Ulrich Foelsche
Gottfried Kirchengast
Andrea Steiner

*Atmosphere and Climate*
Studies by Occultation Methods
Ulrich Foelsche
Gottfried Kirchengast
Andrea Steiner
Editors

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Studies by Occultation Methods

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Preface

Since the early use of the occultation measurement principle for sounding planetary atmospheres and ionospheres, its exploitation in atmospheric remote sensing has seen tremendous advances. In this book we focus on sensors on Low Earth Orbit (LEO) satellites, which exploit solar, lunar, stellar, GNSS (Global Navigation Satellite Systems), and LEO-crosslink signals for observing the Earth's atmosphere and climate.

The methods all share the key properties of self-calibration, high accuracy and vertical resolution, global coverage, and (if using radio signals) all-weather capability. The atmospheric parameters obtained extend from the fundamental variables temperature, density, pressure and water vapor via trace gases, aerosols and cloud liquid water to ionospheric electron density. Occultation data are therefore of high value in a wide range of fields including climate monitoring and research, atmospheric physics and chemistry, operational meteorology, and ionospheric physics.

The 2nd International Workshop on Occultations for Probing Atmosphere and Climate – OPAC-2 – was held September 13–17, 2004, in Graz, Austria. OPAC-2 aimed at providing a casual forum and stimulating atmosphere fertilizing scientific discourse, co-operation initiatives, and mutual learning and support amongst members of all different occultation communities. The workshop was attended by 40 participants from 12 different countries who actively contributed to a scientific programme of high quality and to an excellent workshop atmosphere, which was judged by the participants to have fully met the aims expressed.

The programme included 7 tutorial lectures and 15 invited presentations, complemented by about 30 contributed ones, including 11 posters, and an occultation software demonstration. It covered occultation science from occultation methodology in general via different occultation methods and new concepts to use and applications of occultation data in atmosphere and climate science. The detailed programme and all further workshop information will continue to be available online at the OPAC-2 website at http://www.uni-graz.at/opac2.

This book was compiled based on selected papers presented at OPAC-2 and well represents in its six chapters the broad scope of the workshop. Results from the radio occultation experiment onboard CHAMP, which is now over five years in orbit, are collected in chapter 1 while chapter 2 comprises results from the stellar occultation experiment GOMOS onboard ENVISAT. Wave optics algorithms turned out to be very useful for the processing of radio occultation data in the lower troposphere; they are covered in chapter 3. Chapter 4 deals with future occultation missions and with the novel LEO-LEO crosslink concept. Radio occultation data are now increasingly used in numerical weather prediction and atmos-
pheric studies as well as in climate monitoring and change research. This is reflected by the significant amount of articles in chapter 5 and chapter 6, respectively.

We cordially thank all OPAC-2 colleagues, who contributed as authors and co-authors to the book, for the effort and diligent work invested into their papers and for largely observing the length target. All papers were subjected to a peer review process, involving two independent expert reviewers per paper from the community of OPAC-2 participants and beyond. We also very much thank these reviewers for their important service to coherently ensure scientific correctness and high quality of the book from first to last page.


Special thanks are, furthermore, due to M. Sc. Barbara Pirscher for her tireless support in the final copy editing and formatting of the book and to Dr. Wolfgang Engel, Mrs. Helen Rachner, and Mrs. Agata Oelschläger from Springer Verlag, Heidelberg, for the kind offer to issue this book as Springer publication and the related technical support. Many thanks also to all others who provided support in one or another way, in representation of which we thank the sponsors of OPAC-2 (see the OPAC-2 website noted above for details) and the sponsors of the START Program No. Y103-N03 (Federal Ministry for Education, Science, and Culture; Austrian Science Fund) for providing the material support enabling the realization of the book.

We hope that, in the spirit of the OPAC-2 aims, the book will become a useful reference for the members of the occultation-related community but also for members of the science community at large interested in the present status and future promises of the field of occultations for probing atmosphere and climate.

Graz, January 2006

Ulrich Foelsche
Gottfried Kirchengast
Andrea K. Steiner
# Table of Contents

1. **Radio Occultation with CHAMP: Mission Status, Retrieval, Validation, and Error Analysis** ............................................................... 1

GPS Radio Occultation with CHAMP and GRACE: Recent Results  
*and C. Reigber* .................................................................................................................. 3

Sensitivity of Stratospheric Retrievals from Radio Occultations on Upper Boundary Conditions  
*M. de la Torre Juárez,* and *S. S. Leroy* ........................................................................ 17

Error Characteristics of Refractivity Profiles Retrieved from CHAMP Radio Occultation Data  
*A. K. Steiner, A. Löscher,* and *G. Kirchengast* .................................................................. 27

Refractivity Biases in GNSS Occultation Data  
*and J. Wickert* .................................................................................................................. 37

2. **Stellar Occultation with GOMOS: Retrieval, Validation and Error Analysis** ........................................................................................................... 45

