Minutes of the Kickoff-Meeting of the ESA Study

DEVELOPMENT OF ALGORITHMS FOR RETRIEVAL OF GOME TOTAL OZONE COLUMN "GOTOCORD"

Meeting Place: ESA/ESRIN, Frascati, Italy

Date: 10th October 2002, 9:30h-12h

Participants: Stefano Casadio, Yves-Louis Desnos, Luc Govaert, Claus Zehner (all ESA/ESRIN), Mark Weber (IUP University of Bemen).

Introduction

The kickoff-meeting served the purpose to present the GOTOCORD project, to negotiate and resolve contractual issues, and provide detailed planning of the first phase of this project. The presentation of the GOTOCORD Project was given by Mark Weber, principal investigator of GOTOCORD. Contractual items negotiated during that meeting and summarized in the minutes shall from part of the contract to be signed between the University of Bremen and ESA. The duration of the project is one year starting from the date of this kick-off meeting.

Background

Mark Weber began his presentation by discussing the background and motivation for this ESA study. In the scientific community, particularly among scientists participating in the SPARC (Stratospheric Processes and their Role in Climate) and WMO (World Meteorological Organization) assessment of longterm ozone trend, a controversy on the continuation of the ozone trend in response to the Montreal Protocol and its amendments exists. At the turn of the millennium the stratospheric chlorine loading has reached maximum and its expected to decrease in the near future as a response of the CFC ban as part of the Montreal protocol. It is therefore expected that we move away from a linear trend. Another important issue is the coupling of cllimate change and ozone trend. Associated with global warming (mainly in troposphere) is the expectation of a stratospheric cooling trend which may decelerate the ozone recovery this century. Ozone trend assessments also suffer from inconsistencies between various total ozone data sets provided from the ground and the satellite instruments TOMS and GOME. For instance, TOMS data show a strong hemispheric bias while GOME Version 2.7 shows a quite strong seasonal cycle in the differences to groundbased measurements. The data gap in the TOMS record between 1994 and 1996 could only partially filled by GOME launched in 1995. Results from the Validation Tiger Team (Lambert et al.) showed that Version 3.0 data still exhibit

seasonal variations in the differences to collocated groundbased measurements, although the differences have become smaller. A prerequisite of a longterm trend assessment is the high quality of satellite data (with an overall consistency to within 1%) over the entire lifetime of the instrument. For these reasons a call for an improved total ozone retrieval algorithm for GOME has been initiated by ESA and IUP University of Bremen proposed an advanced total ozone retrieval algorithm, which goes beyond the standard DOAS approach (slant column retrieval and airmass factor calculation). This algorithm shall be developed into a protoype algorithm during this study and it is believed to provide significant improvements in the GOME total ozone retrieval.

Proposal GOTOCORD

In this study IUP is proposing the weighting function DOAS (WF DOAS) approach as a novel retrieval algorithm. The theory behind it is the linearisation (development into a Taylor series) of the DOAS equation about a reference intensity. The vertical column is obtained in a direct fit. All RTM quantities are to be provided in look-up tables (LUT). One emphasis in this study is to find a more appropriate treatment of the Ring effect. At the end of the project a quasi-operational processor shall be delivered including LUT tables and a database of pre-processed data such as cloud information and Lambertian reflectivities. The algorithm will be tested by validation using the so-called reference orbits (about 2200 GOME orbits from the 1995-2001 period) and using the Brewer/Dobson network data contained in the WOUDC database as described in Bramstedt et al. (2002).

Current Status

The WF DOAS algorithm has been implemented in a first version that includes specific adaptations to the UV spectral region (Buchwitz et al. 2000). It is based upon a Fortran90 code and uses as input GDP extracted level-1 data. Current computer facilities (provided at no extra cost) consist of an alpha DEC cluster, Sun Ultra cluster, and a Cray J90 super computer, all available for various computations. The WF DOAS algorithm runs currently on the SUN cluster. During this study additional refinements and optimizations have to be carried out. Particularly important issues to be addressed are the selection of fitting parameters and spectral range, the best choices of cross-sections, and improved treatment of the Ring effect. In addition optimum selection of the design and size of the LUT tables with a fast interface to the retrieval algorithm shall be developed.

