: NO_2 , NO or SO_2 in N_2 ; pure O_2 ; O_3 in a mixture of O_2 and N_2 ; and OCIO in a mixture of O_3 , O_2 and N_2 . The NO_2 , NO and SO_2 are taken from commercial gas bottles (Messer Griesheim) with a certified mixture of 1% NO_2 , NO or SO_2 in N_2 . These mixtures are additionally diluted with nitrogen (N_2 5.0) as carrier gas. The O_3 is generated by flowing oxygen (O_2 5.0) through a commercial ozonizer (Innovatec OG5) containing a silent discharge. The oxygen is also used for the measurements of pure oxygen. The mixing ratios of each trace gas are adjusted to match the different absorption of the gas in the different wavelength regions. After mixing up the gases are cooled prior to entering the cells. In the cells, the pressure is monitored by two capacitive manometer (MKS Baratron) varying between 50 and 900 mbar for the different measurements. After flushing through the cells the ozone is destroyed by a catalytic process, the other gases are trapped by a cryo trap.

For the static measurements another gas system is used, which is separated from the flow system by valves. The core of the cells is filled with gas mixtures of CO, CO_2 , N_2O or CH_4 in N_2 prepared in a special gas mixing system at a total pressure of 500 mbar in the cell and different partial pressures of the trace gases. The H_2O is filled into the cell at its vapour pressure, the H_2CO at slightly reduced vapour pressure in order to avoid saturation effects.

Measurement Procedure

For each temperature and gas mixture the following measurement procedure was applied: First the pixel exposure times in the different channels were optimized for the selected combination of light source, cell and pathlength. Then a shutter after the end of the fibre bundle was closed and the dark current was measured for the chosen pixel exposure times. Thereafter a spectrum of the lamp was recorded without any absorber in the cell. During this measurement the cell was empty or only filled with carrier gas (N_2). Then the cell was filled with the gas mixture to be measured. After having achieved equilibrium conditions in the cell an absorption spectrum was recorded and the gas mixture was pumped out of the cell. At last a lamp spectrum was again measured in order to monitor lamp drifts. Each measurement took 5 times 64 seconds, while the detectors of the different channels were repeatedly read out.

At the beginning and end of each day a spectrum of the CrPtNe-lamp either on CATGAS or built in the SCIAMACHY spectrometer was recorded for wavelength calibration. Once a week a spectrum of the internal White light source in the SCIAMACHY spectrometer was measured.

List of Measurements

Three measurement campaigns were performed with the SCIAMACHY spectrometer. In October 1998 the so-called PI-Period took place and after some modifications of the instrument the Delta-PI-Period (January 1999) and the Delta2-PI-Period (January 2000) were performed. During the Delta-PI-Period and the Delta2-PI-Period only measurements in channels concerned by the modifications were repeated.

Table 1: Measurements during the PI-, the Delta-PI- and the Delta2-PI-period

Molecule	PI-period		Delta-PI-period		Delta2-PI-period	
	Tempera- tures in K	number of partial pressures	Tempera- tures in K	number of partial pressures	Tempera- tures in K	number of partial pressures
O ₃	293, 273, 243, 223, 203	5	–	–	293, 273, 243, 223, 203	3
NO ₂	293, 273, 243, 223, 203	2 (293 K, 203 K), 4 (273 K, 243 K), 3 (223 K)	293	7	293, 273, 243, 223	1 (293 K), 3 (273 K, 243 K, 223 K)
SO ₂	293, 273, 243, 223 203	2	–	–	–	–
OCIO	293	1	–	–	–	–
NO	293	1	–	–	–	–
O ₂	293, 243 203	1	–	–	–	–
H ₂ CO	293	1	–	–	–	–
H ₂ O	293	1	293	2	–	–
CO	293	2	293, 243	3 (293 K), 2 (243 K)	–	–
N ₂ O	293	2	293, 243	2 (293 K), 1 (243 K)	293 K	1
CH ₄	293, 273, 243, 223 203	4 (293 K, 243 K), 2 (273 K, 223 K, 203 K)	293, 243	4 (293 K), 2 (243 K)	–	–
CO ₂	293, 243, 203	4 (293 K), 2 (243 K, 203 K)	293, 243	4 (293 K), 2 (243 K)	293 K	1

DATA REDUCTION

First the readouts of the channels were averaged and for each measurement the dark current was subtracted from the two lamp spectra and the absorption spectrum. Then the uniform and the ghost spectral straylight was calculated for each spectrum using scaling factors for the uniform straylight in the different channels and polynomial coefficients describing the positions and intensities of the different spectral ghosts. The scaling factors and the polynomial coefficients were provided by industry [3]. For channel 1, a special straylight algorithm was applied due to the strong polarization dependence of the straylight in this channel [5]. Once being calculated the straylight was subtracted from the lamp and absorption spectra. By dividing the lamp spectra measured before and after the absorption spectrum through each other, a possible lamp drift during the measurement and the signal-to-noise ratio was monitored. Usually the lamp drift was $\leq 1\%$ and the signal-to-noise ratio was larger than 200 depending on wavelength. The lamp spectra with the smaller drift in relation to the absorption spectrum and with the better signal-to-noise ratio was chosen as reference spectrum $I_0(\lambda)$. At any rate the

lamp spectrum with the smaller signal-to-noise ratio was used. If both lamp spectra were of the same quality, they were weighted and averaged to obtain the reference spectrum $I_0(\lambda)$. Then the optical depth was calculated:

$$\text{optical depth} = \ln \left(\frac{I_0(\lambda)}{I(\lambda)} \right) = \sigma \cdot n \cdot l \quad (1)$$

($I(\lambda)$: absorption spectrum, σ : absorption cross-section, n : number of molecules per volume, l : optical pathlength). If necessary the optical depths were corrected for residual lamp drifts by adding a constant value assuming the lamp drift was linear with time. The O_3 optical depth at 293 K had to be corrected for an additional OCIO absorption and the O_3 optical depths at the other temperatures for some atomic lines in the Chappuis bands caused by the lights in the hall where the measurements took place. The optical depths of NO_2 at 243 K, 223 K and 203 K also comprised absorption of N_2O_4 , which is formed in thermal equilibrium with NO_2 at low temperatures. They had to be corrected for this absorption by a procedure using three different optical depths of NO_2/N_2O_4 and basing on the fact that N_2O_4 negligibly absorbs at wavelengths above 400 nm [6], [7]. During the measurement of the OCIO optical depth O_3 also was in the cell, therefore the O_3 absorption had to be removed from the OCIO optical depth. For each gas the optical depths measured at different partial pressures were scaled to each other and were wavelength-calibrated using a fifth order polynomial. Then the optical depths were concatenated to obtain complete spectra over the whole absorption wavelength range of the measured molecule. The error of the optical depths caused by lamp drifts and noise is 1.1%. In order to calculate absolute absorption cross sections from the optical depths the optical pathlength l and the partial pressure of the trace gas in the cell have to be known very precisely. Due to the limited time available during the PI periods the partial pressures of the trace gases could not be determined exactly. For this reason the optical depths were scaled to absolute absorption cross sections using molecular absorption cross sections from literature. The O_3 optical depths were scaled to absorption cross sections calculated the polynomial coefficients given by Bass and Paur [8]. The NO_2 and the SO_2 optical depth at 293 K were scaled to the absorption cross sections measured by Vandaele et al. [9], [10]. The optical depths at the other temperatures were scaled using the integrated absorption cross section of the electronic transition, which is temperature independent assuming the electronic transition moment independent from the nuclear coordinates [7], [11]. The OCIO optical depth was scaled to the absorption cross sections measured by Kromminga et al. [12] and the O_2 optical depths were scaled using HITRAN data [13]. The error of the absorption cross sections is given by the error of the optical depths, the error of the absorption cross sections used for scaling and the error in the scaling procedure. The error of the O_3 absorption cross sections can be estimated to 3.1%. The error of the NO_2 and SO_2 absorption cross sections depends on the temperature and is 3.2% for the NO_2 absorption cross sections at 293 K, 3.4% for the NO_2 absorption cross sections at lower temperatures, 2.8% for the SO_2 absorption cross sections at 293 K, and 3.0% for the SO_2 absorption cross sections at lower temperatures. The error of the OCIO absorption cross sections is 8.5%.

ABSORPTION CROSS SECTIONS

In this section the measured temperature dependent absorption cross sections are presented. The absorption cross sections vary with temperature because the rotational and vibrational state distribution in the electronic ground state changes with temperature. Generally the differential cross sections increase with decreasing temperature.

Temperature dependent absorption cross sections of ozone are measured from 230 nm to 1070 nm thus containing the band origin of the Wulf bands at 9553.13 cm^{-1} [14] (fig. 1a). In channel 7 and 8 the absorption to highly excited vibrational states can be observed (fig. 1b). The line positions and intensities of these bands are recently measured by high resolution Fourier transform spectroscopy [15], [16], [17], [18], [19]. The temperature dependence of the Hartley, Huggins and Chappuis bands in the O_3 absorption cross section is in agreement with previous studies [11], [20], [21], [22]. Due to the high partial pressures of O_3 used in the measurements and due to the high sensitivity of the SCIAMACHY spectrometer the very weak absorption between 350 nm and 420 nm could also be measured with a good signal-to-noise ratio (fig. 2a). The hot and cold bands in the Huggins bands are clearly visible in this region. The intensity of the hot bands arising from excited vibrational states in the electronic ground state, decreases with decreasing temperature, while the intensity of the cold band increases. With decreasing temperature the edges of the Huggins and the Chappuis bands move towards shorter wavelength and the absorption between these two bands decreases. It is unexplained why this absorption again increases between 223 K and 203 K. This was already observed in the ozone absorption cross sections measured with the GOME FM spectrometer [11] and by Fourier Transform spectroscopy [7], [23], so an error caused by lamp drifts is improbable. Due to the high purity of the used gases, absorption of gaseous impurities is not to be expected. Maybe a weakly bound complex of O_3 and O_2 is formed at lower temperatures.