GOMOS Ozone Profiles at High Latitudes: Comparison with Marambio and Sodankylä Sonde Measurements  
*J. Tamminen, J. A. Karhu, E. Kyrölä,* *S. Hassinen,* *E. Kyrö,* *A. Y. Karpechko,*  
*and E. Piacentini* ............................................................................................................ 47

Ozone and Temperature Retrieval Results from GOMOS Validated with CHAMP and ECMWF  
*C. Retscher, G. Kirchengast,* and *A. Gobiet* ...................................................................... 55

Modeling Errors of GOMOS Measurements: A Sensitivity Study  
*V. F. Sofieva, J. Tamminen, E. Kyrölä,* and *GOMOS CAL/VAL Team* .............. 67
### 3. Wave Optics Algorithms for the Processing of Radio Occultation Data

Asymptotic Wave Optics Methods in Inversion and Direct Modeling of Radio Occultations: Recent Achievements  
*M. E. Gorbunov and K. B. Lauritsen* ................................................................. 81

Processing Radio Occultation Data by Full Spectrum Inversion Techniques: An Overview and Recent Developments  
*A. S. Jensen, H.-H. Benzon, M. S. Lohmann, and A. S. Nielsen* ....................... 95

Evaluation of the Processing of Radio Occultation Signals by Reconstruction of the Real Signals  
*A. S. Jensen, C. Marquardt, H.-H. Benzon, M. S. Lohmann, and A. S. Nielsen* ................................................................. 113

Radio Holographic Filtering of Noisy Radio Occultations  
*M. E. Gorbunov and K. B. Lauritsen* .................................................................. 127

### 4. Future GNSS Occultation Missions and the LEO-LEO Occultation Concept

Preparing for COSMIC: Inversion and Analysis of Ionospheric Data Products  
*S. Syndergaard, W. S. Schreiner, C. Rocken, D. C. Hunt, and K. F. Dymond* ........................................................................................................... 137

The Operational EPS GRAS Measurement System  
*J.-P. Luntama* .................................................................................................. 147

ROSA: The Italian Space Agency GPS Radio Occultation Receiver. Signal Tracking Characteristics and Terrestrial Measurement Campaign  
*R. Notarpietro, A. Zin, G. Perona, L. Corgnati, and M. Gabella* ....................... 157

Tropospheric Water Vapor from LEO-LEO Occultation: Estimation by Differential Attenuation Measurements near 20 GHz  
*F. Argenti, F. Cuccoli, L. Facheris, and E. Martini* ............................................ 169

Processing X/K Band Radio Occultation Data in Presence of Turbulence: An Overview  
*M. E. Gorbunov and G. Kirchengast* ................................................................. 183
# 5. Use of GNSS Occultation Data in Numerical Weather Prediction and in Atmospheric Studies

Assimilation of GNSS Radio Occultation Data into Numerical Weather Prediction  
*P. Poli*  ............................................................................................................. 195

Observation Operators for the Assimilation of Occultation Data into Atmospheric Models: A Review  
*S. Syndergaard, Y.-H. Kuo, and M. S. Lohmann* ........................................... 205

Analysis of Atmospheric and Ionospheric Wave Structures Using the CHAMP and GPS/MET Radio Occultation Database  
*A. G. Pavelyev, J. Wickert, Y. A. Liou, A. A. Pavelyev, and C. Jacobi* ........... 225

Are we Observing Mountain Waves Above the Andes Range from GPS Occultation Profiles?  
*A. de la Torre, P. Alexander, and C. G. Menéndez* ....................................... 243

Analysis of Seasonal and Daily Mid-Latitude Tropopause Pressure Using GPS Radio Occultation Data and NCEP–NCAR Reanalyses  
*B. Bizzarri, I. Bordi, A. Dell’Aquila, M. Petitta, T. Schmidt, A. Sutera, and J. Wickert* .......................................................... 253

CHAMP Radio Occultation Detection of the Planetary Boundary Layer Top  
*A. von Engeln, J. Teixeira, J. Wickert, and S. A. Buehler* ............................ 265

# 6. Use of GNSS Occultation Data for Climate Monitoring and Climate Change Studies

Monitoring Climate Variability and Change by Means of GNSS Data  
*M. Stendel* ........................................................................................................ 275

Climate Benchmarking Using GNSS Occultation  
*S. S. Leroy, J. A. Dykema, and J. G. Anderson* ............................................ 287

Global Climatologies Based on Radio Occultation Data: The CHAMPCLIM Project  
*U. Foelsche, A. Gobiet, A. K. Steiner, M. Borsche, J. Wickert T. Schmidt, and G. Kirchengast* ................................................. 303
Pre-Operational Retrieval of Radio Occultation Based Climatologies
  M. Borsche, A. Gobiet, A. K. Steiner, U. Foelsche, G. Kirchengast,
  T. Schmidt, and J. Wickert.................................................................315

Assimilation of GNSS Radio Occultation Profiles into GCM Fields for Global
Climate Analysis
  A. Löscher and G. Kirchengast............................................................325