Work Package Breakdown

Apart form technical and administrative management (WP 100 and 200), three major scientific work packages are defined:

WP 300 Phase 1: Sensitivity Study and Optimization (WP Manager R. De Beek)

WP 400 Phase 2: Algorithm Implementation (WP Manager M. Coldewey)

WP 500 Phase 3: Validation (WP Manager M. Weber)

Deliverables as requested in the ITT are the ATBD, Software Requirement Document, Software User Document, Validation Report, and a data CD containing the WF DOAS software and LUT tables.

Contractual Issues/ Request

Since the algorithm approach differs from that assumed in the ITT, IUP suggests to extend the first phase to four months and, therefore, reduce the second phase to six months (ITT: two months and eight months, respectively). It was agreed that the first progress meeting will still take place after two months and that the contractor tries at least to complete the most critical issues of the sensitivity study to a point that a decision on the adopted procedure in the WF-DOAS retrieval can be made at the first progress meeting.

IUP requested from ESA all reference orbits (level1 and level2) used in the Tiger Team Validation collected on a storage media, preferably CDs. Claus Zehner agreed to send only the GDP Version 3 Level-2 data. Other requests to ESA include access to a global topography and ISCCP cloud climatology database. This may be provided as part of the GDP database. Claus Zehner suggested to use the new ground altitude database from the ERS radar altimeter and he is checking on the availability of this dataset. He indicated that the database may have to be purchased from ESA. It was agreed that ESA provides the requested data sets by mid-November.

Luc Govaert asked for an update of the financial plan due to the agreement to hold the midterm progress meeting (after six months) in Bremen and due to the fact that only one person attended the kickoff meeting. Progress meeting 1 (after two months) and the final meeting (after a year) will be held at ESRIN in Frascati. It was agreed to hold the first progress meeting in conjunction with the ENVISAT Geophysical Validation Meeting. The update in the financial plan is given in Appendix A.

Study Team

The members of the core team are John Burrows (GOME expert/advisor), Rüdiger De Beek (researcher and WP 300 manager), Melanie Coldewey-Egbers (researcher and WP 400 manager) and Mark Weber (PI and WP 500 manager). The core team is supported by an advisory team consisting of Michael Buchwitz (expert on WF-DOAS), Vladimir Rozanov (radiative transfer expert), and Marco Vountas (Ring expert). All members from the core and advisory team are from IUP.

Company Profile

The IUP is one of the largest institutes within the Department of Physics and Electrical Engineering at University of Bremen. Currently 105 people are employed at IUP (48% PhD candidates and students, 38% scientists, 14% technical staff). Research at IUP is regularly funded by EU, German Secretary of Education and Research (BMBF), and the State of Bremen. Main research area of IUP are atmospheric remote sensing, land/sea ice imaging, and tracer oceanography. IUP participated in a leading role in several satellite projects, e.g. SCIAMACHY, GOME, and shuttle MAS. About two years ago IUP started an Postgraduate Environmental Physics (PEP) program, which enables international students to obtain a Master degree (2 year program) or a certificate in Environmental Physics (1 year program). All classes in PEP are taught in English.

Phase 1 Plan

Mark Weber presented viewgraphs prepared by Melanie Coldewey-Egbers on some preliminary activities and plans to Phase 1 of this study. The major emphasis here is on sensitivity studies for optimizing the WF-DOAS retrieval. After summarizing the basic equations for WF-DOAS the iterative scheme was discussed. The RTM quantities, reference intensity and weighting functions are selected using solar zenith angle, line of sight, topographic height, Lambertian reflectivity, and total ozone information. Some of the parameters are provided from GDP. Total ozone information is needed to obtain the proper profile shape. For this purpose the TOMS V7 profile climatology which is parameterized according to total ozone is used. If the a-priori total ozone grid point is not the closest one to the retrieved total ozone the DOAS fit is repeated by using an updated a-priori value. After retrieval a cloud correction to the retrieved column is carried out. Several other issues were discussed in the following.

Selection of relevant Input Parameters

In the retrieval weighting functions for ozone, NO2, and BrO columns can be included. For saving space in the LUT, a slant column (SC) fitting for the minor trace gases may suffice. Additional fit parameters are effective SC for undersampling and Ring effect. Some preliminary checks showed that temperature weighting functions should be included. Albedo weighting functions, however, show strong correlations with ozone WF and should, therefore, not be included in the fit. Nevertheless, reference intensities in the LUT have to be tabulated for various albedo values. The use of neutral density WF (surface pressure WF) have still to be investigated.