The temperature dependence of the Wulf bands is first measured at more than two temperatures and over a broad spectral range (fig. 2b). In this region the differential absorption cross sections vary for 20% between 293 K and 203 K in the

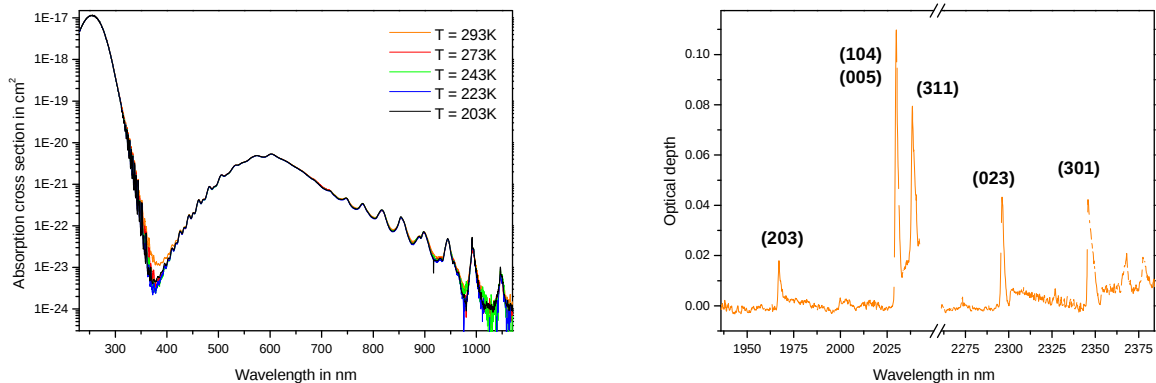


Fig. 1: a) Temperature dependent absorption cross sections of O₃ between 230 nm and 1070 nm. b) Optical depths of O₃ at 293 K in the channels 7 and 8.

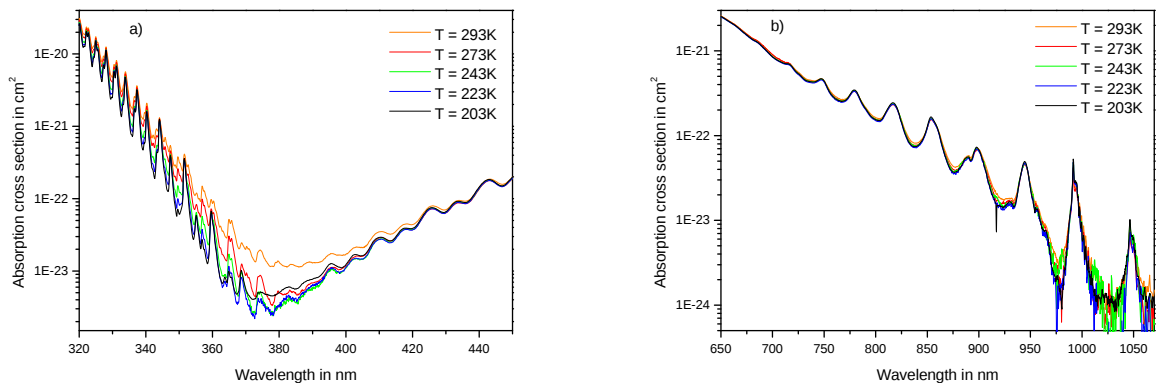


Fig. 2: a) Temperature dependent absorption cross sections of O₃ in the Huggins bands. b) Temperature dependent absorption cross sections of O₃ in the Wulf bands.

maxima of the absorption peaks.

Absorption cross sections of NO₂ are also measured between 203 K and 293 K (fig. 3). The temperature dependence in the wavelength region used for atmospheric detection is shown in fig. 3b. The absorption cross sections measured by the SCIAMACHY spectrometer are compared with absorption cross sections measured by the GOME spectrometer over a similar spectral range (231–794 nm) and at similar temperatures (221–293 K) [24]. The absorption cross section measured by the GOME spectrometer are smaller at all temperatures than the SCIAMACHY absorption cross sections but except for the differences in the absolute values the absorption cross sections well agree over a broad wavelength range. This shows that both sets of temperature dependent absorption cross sections do not contain residual N₂O₄ absorption and errors caused by lamp drifts.

In fig. 4 absorption cross sections of SO₂ and their temperature dependence in the 295–320 nm wavelength range are shown. At 293 K the absolute absorption cross sections agree within 5% with the absorption cross sections measured by Vandaele et al. [10] and by Hearn and Joens [25], the differential cross sections measured by the SCIAMACHY spectrometer are slightly larger.

In fig. 5 absorption cross sections of O₂ and OClO are shown. The OClO absorption cross sections are scaled to the absorption cross sections measured by Kromminga et al. [12] and therefore about 10% smaller than the absorption cross sections measured by Wahner et al. [26].

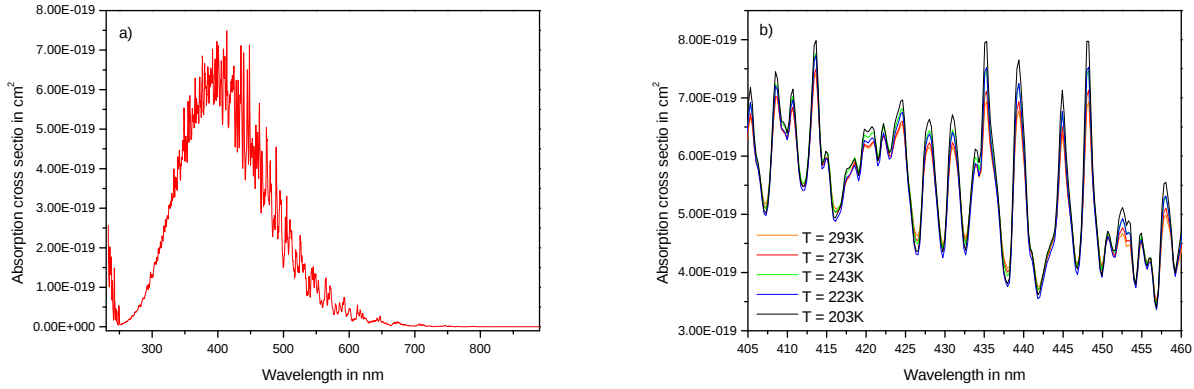


Fig. 3: a) Absorption cross sections of NO₂ at 273 K. b) Temperature dependent absorption cross sections of NO₂ in the 405–460 nm wavelength range.

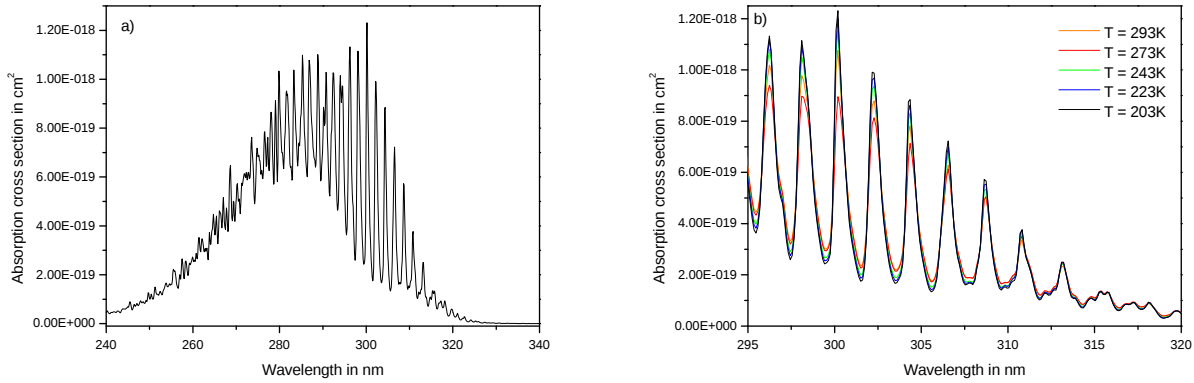


Fig. 4: a) Absorption cross sections of SO₂ at 203 K. b) Temperature dependent absorption cross sections of SO₂ in the 295–320 nm wavelength range.

TEMPERATURE PARAMETRIZATION OF THE ABSORPTION CROSS SECTIONS

Absorption cross sections are usually measured at selected temperatures. In order to characterize their temperature dependence and to calculate absorption cross sections at intermediate temperatures a temperature parametrization is applied to the measured absorption cross sections. Thereby the noise in the spectra as well as small uncertainties due to lamp drifts and to unrecognized straylight are also reduced.