Author Index..........................................................................................335
Radio Occultation with CHAMP
Mission Status, Retrieval, Validation,
and Error Analysis
GPS Radio Occultation with CHAMP and GRACE: Recent Results


GeoForschungsZentrum Potsdam (GFZ), Department 1, Geodesy & Remote Sensing, Potsdam, Germany
wickert@gfz-potsdam.de

Abstract. The German CHAMP (CHAllenging Minisatellite Payload) satellite provides continuously GPS radio occultation data since February 2001. The measurements are analyzed by an operational orbit and occultation processing system at GFZ. In total ~170 000 high quality globally distributed vertical profiles of refractivity, temperature and water vapor are provided as of October 2004. The ground infrastructure from GFZ allows for the demonstration of a rapid data analysis since February 2003. The average delay between each measurement and provision of atmospheric excess phase data was reduced to ~4 hours by mid April 2004 and is continuously reached. The complete set of the available refractivity profiles is compared with corresponding analysis data from the European Centre for Medium-Range Weather Forecasts (ECMWF) between 0 km and 30 km altitude. The comparison shows nearly bias-free refractivity between ~7 km and 30 km, the standard deviation is ~1 %. The known negative refractivity bias of the CHAMP data in relation to ECMWF is significantly reduced in comparison to earlier product versions by applying the Full Spectrum Inversion (FSI) method for the data analysis in the lower troposphere. First radio occultation measurements from the GRACE-B (Gravity Recovery And Climate Experiment) satellite are available for a 25 h period on July 28/29, 2004. The stability of the satellite clock from GRACE-B is significantly improved in relation to CHAMP. This allows for precise occultation analysis using 30 s clock solutions applying a zero difference technique. Thus the disadvantageous use of a reference GPS satellite link to eliminate the clock error from GRACE-B can be avoided.

1 Introduction

Atmospheric profiling aboard the German CHAMP (Reigber et al. 2005) satellite was activated on February 11, 2001 (Wickert et al. 2001b). The experiment brought significant progress (Hajj et al. 2004; Kuo et al. 2004; Wickert et al. 2005c) for the innovative GPS (Global Positioning System) radio occultation (RO) technique (e.g., Kursinski et al. 1997) in relation to
the pioneering GPS/MET (GPS/METeorology) mission (Ware et al. 1996; Rocken et al. 1997). Main advantages of the calibration-free RO method are global coverage, high vertical resolution and all-weather capability combined with high accuracy. These properties allow for various applications in atmospheric/ionospheric research (e.g., Hajj et al. 2000; Ratnam et al. 2004; Wickert et al. 2004b; Wang et al. 2004; Wickert 2004; Kuo et al. 2005), weather forecast (e.g., Kuo et al. 2000; Healy et al. 2005; Healy and Thepaut 2005) and climate change detection (e.g., Randel et al. 2003; Schmidt et al. 2004, 2005a; Foelsche et al. 2005). Together with CHAMP, several upcoming RO missions will provide thousands of occultations daily and will extend the prospects of this promising technique (e.g., EQUARS (EQUatorial Atmosphere Research Satellite, Takahashi et al. (2004)); COSMIC (Constellation Observing System for Meteorology, Ionosphere and Climate, Rocken et al. (2000)) or Metop (e.g., Loiselet et al. 2000; Larsen et al. 2005)). We review recent results from the CHAMP RO experiment and present first results from the activation of GPS RO aboard the U.S. American/German GRACE mission (Dunn et al. 2003; Tapley and Reigber 2004).

## 2 Status of the CHAMP RO Experiment

Occultation measurements were performed during 1 238 days since February 2001 as of November 2, 2004; giving a total of 271 012 recorded events (∼219
daily). For \(\sim 74.9\%\) of the occultations (203,118) atmospheric excess phases are available (see Fig. 1). Vertical profiles of atmospheric parameters were derived for 169,767 occultations (\(\sim 62.6\%\)). The yield of the profiles in relation to the number of measurements is currently investigated in more detail within the framework of the Radio Occultation Sensor Evaluation activity (ROSE), jointly initiated by GFZ, Jet Propulsion Laboratory (JPL) and University Corporation for Atmospheric Research (UCAR) (Ao et al. 2003b; Wickert et al. 2005a). ROSE is aimed to evaluate and optimize the quality of CHAMP’s analysis results and to improve the involved occultation processing systems.