Ghost Vertical Column

Using cloud fraction and cloud-top-height from ICFA/ISCCP and/or FRESCO, an estimate for the hidden tropospheric column can be made. It is proposed to use Labow's zonal profile climatology for tropospheric ozone estimates.

Profile Shape dependency

Melanie Coldewey showed that the use of the incorrect profile shape can lead to errors of up to 4% using simulated data. The profile shape dependency will be taken into account by use of the TOMS V7 profile climatology.

Scan Simulation

It can be shown that co-adding of three line-of-sights intensities and WF may be necessary to accurately simulate the large ground pixel of GOME (320X40 km2).

First Setup of LUT

A first proposal for the extent and size of the LUT has been presented with 26 total ozone values (in steps of 50 DU and three zonal bands), 30 solar zenith angles

(spacing of 5° below 70°SZA and 1° above 70°SZA), seven line-of-sights (11° spacing between –34.5 and 34.5°), six albedo values (between 0.05 and 0.98), and four ground altitudes (between 0 and 6 km). For each combination of theses parameters WF and reference intensities have to be tabulated (albedo: only reference intensities). In Phase1 the extent and spacing of the table has to be optimized in terms of accuracy and computation speed.

Ring Effect Studies

Both Fraunhofer and molecular filling-in contribute to the spectral signature due to the Ring effect. It can be shown that the use of the incorrect ozone profile shape in the Ring simulation can lead to errors on the order of 3% under ozone hole condition (large SZA). In Phase 1 the extent of the Ring spectral database has to be investigated. Since the computational cost is much higher for the Ring simulation, a Ring spectrum for each of the entries in the LUT is not feasible. The effect of clouds, SZA, profile shape, albedo and clouds will be investigated in order to find the optimum set of representative Ring spectra to be used in the fitting. Ring simulation for a representative set of geo-temporal scenarios using realistic trace gas profiles from a chemistry-transport model have been initiated and will be used in this study.

Preliminary Validation

Comparison between GOME WF-DOAS results and data from Neumayer, Antarctica (70°S, 8°W) show a reduced bias in the total column compared with V2.7 data under ozone hole condition. A comparison to collocated Dobson data at Hradec Kralove (Czech Republic, 50°N, 15°E) from 1996 to 2001 show excellent agreement and almost no seasonal cycle as in the differences to V2.7 data is observable, indicating the potential of the WF DOAS algorthm.

Activities during Phase 1

The following investigations are planned during Phase 1:

- Selection of optimum spectral range and number of spectral points for WF DOAS fitting
- Selection of RTM (SCIATRAN or spherical CDI)
- Definition of optimum parameter space for LUT (reference spectra and WF)
- Selection of optimum number of parameters included in the fitting procedure
- Definition of an optimum Ring data base
- Investigate necessity of shift-and-squeeze and fixed-shift approach
- Decision of default ghost vertical column calculation (ICFA or FRESCO) and climatology data base (Labow or TOMS V7)
- Selection of appropriate viewing geometry (ground or top-of-atmosphere)
- Selection of cross-section (GOME FM98 or Bass-Paur)

Bremen, 23rd October 2002

Signature

(Mark Weber)

Appendix A: Update of Financial Plan

Additional labor of 90 man hours goes into WP 300 for Ring effect studies. In turn the travel budget has been reduced to 5,589€ to reflect the fact that the midterm meeting will take place in Bremen and only one person from Bremen attended the kickoff meeting . All prices given in Table 1 are in €. No changes are required in the Payment Plan.

Table 1: Updated Financial Plan for GOTOCORD

Labor & Administration		
13.6 Man Months (2170 hrs X 35,40 €)	**76,818.00**	A
Consumable Items		
telephone, fax, computer accessories, stationaries	**1,000.00**	B
Travel		
Kickoff	1,043.60	
Phase 1 Meeting	2,115.00	
Midterm Meeting	0.00	
Final Workshop	2,430.00	
	5,588.60	C
Total (A+B+C)	**83,406.60**	D
Overhead (20% of Total)	**16,681.32**	E
Grand Total (D+E)	**100,087.92**	