For the SO₂ absorption cross sections an exponential function is applied to describe the temperature dependence:

$$\sigma(\lambda, T) = \exp(x_1(\lambda) - \frac{x_2(\lambda)}{T}). \quad (2)$$

The two wavelength-dependent parameters $x_1(\lambda)$ and $x_2(\lambda)$ are adjusted by a nonlinear least-squares fitting routine in the wavelength range between 260 nm and 335 nm. The absorption spectrum at 273 K is excluded from the fit because of problems caused by larger lamp drifts. For this temperature it is recommended to use the modelled spectrum. The agreement between the measured and the modelled spectra is better than 2% between 260 and 320 nm. For smaller wavelength the larger deviations result from small lamp intensities and therefore larger lamp drifts, for longer wavelengths the deviations result from small absorbances. A theoretical interpretation of the parameters $x_1(\lambda)$ and $x_2(\lambda)$ needs further investigation.

For the O₃ and NO₂ absorption cross sections a third wavelength dependent parameter $x_3(\lambda)$ has to be introduced to

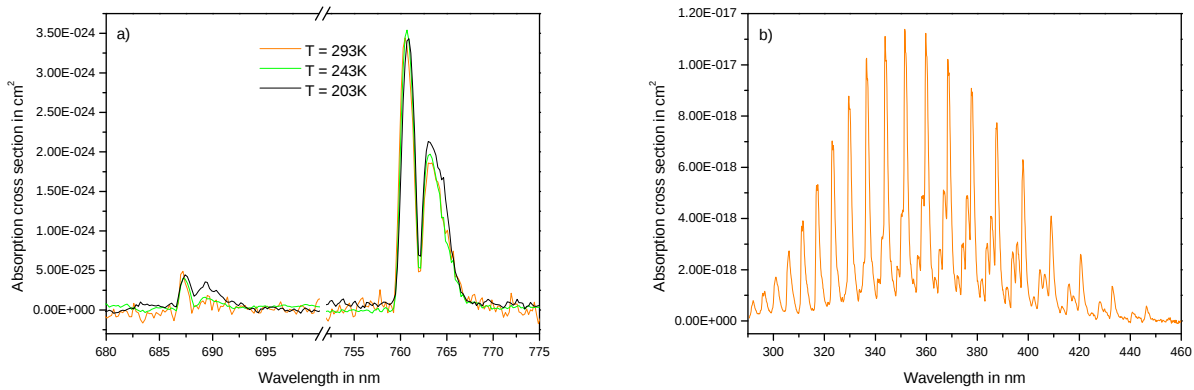


Fig. 5: a) Temperature dependent absorption cross sections of O₂ in the visible wavelength region. b) Absorption cross sections of OCIO at 293 K.

describe adequately the temperature dependence:

$$\sigma(\lambda, T) = \exp(x_1(\lambda) - \frac{x_2(\lambda)}{T} - x_3(\lambda) \cdot T). \quad (3)$$

The temperature parametrization was applied to the NO₂ absorption cross sections in the 400–600 nm wavelength region and to the O₃ absorption cross sections in the 320–350 nm wavelength region. The modelled spectra agree better than 2% with the measured spectra within these wavelength regions.

INSTRUMENT CHARACTERIZATION

Wavelength Calibration

The wavelength calibration of the SCIAMACHY spectrometer is performed using the spectral lines of an external CrPtNe-lamp [3]. However, the spectral lines are not evenly spread over the wavelength range of the SCIAMACHY spectrometer (fig. 7a). Especially at the borders of the channels and in channel 7 lines useful for calibration are failing and the polynomials for calibration have to be extrapolated. In this regions molecular absorption lines can be used for wavelength calibration (fig. 7b). To determine the pixel positions of the molecular lines the molecular optical depth depending on

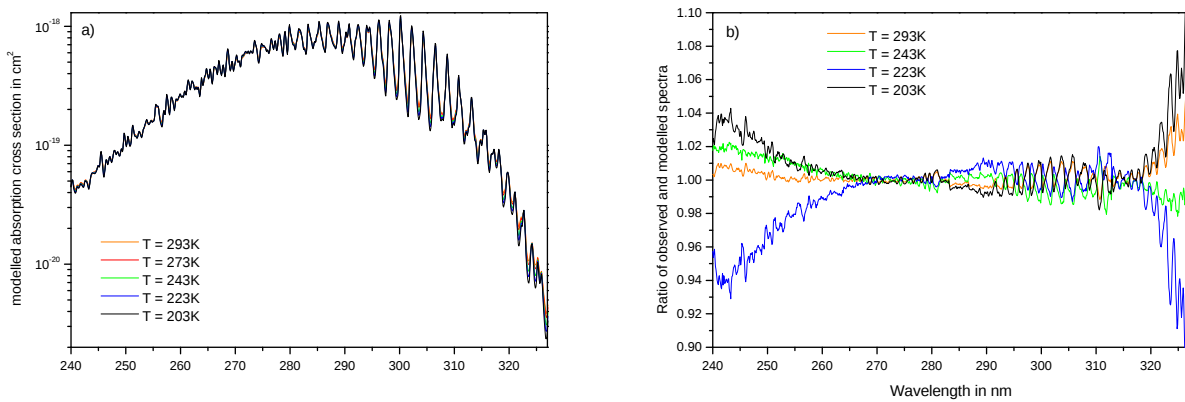


Fig. 6: a) Modelled absorption cross section of SO₂. b) Ratio of the modelled and measured absorption cross section of SO₂.

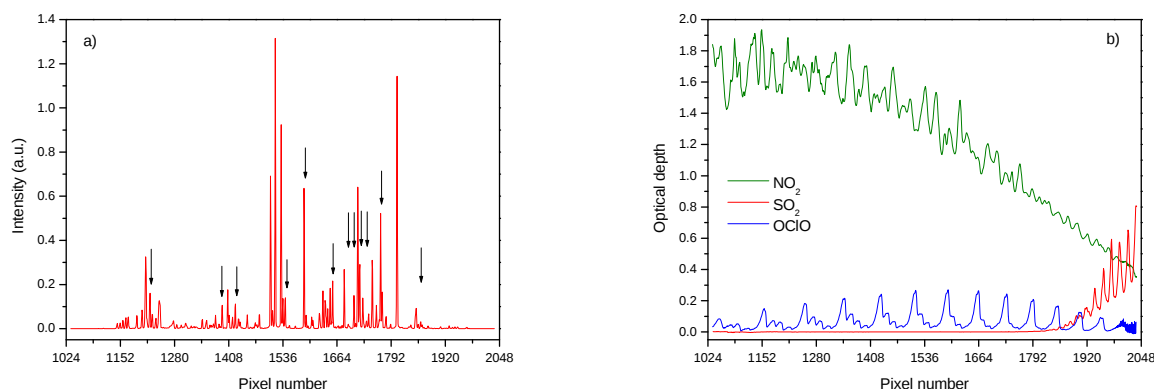


Fig. 7: a) Spectral lines of the CrPtNe-lamp. The spectral lines of the CrPtNe-lamp used for calibration are indicated by arrows. b) Optical depths of OClO, NO₂, and SO₂ in channel 2 used for wavelength calibration.

pixel are interpolated on a finer grid depending on the spectral stability of the channels using splines. The wavelengths of the lines are determined using well calibrated molecular spectra measured by a Fourier transform spectroscopy at the same temperatures [7], [10], [12] and convoluted with the SCIAMACHY slit function. A fifth order polynomial is fitted to the data using a linear least-square fit. The residuals are smaller than 0.01 nm in the middle of the channels and slightly larger at the borders of the channels.

Slit Function

The slit function is determined for each channel by fitting different functions to the spectral lines of a CrPtNe-lamp. For channel 1–6 the type of the slit function (Simple hyperbolic function for channel 1–5 and a Gaussian function for channel 6) and its full width at half maximum (FWHM) was provided by industry [3]. Highly resolved molecular spectra measured by Fourier transform spectroscopy [7], [9], [10], [12], [23] were convoluted with the slit function assuming that the FWHM is constant for each channel and compared to the spectra measured with the SCIAMACHY spectrometer. The agreement was generally good, except for channel 1. In this channel the convolution with the same slit function but with a smaller FWHM results in a better agreement.

The slit function in the channels 7 and 8 is derived from measurements performed during the Delta-PI period after realignment of these channels. Different analytical functions are fitted to the spectral lines of the CrPtNe-lamp using a nonlinear least square fitting routine. From the fits the type of the slit function is determined. The slit function in Channel 7 is a Gaussian function (FWHM 1.7 pixel) and in channel 8 a Voigt profile (FWHM 1.3 pixel). Because there are only a few spectral lines in each channel the wavelength dependence of the FWHM of the slit function can not be determined. For this purpose molecular spectra can be analyzed because they show bands of regularly spaced lines over the whole channels. The molecular spectra were measured at a total pressure of 500 mbar using N₂ as buffer gas in order to broaden the spectral lines and to prevent their saturation. Using the molecular spectra for characterizing the slit function the pressure broadening has to be taken into account. The FWHM of the pressure broadened lines is between 0.2 and 0.4 pixels and 0.02 and 0.06 nm, respectively. Because of the pressure broadening the molecular lines in channel 7 also have to be fitted using a Voigt profile because the convolution of the Lorentzian line shape of a pressure broadened molecular line with the Gaussian slit function is a Voigt profile. The analysis of the molecular spectra is currently under investigation.