3 Operational Data Analysis

The occultation data aboard CHAMP are recorded by the “BlackJack” GPS flight receiver provided by JPL. The ground infrastructure of GFZ is used for a fully automated data analysis. Details on the infrastructure and on the orbit and occultation processing system can be found in Wickert et al. (2004a,c); König et al. (2005); Schmidt et al. (2005b). A Near-Real-Time (NRT) provision of atmospheric excess phases is continuously demonstrated since February 2003. An average delay of \(\sim 5\) hours between each measurement and provision of corresponding analysis results was reached. Optimized GPS ground station data handling for the precise orbit determination reduced this delay to \(\sim 4\) hours since mid April 2004. For some measurements per day the delay is \(\sim 2.5\) h (see Fig. 2). Further reduction is possible due to the use of a polar satellite receiving antenna at Ny Aalesund, Spitsbergen, (access to the satellite data every \(\sim 1.5\) h) and a global low latency GPS ground network (access to the ground data every \(\sim 15\) min), but requires further optimization concerning precise satellite orbit generation and occultation processing. The demonstration of NRT data analysis is an important milestone for the future assimilation of GPS RO data in numerical weather models. A positive impact of CHAMP data on global weather forecasts was already shown by Healy et al. (2005) and Healy and Thepaut (2005).

CHAMP data are analyzed using the standard double difference method to eliminate satellite clock errors (Wickert et al. 2001a). Atmospheric bending angles are derived from the time derivative of the excess phase after appropriate filtering. The ionospheric correction is performed by linear combination of the \(L_1\) and \(L_2\) bending angle profiles (Vorob’ev and Krasil’nikova 1994). The Full Spectrum Inversion (FSI) technique (Jensen et al. 2003), a wave optics based analysis method, is applied below 15 km to correct for the effect of lower troposphere multipath.

Vertical profiles of atmospheric refractivity are derived from the ionosphere corrected bending angle profiles by Abel inversion. For dry air, the density profiles are obtained from the relationship between density and refractivity. Pressure and temperature (“dry temperature”) are obtained applying the hydrostatic equation and the equation of state for an ideal gas. More details
Fig. 2. Time delay between CHAMP occultation measurements and availability of analysis results at GFZ from February 2003 until mid May 2004. Black diamonds indicate the daily mean of the time delay between each measurement and the availability of the corresponding calibrated atmospheric excess phases. An average of ∼5 hours for nearly the entire period is reached. The minimum time delays are marked by gray triangles. Due to improvements in the satellite orbit provision the mean delay was reduced to ∼4 hours since end of April 2004.

on the retrieval are given by Wickert et al. (2004c). Basics of the GPS radio occultation technique and the derivation of atmospheric parameters are described, e.g., by Kursinski et al. (1997). The refractivity and dry temperature profiles (Product:CH-AL-3-ATM) are provided via the CHAMP data center at GFZ (http://isdc.gfz-potsdam.de/champ/).

Background information from ECMWF is used to derive vertical humidity profiles from the CHAMP refractivities. Two methods for the water vapor derivation were implemented to the operational data analysis. In addition to a standard 1Dvar retrieval (Healy and Eyre 2000) a new direct method (DWVP), introduced by Heise et al. (2005), is implemented. Here the background temperature and pressure information are used to calculate water vapor pressure $p_w$ directly from the refractivity measurements using the Smith-Weintraub formula (Smith and Weintraub 1953). Both methods come to statistically comparable results and reveal a bias of less than 0.2 g/kg and a
standard deviation of less than 1 g/kg specific humidity in relation to radiosonde measurements in the mid troposphere. As an application example for the operational water vapor retrieval with CHAMP data, Fig. 3 shows the seasonal mean of the global water vapor distribution for northern summer (2002) and winter (2002/2003) at 500 hPa. The specific humidity data are derived using the DWVP method.

4 Recent Validation Results for CHAMP

The complete set of CHAMP measurements was reprocessed using the recent version (005) of GFZ occultation analyses software. The resulting set of refractivity profiles (∼170000) is compared with corresponding analysis data from ECMWF (Gaussian grid with 0.5° × 0.5° resolution at the Equator, 60 altitude levels) between 0 km and 30 km.

The comparison shows nearly bias-free refractivity between 10 km and 30 km (see Fig. 4). The standard deviation is ∼1%. The deviations show different characteristics in latitude (e.g., wave-like vertical structures of the bias above the south polar region with a period of ∼6 km). This fact suggests weaknesses of the analyzed data, introduced by the ECMWF assimilation scheme (e.g., Gobiet et al. 2005). Our validation results are, as expected, in good agreement with earlier validation studies (ECMWF and radiosonde data) using the previous product version 004 (Schmidt et al. 2004; Wickert et al. 2004c), since FSI is applied only below 15 km.

The major advantage of the recent version (in relation to earlier ones) of GFZ analysis software is the implementation of the FSI method (Jensen et al. 2003) to eliminate the effect of atmospheric multipath to the occultation data. The resulting bias and rms of the comparison with ECMWF is depicted in Fig. 5. The negative refractivity bias of the CHAMP data depends on latitude and is most pronounced in the tropics, where it reaches a value of 5% at 1 km. However in mid latitude and polar regions the CHAMP data are nearly bias free throughout the entire troposphere. The rms also depends on the latitude. In the tropics values of ∼3% are observed. In mid latitudes and
Fig. 4. Comparison of CHAMP refractivity data with corresponding ECMWF analyses (zonal means with 5° resolution) in the upper troposphere/stratosphere (left: bias; right: rms) between May 14, 2001 and November 3, 2004 (∼170 000 profiles).

Fig. 5. Comparison of CHAMP refractivity data with corresponding ECMWF analyses (zonal means with 5° resolution) in the troposphere (left: bias; right: rms) between May 14, 2001 and November 3, 2004 (∼170 000 profiles).

Polar regions the rms is below 1% almost down to the Earth’s surface. The negative refractivity bias is a known phenomenon of the CHAMP data and is discussed in more detail by Ao et al. (2003a); Beyerle et al. (2003a,b, 2005b). Causes of the bias are, beside multipath propagation, also signal tracking errors of the GPS receiver and critical refraction, a physical limitation of the RO technique. Further progress in reducing the bias is expected by the application of advanced signal tracking methods (“open loop” technique, see, e.g., (Sokolovskiy 2001; Beyerle et al. 2005b)) and improved signal strength due to the use of more advanced occultation antenna configuration (foreseen, e.g., for COSMIC or Metop). We note, that first investigations of the global map of fractional refractivity errors between CHAMP and ECMWF also reveal complex zonal and meridional structures (Beyerle et al. 2005b).
Monitoring of Tropopause Parameters

CHAMP temperature data in the tropopause region are not affected by background temperature fields. In conjunction with its high vertical resolution the RO technique provides a nearly perfect tool for precise monitoring of tropopause characteristics (altitude, pressure and temperature) on a global scale.

The tropopause has received increasing interest from climate change researchers during the last three decades. Changes in tropopause parameters (altitude, pressure and temperature) were used as indicators for climate change. Hereby it was shown, that these parameters have the potential to provide a more clear signal for the global warming than the surface temperature (e.g., Sausen and Santer 2003). Therefore, we use the CHAMP data to monitor tropopause parameters.

As an example for these studies Fig. 6 shows the latitudinal-longitudinal structure of the tropical tropopause derived from CHAMP RO data for the Northern Hemisphere winter months. The plots represent a mean over 3 winter seasons. The results are consistent with climatologies based on radiosonde measurements and meteorological analyses, as discussed by Schmidt et al. (2004): The highest lapse rate tropopause altitudes during December to February of >17.0 km are observed in the tropical Western Pacific and the northern part of South America (Fig. 6a). The coldest temperatures (Fig. 6b), less than $-82^\circ$C, are correlated with the maximum lapse rate tropopause altitudes. In
6 First Results from GRACE

The “BlackJack” GPS receiver (provided by JPL) aboard the GRACE-B satellite (aft-looking antenna to observe setting occultations) was activated for the first time in atmospheric sounding mode from July 28, 06:00 UTC until July 29, 07:00 UTC, 2004. 120 occultations (parallel tracking of occultation and reference satellite ≥20 s) were recorded during this 25 h interval. The data were analyzed using the orbit and occultation processing system for CHAMP (see Sect. 3). The quality of the GRACE orbits was evaluated by comparisons with Satellite Laser Ranging (SLR) data. The rms was around 4cm to 5 cm and is slightly lower than the rms for CHAMP orbits (currently 5 cm).

The location of the first occultation measurement from GRACE is not far from the geographical center of Europe (54.85°N, 25.32°E, nearby Vilnius, Lithuania). Figure 7 shows the retrieved profiles of dry temperature and specific humidity, and the corresponding ECMWF profiles for the first occultation measurement from GRACE.

The significantly improved stability of the satellite clock from GRACE-B in relation to CHAMP (absence of periodic clock adjustments) allows for

the Western Pacific region tropopause temperatures reach values of less than −86 °C.
the application of a zero differencing technique. This avoids the disturbing influence of the additional link to a referencing GPS satellite and reduces the onboard data amount. The method was first applied and is described in more detail by Beyerle et al. (2005a). For the operational GRACE data analysis we apply an implementation of the zero difference technique using the 30 s clock solutions (Wickert et al. 2005b) provided by the precise orbit determination facility from GFZ (König et al. 2005). We processed the first GRACE occultations applying the standard double, the single (Wickert et al. 2002) and the zero differencing technique and compared the resulting vertical refractivity profiles with ECMWF (see Fig. 8). The comparison results for these three datasets are nearly identical and show no discernable differences. This finding does not confirm the early results from Wickert et al. (2005b), which indicated a better agreement of the zero difference results with ECMWF. In contrast to these preliminary results we’ve analyzed the first measurements from GRACE-B within the available study taking into account the reset of the GRACE-B clock by 14 ms on July 28, 16:00 UTC.

**Fig. 8.** Statistical comparison between 87 refractivity profiles, derived from GRACE measurements and 6-hourly ECWMF analyses during July 28 and 29, 2004. The differences (GRACE - ECMWF) are plotted for the profiles derived using (a) double differencing, (b) single differencing and (c) zero differencing (please note the difference compared to Fig. 4 of Wickert et al. (2005b), for details see text).
7 Atmospheric Sounding with CHAMP and GRACE

CHAMP and GRACE will form a satellite configuration for precise atmospheric sounding after the operational activation of the GRACE occultations. The GRACE measurements will be analyzed by the operational processing system at GFZ and the analysis data will be provided to the international scientific community via the data center at GFZ (http://isdc.gfz-potsdam.de).