Straylight Properties

Especially in the ultraviolet wavelength region a good suppression of any straylight in the spectrometer is necessary because the solar radiance varies over about two orders of magnitude in this wavelength region and the earthshine radiance over approximately four orders. To investigate the straylight properties of the instrument filter measurements are used. Gases in a cell at appropriate partial pressures are good filters in some special wavelength regions. A small amount of ozone in the cell can be used to absorb any light in the ultraviolet wavelength region by the strong absorption of the Hartley band and let pass the light in the other wavelength regions. Such measurements are performed to quantify the straylight

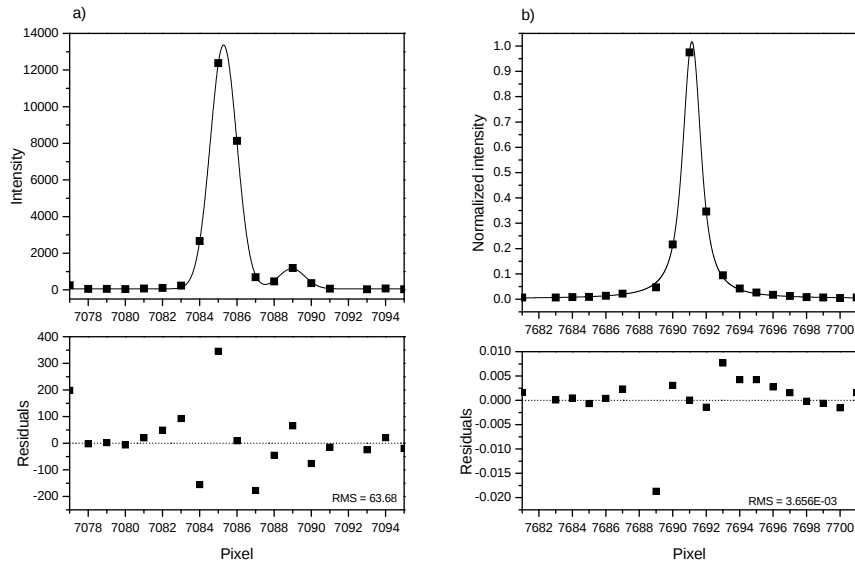


Fig. 8: a) Spectral lines of the CrPtNe-lamp in channel 7 fitted by a Gaussian function and according residuals of the fit. b) Spectral line of the CrPtNe-lamp in channel 8 fitted by Voigt profile and according residuals of the fit.

before and after the modification of the SCIAMACHY channel 1 (230–314 nm): after the modification the straylight was reduced by the factor of 30 (fig. 9).

RESULTS

A new data set of absorption cross sections for atmospheric remote sensing is presented. The absorption cross sections are measured at medium spectral resolution over a broad spectral range and at temperatures between 203 K and 293 K. They show a high signal-to-noise ratio, a high baseline stability and a good wavelength calibration. For O_3 , NO_2 , and SO_2 a temperature parametrization is applied to the absorption cross sections. With this parametrization the absorption cross sections in certain wavelength regions can be calculated at intermediate temperatures with an error smaller than 2%. The absorption cross sections were successfully used to improve the wavelength calibration of the SCIAMACHY spectrometer

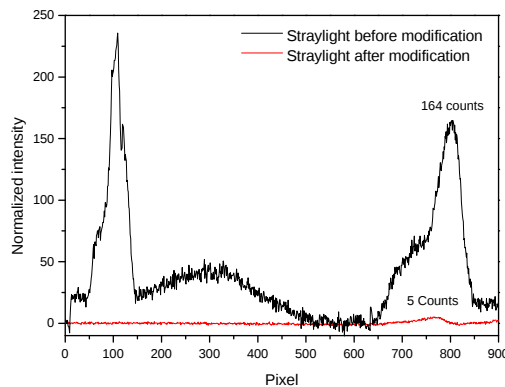


Fig. 9: Straylight before and after the modification of channel 1.

and to characterize the slit function and the straylight properties of the instrument.

ACKNOWLEDGEMENTS

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Anhang 3

W. Gurlit, Study of the REDGRASS phenomenon, Final Report, University of Bremen,
November 2000

Study of the REDGRASS phenomenon

Final Report,

November 2000

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This study is based on documents from the years 1998-1999 prepared by SRON which describe the redgrass phenomenon found on the detectors of the SCIAMACHY instrument. During the past months since the progress report from march 2000, more data provided by SRON have been screened and analysed to improve the statistical relevance of the results.

Summary

All additional data from SRON show redgrass mainly in channels 1 and 2. Some redgrass can be found in channel 4 and 5, while channel 3 seems to be almost perfectly clean in all data screened so far. Redgrass has also been observed in dark signals provided by SRON. The effect of redgrass on the DOAS retrieval depends strongly on the distribution (correlation) relative to the spectral features observed. Retrieval errors of greater than 10 % are possible for worst-case situations. A software algorithm to remove the RG from the data without any damage to spectral information is proposed and demonstrated. It is based on the RG finder program described in detail in the progress report of March 2000.

These points will be addressed in the report:

- | | |
|--|---------|
| 1) Survey of data records provided by SRON | page 2 |
| 2) Interpretation of the results of the RG screening | page 4 |
| 3) Automatic redgrass-repair | page 8 |
| 4) Effects of redgrass on the DOAS trace gas retrieval | page 12 |
| 5) Annex : Qbasic listing of "Redgrass-repair 1.1" | page 15 |

1. Survey of data records provided by SRON

Each of the 9 data records provided by SRON for additional RG analysis consists of 6 scans with 8192 pixels each. The first 3 scans (fileX1.dat.....fileX3.dat) are dark signals, the second 3 scans of each record (fileX4.dat.....fileX6.dat) are WLS-signals. Prior to RG analysis, the records were converted to ASCII files. RG screening was made with the algorithm described previously in the "Redgrass Progress Report"(march 2000). Table 1 below shows the results channel-wise (RG-pixels per channel). An interpretation of the results is also given below.

a) record : OP4_8FM_ait2_wls_c001

file	CH1	CH2	CH3	CH4	CH5	
file11.dat	948	48	0	216	28	dark
file12.dat	964	44	0	204	28	dark
file13.dat	946	36	0	206	28	dark
file14.dat	564	12	2	12	12	wls
file15.dat	594	4	0	18	12	wls
file16.dat	628	4	0	18	12	wls

b) record : TVT_8FM_ait2_wls_c001

file	CH1	CH2	CH3	CH4	CH5	
file21.dat	940	226	0	406	66	dark
file22.dat	944	244	0	400	68	dark
file23.dat	958	236	0	400	70	dark
file24.dat	588	146	2	22	26	wls
file25.dat	590	72	0	28	26	wls
file26.dat	580	72	0	34	24	wls

c) record : TVT_8FM_ait2_wls_c003

file	CH1	CH2	CH3	CH4	CH5	
file31.dat	942	412	0	524	120	dark
file32.dat	942	444	0	538	118	dark
file33.dat	940	420	0	510	110	dark
file34.dat	572	200	10	32	36	wls
file35.dat	552	114	0	42	24	wls
file36.dat	588	128	2	44	20	wls

d) record : TVT_8FM_ait2_wls_c005

file	CH1	CH2	CH3	CH4	CH5	
file41.dat	960	44	0	158	30	dark
file42.dat	956	52	0	178	30	dark
file43.dat	962	46	0	158	32	dark
file44.dat	598	10	0	16	12	wls
file45.dat	606	4	0	18	12	wls
file46.dat	598	2	0	16	12	wls

Table 1: RG screening of data records provided by SRON (cont'd on page 3) The results show the number of RG-pixels per channel, as detected by software algorithm "RGfinder".

e) record : TVT_8FM_ait2_wls_c007

file	CH1	CH2	CH3	CH4	CH5	
file51.dat	948	20	0	152	28	dark
file52.dat	956	32	0	150	28	dark
file53.dat	940	24	0	152	28	dark
file54.dat	606	0	0	18	12	wls
file55.dat	616	8	0	18	12	wls
file56.dat	604	4	0	16	12	wls

f) record : TVT_8FM_ait2_wls_c009

file	CH1	CH2	CH3	CH4	CH5	
file61.dat	954	28	0	198	28	dark
file62.dat	934	34	0	204	28	dark
file63.dat	964	26	0	202	28	dark
file64.dat	574	26	0	18	12	wls
file65.dat	588	4	0	18	12	wls
file66.dat	600	2	0	18	12	wls

g) record : TVT_8FM_ait2_wls_c011

file	CH1	CH2	CH3	CH4	CH5	
file71.dat	954	20	0	208	26	dark
file72.dat	960	18	0	206	28	dark
file73.dat	944	32	0	208	26	dark
file74.dat	570	92	0	18	18	wls
file75.dat	610	40	0	18	18	wls
file76.dat	570	30	0	18	16	wls

h) record : TVT_8FM_ait2_wls_c013

file	CH1	CH2	CH3	CH4	CH5	
file81.dat	946	32	0	220	26	dark
file82.dat	946	24	0	210	28	dark
file83.dat	948	24	0	204	28	dark
file84.dat	590	70	2	18	16	wls
file85.dat	568	36	0	22	14	wls
file86.dat	614	32	0	16	14	wls

i) record : TVT_8FM_ait2_wls_c015

file	CH1	CH2	CH3	CH4	CH5	
file91.dat	962	42	0	244	28	dark
file92.dat	952	30	0	240	28	dark
file93.dat	944	32	0	236	28	dark
file94.dat	624	38	0	16	18	wls
file95.dat	562	32	0	18	16	wls
file96.dat	632	30	0	18	16	wls

Table 1: RG screening of data records provided by SRON. The results show the number of RG-pixels as detected automatically by the RGfinder algorithm.