Considering RO data from CHAMP and GRACE, the number of continuously available occultation measurements in comparison to the current stage (only CHAMP) can be doubled. A first impression of the global occultation distribution from the CHAMP/GRACE constellation is given by Fig. 9. In total 338 occultations (218 from CHAMP, 120 from GRACE) were recorded during the 25 h activation of the GRACE occultations. The number of GRACE-B measurements was intentionally reduced during the test (reduction of the viewing angle of the occultation antenna to 40°). Working in nominal mode, the same number of measurements as from CHAMP can be expected.

8 Conclusions and Outlook

After more than three and a half years of GPS radio occultation with CHAMP about 270 000 occultation measurements are available. As the mission is ex-
pected to last at least until 2007, the first long-term dataset of GPS RO data is anticipated. The data and results of the operational data analysis are available at the data center at GFZ (http://isdc.gfz-potsdam.de/champ). A NRT occultation data transfer and analysis is continuously demonstrated since February 2003. The average delay of ∼5 hours between each measurement aboard CHAMP and data product provision was reduced to ∼4 hours since mid April 2004. The long-term dataset of CHAMP is the base for the preparation of future occultation missions and the related processing systems, impact studies to improve the global weather forecasts, studies with relevance to detect climate change and other applications for atmospheric/ionospheric research. Validation results indicate that refractivities in the upper troposphere and lower stratosphere agree well with ECMWF. Mean deviations are below 0.5% and standard deviations below 1%. These deviations show latitudinal dependent characteristics. A negative refractivity bias in the lower troposphere is observed. This was significantly reduced by using advanced retrieval methods, which were implemented to generate the current version of data products (005). CHAMP dry temperature data are used for a precise monitoring of tropical tropopause characteristics. First measurements from the GRACE-B satellite are analyzed. The GRACE-B clock is stable enough to be modeled by 30 s clock solutions which can be used for the precise occultation processing applying zero differencing. A significant improvement of the GRACE-B analysis results by applying zero differencing, as indicated by the early results, cannot be confirmed. CHAMP and GRACE will form a promising constellation for operational sounding of the Earth’s atmosphere on a global scale. Recent information on the status of the RO experiments aboard CHAMP and GRACE, the operational data analysis at GFZ and current validation results can be obtained via WWW (http://www.gfz-potsdam.de/gasp).

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Sensitivity of Stratospheric Retrievals from Radio Occultations on Upper Boundary Conditions

C. O. Ao\textsuperscript{1}, G. A. Hajj\textsuperscript{1}, B. A. Iijima\textsuperscript{1}, A. J. Mannucci\textsuperscript{1}, T. M. Schröder\textsuperscript{1}, M. de la Torre Juárez\textsuperscript{1}, and S. S. Leroy\textsuperscript{2}

\textsuperscript{1} Jet Propulsion Laboratory, California Institute of Technology, Pasadena, USA
\textsuperscript{2} Department of Chemistry and Chemical Biology, Harvard University, Cambridge, USA

Abstract. The main uncertainty in the stratospheric retrievals from GPS radio occultation (RO) measurements comes from the lack of reliable measurements in the upper stratosphere and above where the bending due to the neutral atmosphere is weak and residual ionospheric effects are strong. In this work, we quantify the bias and uncertainty of the refractivity and temperature retrievals due to different upper boundary strategies using a simulation study. We use refractivity profile derived from lidar pressure and temperature profiles as the input states in generating the synthetic occultations. Random noise levels commensurate with the CHAMP RO measurements are added to the simulated data. We examine the sensitivity of stratospheric retrievals to two different upper boundary methods, one based on exponential extrapolation and the other on MSIS climatology. The simulation results show that both methods lead to comparable levels of temperature bias (less than 0.5 K below 30 km altitude), provided that the upper boundary heights are set above 55 km.

1 Introduction

GPS radio occultation (RO) has been touted as one of the most promising remote sensing techniques in climate monitoring because RO measurements are self-calibrating and are not subject to time-dependent biases due to instrumental drifts (Goody et al. 1998). Over the years, the precision, accuracy, and resolution of the measurements, especially in the altitude range of 5 km to 25 km, has been well-established through theoretical considerations (e.g., Kursinski et al. 1997), validation studies (e.g., Rocken et al. 1997), and intersatellite comparison (Hajj et al. 2004). However, stratospheric retrievals at altitudes higher than 25 km are more uncertain. This is mainly due to the lack of reliable measurements in the upper stratosphere and above where the
bending due to the neutral atmosphere is weak compared with various error sources including thermal noise, orbital and local multipath errors, and perhaps most significantly, uncorrected ionospheric effects (Kursinski et al. 1997). A solution for this problem is to replace the noisy bending angles at high altitudes (typically above 40 km to -60 km) with “modeled” bending angles obtained from a climatology such as MSIS (Picone et al. 2002). The influence of the modeled bending angles decreases as the altitude decreases. The possible problem with this approach is that the retrievals could become biased toward the adopted climatology. An alternative, climatology-independent approach is to extrapolate the data at lower altitudes upward to altitudes where the data are not trustworthy. The problem with the extrapolation approach is that it relies on questionable assumptions regarding the characteristics of the stratosphere and mesosphere.

While there have been numerous published works addressing the upper boundary treatments and the retrieval errors associated with them (Kursinski et al. 1997; Hocke 1997; Steiner et al. 1999; Healy 2001; Rieder and Kirchengast 2001; Gorbunov 2002; Gobiet and Kirchengast 2004), the present study is unique in that the retrieval errors are examined with a simulation study which is based on atmospheric profiles from lidar measurements. The lidar profiles are more representative of the real stratospheric and mesospheric conditions than available models (albeit much more localized spatially and temporally) and are relatively independent of climatology. Thus they can be used to assess more quantitatively the errors due to the use of climatology as upper boundary conditions. The focus of this paper is to evaluate and compare the sensitivity of RO retrievals to the extrapolation and climatology approaches. We consider random bending angle noise at levels that are representative of CHAMP measurements.

The rest of the paper proceeds as follows. In Sect. 2, we give more details on the data and methodology used in this study. The numerical results are presented in Sect. 3, where we show refractivity and temperature errors under different upper boundary conditions. Finally, we summarize the main findings in Sect. 4 and discuss future work.

2 Data and Methodology

The input atmosphere used in the simulations is based on one year of lidar observations from Mauna Loa, Hawaii (19.5°N, 155.6°W) (Leblanc and McDermid 2001). The retrieved lidar profiles are freely accessible from the Network for the Detection of Stratospheric Change (NDSC) web site (http://www.ndsc.ucmp.noaa.gov). In the year 2001, a total of 156 profiles covering the altitude range 20 km to 90 km are available. Since the contribution of water vapor to refractivity is negligible in the stratosphere and above, the refractivity profile can be derived simply from the lidar temperature and
pressure profiles with the standard expression \( N = 77.6(P/T) \), where \( P \) is the pressure in hPa and \( T \) is the temperature in Kelvin.

From the refractivity profile, and assuming local spherical symmetry, the bending angle can be obtained with the forward Abel integral (e.g., Kursinski et al. 1997)

\[
\alpha(a) = -2a \int_a^{\infty} \frac{da'}{\sqrt{a'^2 - a^2}} \frac{d\ln n}{da'}
\]

where \( a = n(r)r \) is the impact parameter and \( n(r) = 1 + N(r) \times 10^{-6} \) is the index of refraction. Since input profiles only reach altitudes of \( \approx 90 \) km, we extend the refractivity profiles beyond the maximum lidar altitude with exponential extrapolation. Because the atmosphere is so tenuous at these altitudes, the results presented here are not sensitive to the exact manner in which these profiles are extended.

The next step is to add realistic level of noise to the simulated bending angles.

\[
\alpha_{\text{obs}}(a) = \alpha(a) + \alpha_n(a)
\]

Note that we have ignored the ionosphere in the computation of \( \alpha(a) \). Thus we regard \( \alpha_{\text{obs}}(a) \) as the ionosphere-free bending angle. Any residual calibration and ionosphere errors should be modeled in \( \alpha_n(a) \). The choice of \( \alpha_n(a) \) will be discussed more below.

In the presence of noise, \( \alpha_{\text{obs}}(a) \) can be trusted only below certain impact parameter \( a_u \) where the bending signal is large compared to the noise level. However, to obtain the refractivity at \( a < a_u \), the bending angles at all impact parameters above it are required. Thus, \( \alpha_{\text{obs}}(a) \) for \( a > a_u \) should be replaced with external data or a priori model, \( \alpha_{\text{mod}}(a) \). The refractivity profile is obtained from the Abel inversion integral as

\[
\ln n(a) = \frac{1}{\pi} \int_a^{h+R} da' \frac{\alpha_{\text{obs}}(a')}{\sqrt{a'^2 - a^2}} + \frac{1}{\pi} \int_{h+R}^{\infty} da' \frac{\alpha_{\text{mod}}(a')}{\sqrt{a'^2 - a^2}}
\]

where \( R \) is the local radius of curvature of the Earth and \( h = a_u - R \) is the impact parameter height corresponding to the transition from data to model.

The specification of \( \alpha_{\text{mod}}(a) \) above \( h \) used (including the choice of \( h \)) will henceforth be referred to as the Abel boundary condition (ABC). As discussed in Sect. 1, current approaches to ABC can be grouped into two categories: extrapolation (EXT) and climatology (CLI). The ideal ABC should be able to minimize the propagation of noise in the retrieved refractivity to lower altitudes while producing little or no bias.