2) Interpretation of the results of the RG screening

2.1 RG in dark signals

The first three scans of each record are dark signals. The high number of pixels especially in channel 1 of all records is surprising (table 1). As so far RG was understood as an effect caused or triggered by incoming light, one might simply say that dark signals cannot show RG by definition. At this point, the working principle of the RG detection algorithm used here should be remembered. It is the direct implementation of all information available about RG from the documents provided by SRON.

RG was defined as a periodic (pixel-to-pixel) deviation from the correct signal level, with even pixels deviating down (lower value) and odd pixels deviating up (higher value). This effect has to be seen in five neighboring pixels to set the RG flag for the central pixel (check for periodicity). The amplitude of the deviation is typically 1×10^{-4} of the signal value (expected value from SRON-documents). The detection algorithm used here checks for a deviation (RG amplitude) of at least 4×10^{-5} compared to the maximum signal value of each channel, however the choice of this value is not critical. In a 16 bit AD-conversion system, this value is close to the LSB (least significant bit). Smaller digital signals are likely to be artefacts and noise. The algorithm can thus be understood as a phase-sensitive detection of periodic signals of given frequency. The RGFINDER algorithm is described in detail in the "Redgrass Progress Report"

The RG detected in the almost entire channel 1 dark currents of all data records (example shown in fig. 1, detail in fig. 2) might be interpreted as normal noise, equal in phase and frequency to (expected) RG, amplitude is $3 \dots 5 \times 10^{-3}$ of the signal value. Obviously, the channels 2 and 3 exhibit a larger and more constant dark signal, while in channel 4 similar but less significant than in channel 1, many pixels were found that were in agreement with the RG definition.

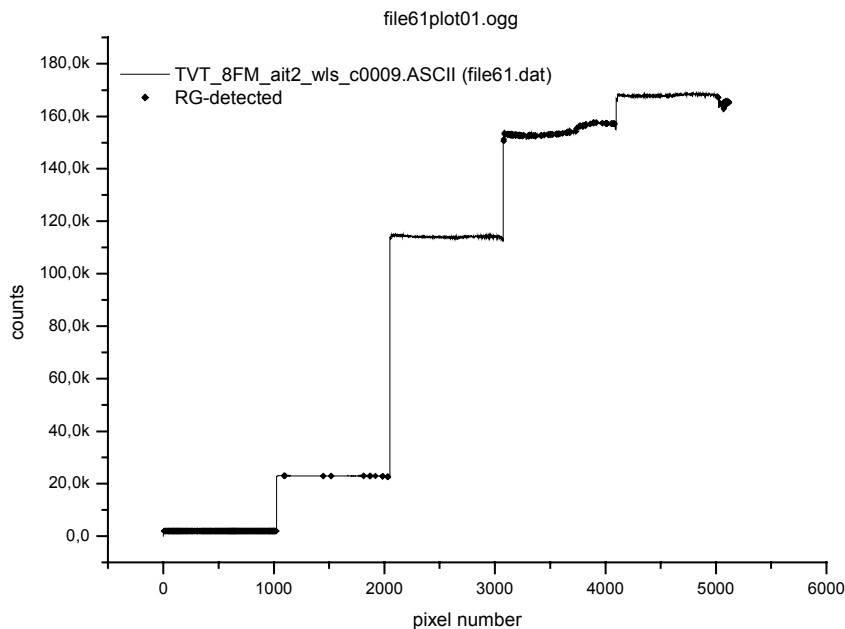


Fig. 1 : Redgrass found in the dark signals of channels 1 – 5 (marked in black)

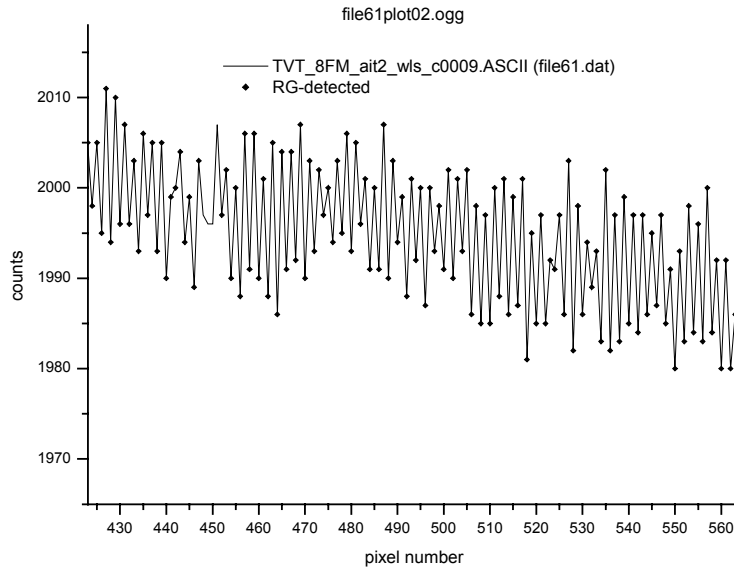


Fig. 2 : Redgrass in dark signal of channel 1, detail from fig. 2

2.2 RG in wls signals

A WLS-scan from channel 1 to 5 is shown in fig. 3, again with many RG pixels detected in channel 1. A detail from channel 1 is shown in fig. 4. Again, the noise signal in agreement with the RG-definition might be caused by dark current due to the low intensity of the incoming light. As can be seen from table 1 however, the number of RG pixels is already reduced compared to the pure dark signal.

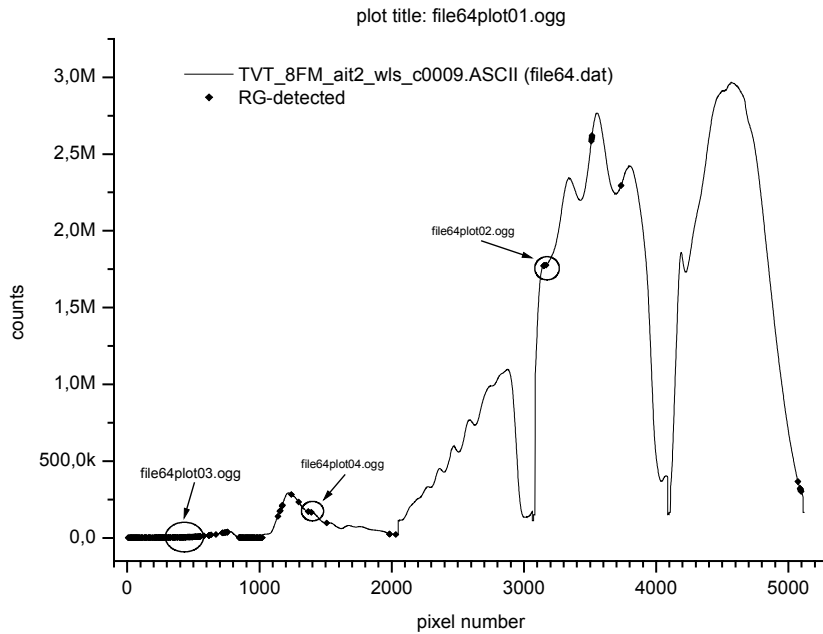


Fig. 3 : WLS – scan with RG detection mostly in channel 1

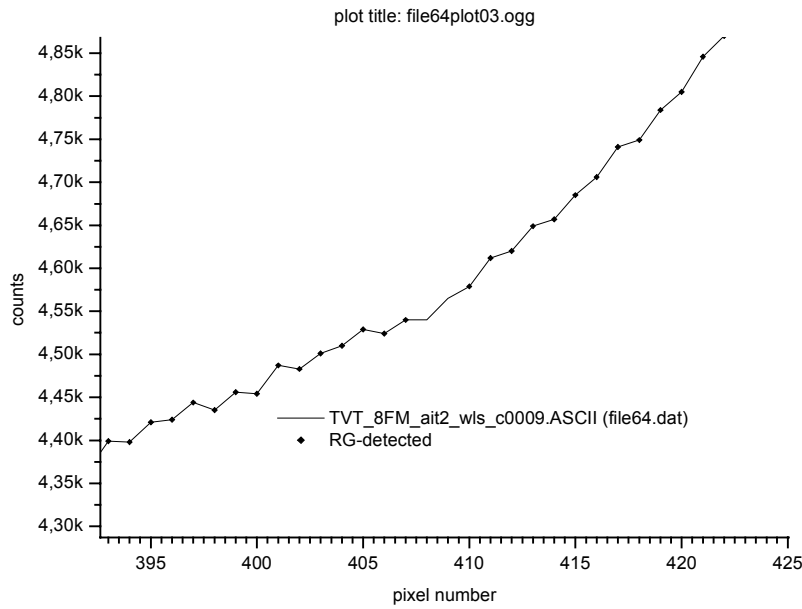


Fig. 4 : RG in channel 1, detail from fig. 3

Channel 3 is almost perfectly clean in all data records examined so far. Even a reduction of the detection threshold from 4×10^{-5} (used in all screening here) to 1×10^{-5} does not show RG for channel 3, while the number of pixels detected for the other channels is increased.

Some RG can be found in channel 4. It is interesting that for three different scan signals (fig. 5-7) exactly the same pixels show RG. However, this does not seem to be a general rule throughout greater portions of the data sets. Please note, that pixels between the two groups of RG-marks do not satisfy the phase-condition (even pixels low, odd pixels high).

Very few RG pixels can also be found in channel 5.

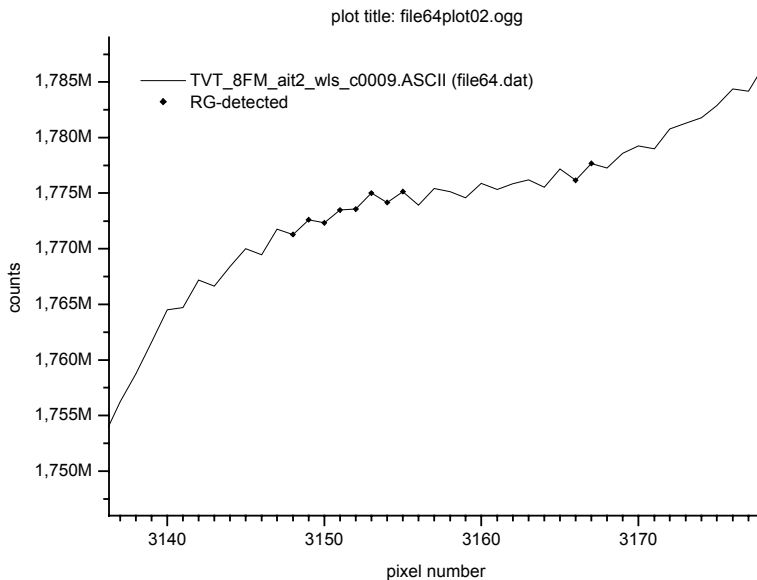


Fig. 5: RG pixels in channel 4, compare with fig. 6 and 7

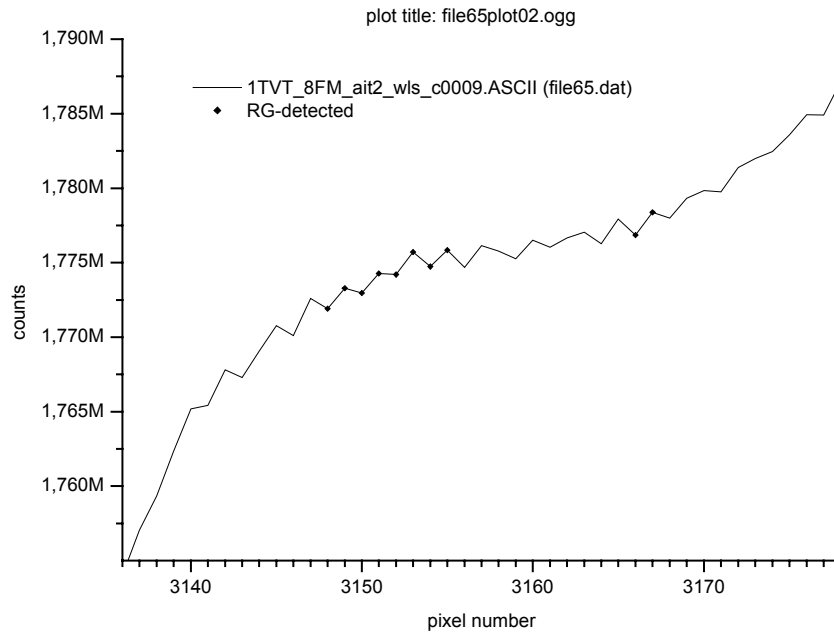


Fig. 6: different data, same RG-pixels (compare to fig. 5 and 7)

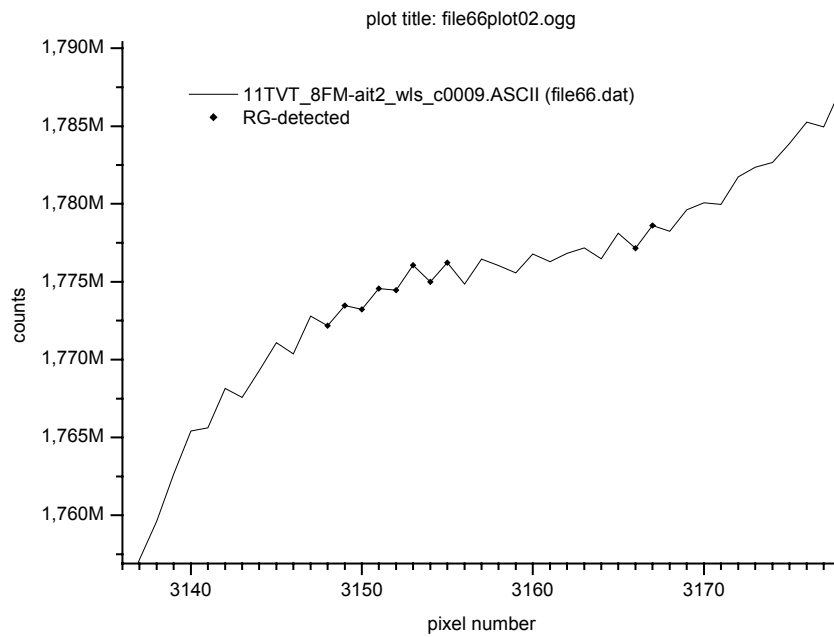


Fig. 7: different data, same RG pixels (compare to fig. 5 and 6)

3) Automatic redgrass-repair

Though it is sometimes hard to discriminate between RG and "normal noise", (especially in dark signals), it can be concluded that all of the 9 data records provided by SRON show RG. However, data containing RG should not be used for the calibration of the optical sensors of SCIAMACHY.

To solve this problem, a "repair algorithm" for data affected by RG has been written and implemented. It is based on the RGFINDER detection algorithm. Target features are :

- no loss of spectral information
- only RG pixels are modified
- no filtering or smoothing

This algorithm works adaptive only on the pixels where RG was detected, all other pixels are left untouched. The algorithm cures all RG found by the automatic detection, this means that also the phase-locked noise in the dark signals can be removed. Because any overall filtering or smoothing was avoided, there is no adverse effect on wavelength calibration or spectral resolution. The "RG-repair" works in 4 steps which are explained below :

- 1) The detector readout file for channels #1 to #5 is read into a data field (black line)
For each channel, the maximum value is detected and stored in a data field.
- 2) for each pixel (excluding pixels #1 and #5200), the 3-pixel average is calculated and stored in another data field.
- 3) For each pixel, a comparison is made between the original value and the averaged value.
As RG appears a periodic signal, there is a phase-shift between the original and the filtered pixel. This means that in the presence of RG,
 - a) even pixels have lower values than their 3-pixel average
 - b) odd pixels have higher values than their 3-pixel average.

This is probed by the algorithm for each pixel and its two neighbours to the left and to the right. If the criteria is "true", the central pixel (out of this 5-pixel group) is marked as "RG" by the algorithm. The detection principle thus can be seen as a phase-sensitive detection of a periodic signal of known frequency. Periodicity is checked by marking only the pixels, that have the criteria a) and b) true also for their neighbours. Out of a group of for example 100 pixels that probably have RG, the first two pixels and the last two pixels will not be detected. This careful approach ensures the complete protection of small and narrow spectral features that might be falsely detected as RG with a less strict definition of periodicity.

The maximum readout value from step 1 is used to adjust the sensitivity of the detection. The adjustment is not very critical, but in general it is assumed that RG produces a greater variation of the signal amplitude than the other noise sources.

4) The approach to correct the negative effect of RG on the data is very straightforward: For even pixels detected as RG, the signal value is increased, for odd pixels it is decreased by the algorithm. The amount of this small modification is derived from the channel's maximum signal value: it is $(\max/10^5)$. As this is a one-pixel operation, there is no loss of spectral information or calibration, unlike smoothing or filtering.

After this modification of the RG-pixels, the detection starts again. A lowered number of RG-pixels then will be found. The correction then works again on these remaining pixels. This iterative process is repeated until no more RG is found by the detection algorithm. Typically 3 to 5 iterations are needed to remove all RG from the data.

The operation of these 4 steps is illustrated in (fig. 8). The original data (fine trace) are from the internal line-source, channel 4, recorded in the delta2-PI period. Redgrass can be clearly seen as a pixel-to-pixel oscillation.

The bold trace shows the result of the correction algorithm. The redgrass has been removed from the data record, while there is no loss of spectral resolution or calibration. The narrow lines of the internal line source are identical in the original data and in the repair result. RG has even been removed on the slope of one of the lines.

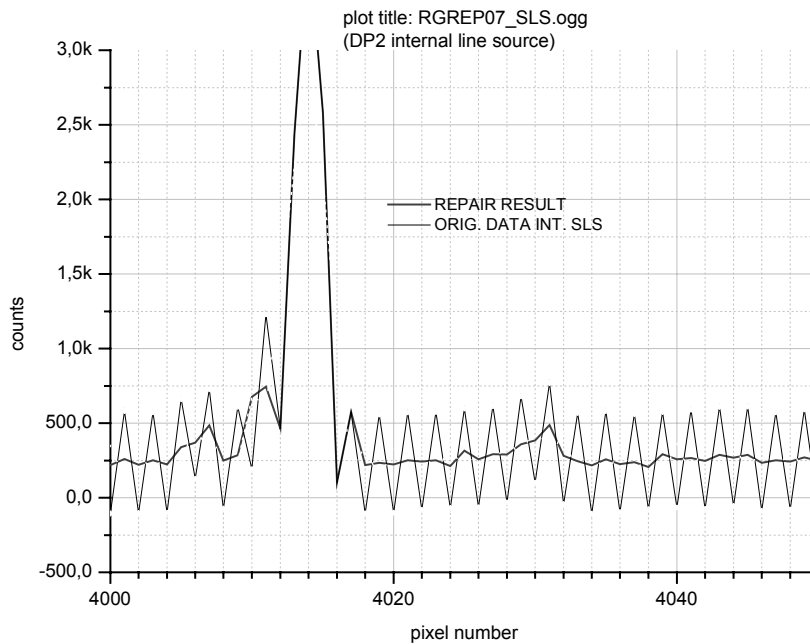


Fig. 8: RG repair (bold trace) and original data (fine trace), SLS signal

Another example from the internal line source is shown in (fig. 9). Also in this greater portion of channel 4 it can be seen that RG is removed while the spectral features remain unchanged.