In the EXT approach, the bending angle in the region below \( h \) is used to extrapolate the data to higher altitudes. No other external information is needed other than the functional form assumed in the extrapolation. We use a simple exponential function \( \exp(b_0 + b_1a) \) to characterize the bending angle above \( h \) with the parameters \( b_0, b_1 \) determined from fitting the data from \( \approx (h - 10 \) km) to \( h \). The exponential functional form approximates an
isothermal atmosphere. The effectiveness of this approach depends on how well such an approximation works as well as how well the fitting parameters can be determined. In the CLI approach, the observed bending angle in the region above $h$ is replaced with bending derived from a climatology such as MSIS (computed at the time and location of each occultation profile). Thus the replacement is completely independent of the observed bending angle and is not susceptible to noise in the data. On the other hand, the MSIS profiles are likely biased relative to the true states of the atmosphere. For instance, compared with the Mauna Loa lidar profiles used in the simulation, the MSIS refractivity is larger in the mesosphere, with a peak average difference of approximately 7% at 60 km. The MSIS temperature is colder in the mesosphere, with a peak average difference of about 2 K at 60 km. The use of MSIS in modeling the bending angles at high altitudes can lead to systematic biases in the retrievals (cf. Sect. 3).

Note from Eq. (3) that we have used a “hard” boundary where the $\alpha(a)$ switches from $\alpha_{\text{obs}}(a)$ to $\alpha_{\text{mod}}(a)$ at a fixed impact parameter height $h$. An alternative approach is to adopt the so-called statistical optimization method where the measured and modeled bending angles are linearly combined to minimize the root-mean-square (rms) error in the bending angles (see e.g., (Gobiet and Kirchengast 2004) and references therein). The effective application of optimization method requires reasonable estimates of the variance and covariance characteristics of the measurements and model, which is a non-trivial task. The hard boundary is applied here because the results are much simpler to interpret.

A key ingredient in the simulation study is to come up with a realistic representation of the bending angle noise $\alpha_{\text{nl}}(a)$. This, however, proves difficult because of the multitude of random and systematic error sources that might contribute to the ionosphere-free bending angle (Kursinski et al. 1997). For simplicity, we assume that the noise is characterized by a random Gaussian process with standard deviation which is independent of altitude. The level of random noise can be determined through the examination of CHAMP bending angles. Figure 1 shows the rms residual of the ionosphere-free bending angle obtained by linearly detrending $\alpha_{\text{obs}}(a)$ with impact parameter heights between 50 km and 55 km. Interesting seasonal and latitudinal variations can be noted, with significantly more scatters in the polar regions. From the figure, it can be concluded that bending angle residuals for most of the CHAMP occultations fall between 1 $\mu$rad and 4 $\mu$rad. For comparison, the U.S. Standard atmosphere gives a bending angle of about 5 $\mu$rad at 60 km and 8 $\mu$rad at 45 km. To obtain a reasonable upper bound on the averaged errors, we consider in the following bending angle noise with 4 $\mu$rad standard deviation and examine the retrieved refractivity and temperature profiles resulting from ABC strategies with upper boundary heights from 45 km to 60 km.
Fig. 1. Residuals of the ionosphere-corrected bending angle from four months of CHAMP data. Solid line indicates the median values within 20° latitudinal bands while dashed lines indicate the mean absolute deviation values about the median.

3 Simulation Results

3.1 Refractivity Errors

Consider first the noiseless case. Figure 2 shows the mean and rms fractional refractivity errors corresponding to different ABC strategies (EXT and CLI approaches, with upper boundary heights $h = 45, 50, 55, 60$ km). These results are obtained by averaging the errors over the 156 simulated occultations. In the noiseless case, the refractivity errors are entirely due to the inaccurate modeling of the atmosphere above $h$. As expected, the mean and rms errors increase as $h$ decreases. The bias is positive for the CLI approach and mostly negative for the EXT approach.

Figure 3 shows the corresponding results for the case with 4 $\mu$rad bending angle noise. While the mean errors remain at about the same level as the noiseless case, the rms errors are now several times larger. It should be noted that lowering the upper boundary height $h$ has relatively little impact on reducing the rms errors, indicating that the rms errors are dominated by the bending angles below 45 km impact parameter heights.

These results show that for both EXT and CLI approaches, it is far better to use an upper boundary height which is in the range of 55 km to 60 km. These strategies yield the smallest biases without introducing significantly larger rms errors. For the 4 $\mu$rad noise case, $h = 55$ km gives a refractivity bias of $-0.05\%$ and rms error of $0.71\%$ at $z = 30$ km for EXT. For CLI, the
Fig. 2. Fractional refractivity errors for EXT and CLI strategies with upper boundary heights at 45, 50, 55, 60 km: noiseless case.

Fig. 3. Fractional refractivity errors for EXT and CLI strategies with upper boundary heights at 45, 50, 55, 60 km: 4 μrad case.

corresponding refractivity bias is 0.14 % with rms error of 0.61 %. Thus EXT and CLI results are quite comparable, with CLI yielding a smaller rms error at the cost of a larger bias.