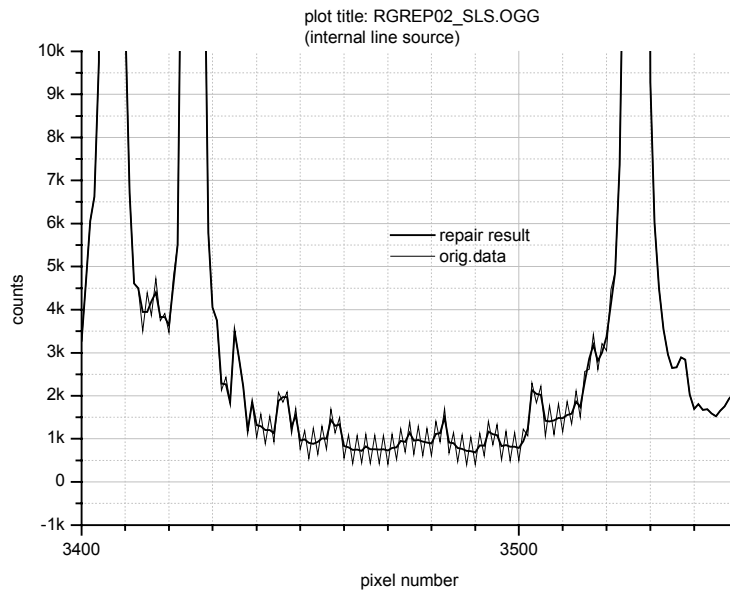


Fig. 9: RG repair with SLS-data, lineshape and position remain unchanged

A program run with WLS-data from the D2-PI period is shown in (fig. 10). Again, the original data are plotted as a fine trace, while the repair result has a bold trace. This result illustrates the ability of the RG-repair to work on structured backgrounds

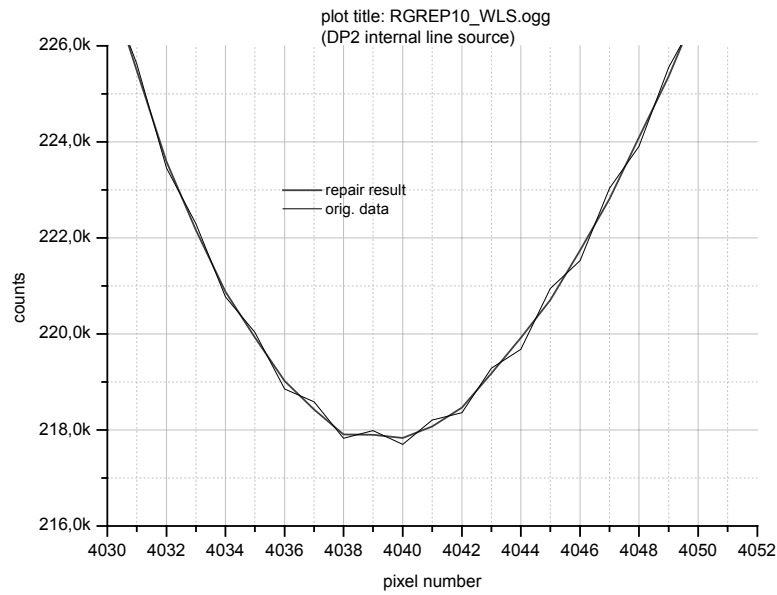


Fig. 10: RG repair (bold trace) on structured background using wls-data

Finally, an example is shown using dark data as input. A phase-locked noise generation according to the RG-definition is clearly active. While one may discuss the relevance of RG in dark files, the result is that the noise can be removed from the signals without adverse effects (fig.11).

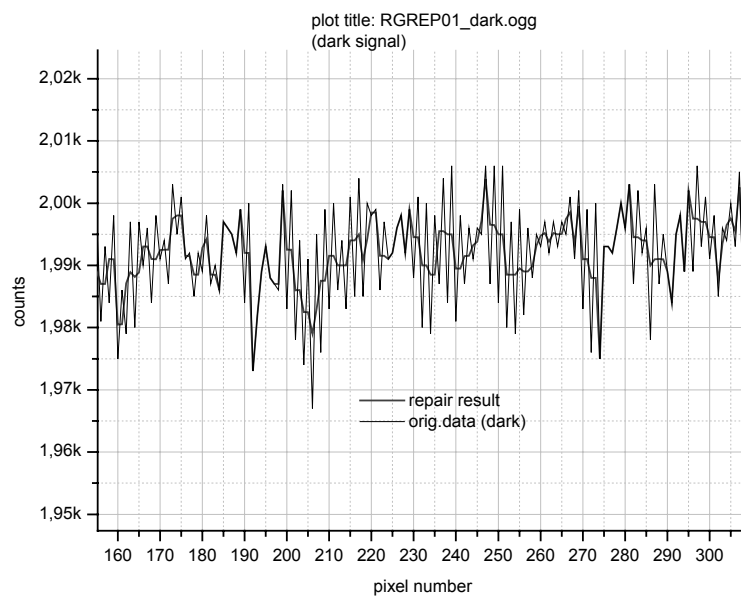


Fig. 11: RG-repair (bold trace) working on dark signal from channel 1

4) Effects of redgrass on the DOAS trace gas retrieval

The model experiments described briefly here have been made in cooperation with R. deBeek, they are also described in "Sciamachy's ATBD review, progress report 2" (june 2000).

A constant signal ratio spectrum was corrupted with 30 different RG patterns. These patterns were provided by a RG-generation program. RG amplitude was always constant (10^{-4} of the signal amplitude), while the distribution of the parts corrupted with RG in the fit-window was changed.

As one can expect intuitively, the maximum error depends not so much on the number of RG pixels but on the distribution. If for example RG is present throughout the entire fit-window, there is almost no effect on the DOAS retrieval. The worst case results appear, when the RG-parts are strongly correlated with the spectral features under interest. These worst case results for five atmospheric trace gases are given in table 2. From a statistical point of view, the errors listed below are not very likely to happen for extended periods of time. However, a RG alarm or repair algorithm should be implemented to remove or at least reduce this additional uncertainty.

Trace Gas	Fit Window	Max. Error (%)	see Figure
SO ₂	314-327 nm	12	12
HCHO	336-354 nm	-7	13
BRO	340-360 nm	6	14
OCLO	350-380 nm	3	15
NO ₂	425-450 nm	1	16

Table 2: Maximum errors as percentage ratio wrt. typical midlatitude abundancies achieved by retrieving RG corrupted signal ratios. Figures below show the according spectral fits and residuals.

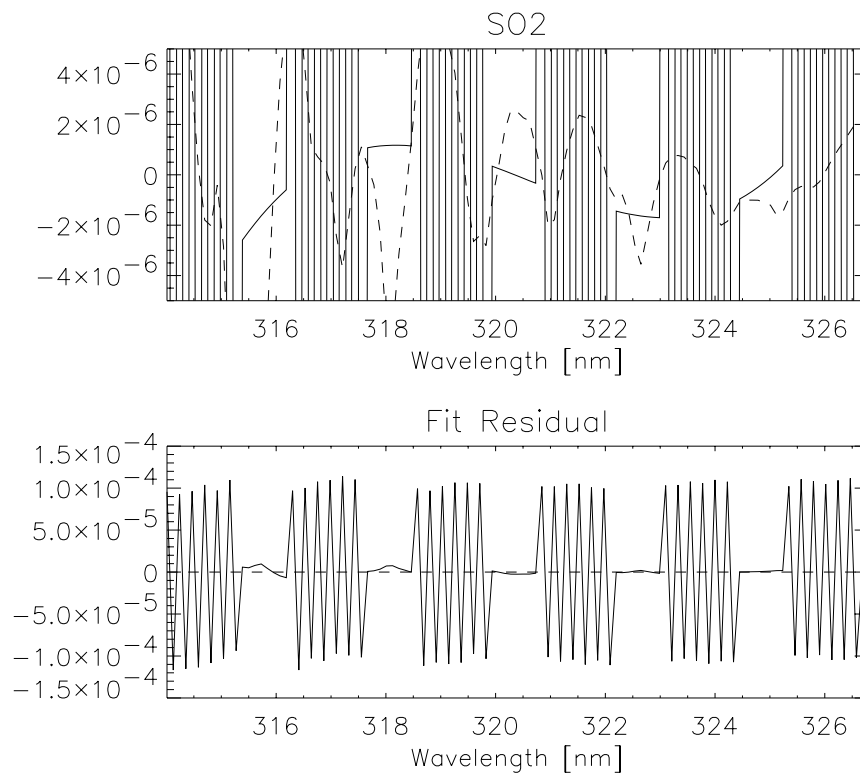


Fig. 12: SO₂ absorption cross sections fitted to RG corrupted signal ratios (top) and the according residual spectrum (bottom)

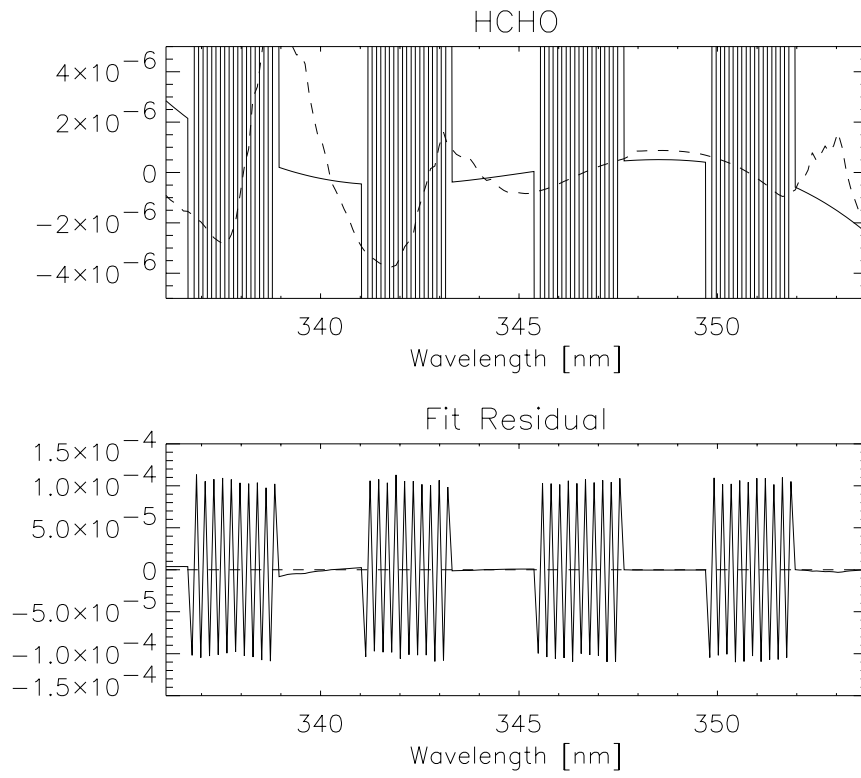


Fig. 13: HCHO absorption cross sections fitted to RG corrupted signal ratios (top) and the according residual spectrum (bottom)

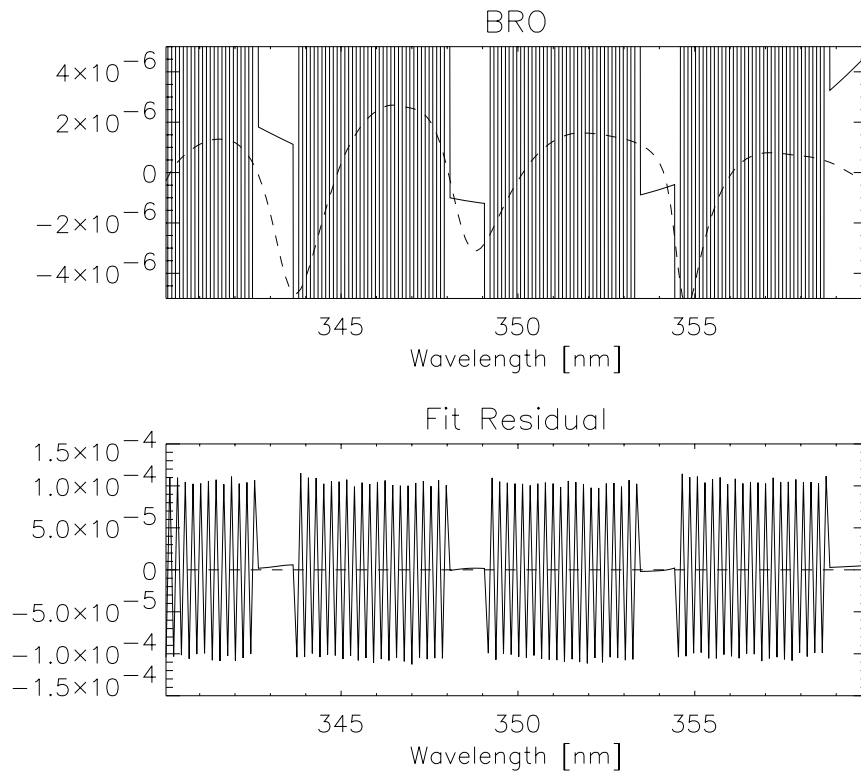


Fig. 14: BrO absorption cross sections fitted to RG corrupted signal ratios (top) and the according residual spectrum (bottom)

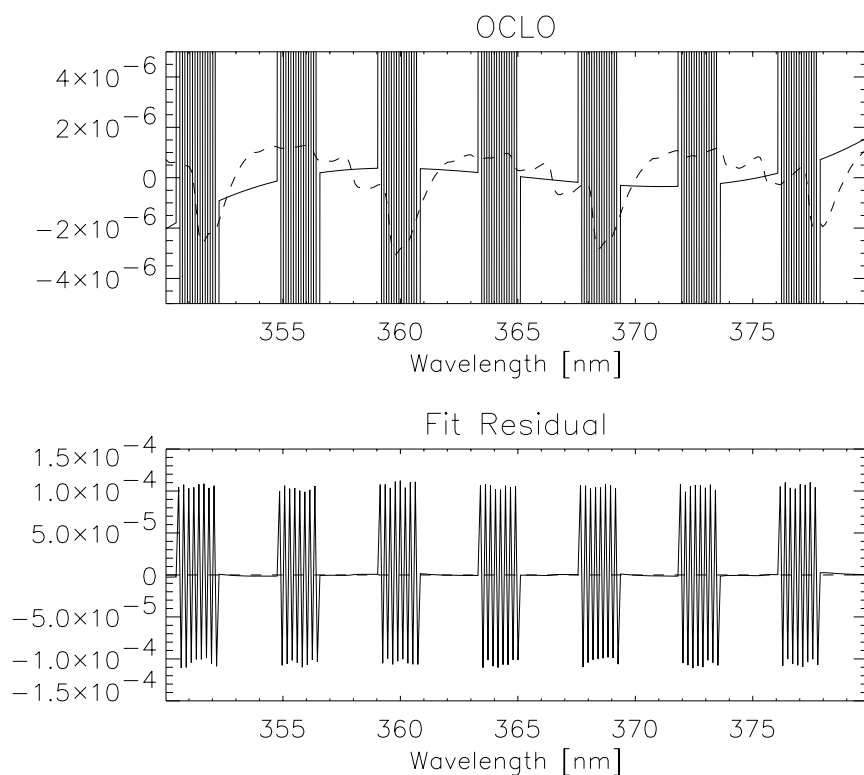


Fig. 15: OCLO absorption cross sections fitted to RG corrupted signal ratios (top) and the according residual spectrum (bottom)

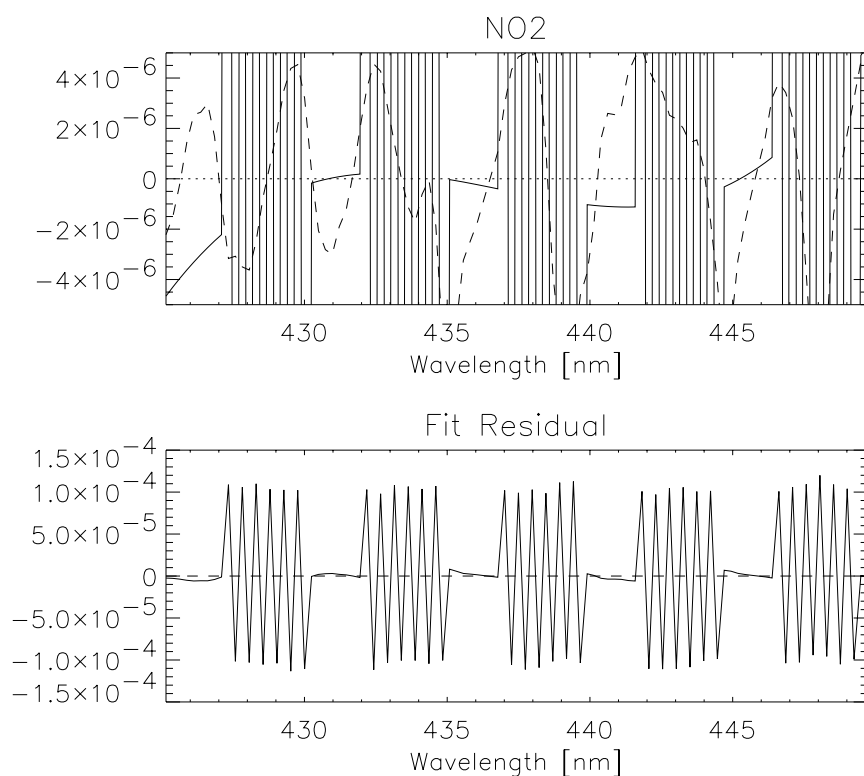


Fig. 16: NO₂ absorption cross sections fitted to RG corrupted signal ratios (top) and the according residual spectrum (bottom)