

ADVANCEMENTS OF GNSS OCCULTATION RETRIEVAL IN THE STRATOSPHERE FOR CLIMATE MONITORING

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ABSTRACT

Radio occultation (RO) observations promise to become a valuable basis for global climatologies of temperature, humidity and geopotential height in the near future. First results from the “GNSS-CLIMATCH study”, aimed at evaluation of the climate monitoring and trend detection ability of RO data, show promising results (temperature bias < 0.6 K in most regions between 8 and 40 km altitude) and the continuous RO data stream from the CHAMP mission enables to create such climatologies for the first time. Both, GNSS-CLIMATCH and first retrieval results from CHAMP are encouraging, but show distinct weaknesses of RO retrieval at high altitudes (increasing temperature bias above 35 km in the GNSS-CLIMATCH study, and above 20 km in the profiles from CHAMP) and a systematic lack of retrieval performance in some geographical regions. We performed a systematic end-to-end simulation study to evaluate state-of-the-art high altitude RO retrieval schemes. The results show a good performance of the commonly applied ionospheric correction scheme, the necessity for the use of statistical optimisation methods involving background data from climatology, and the sensitivity of high altitude RO retrieval products to biases in the background. Considering this, an enhanced background bias correction scheme was developed and evaluated. It proved to be very effective, especially in the former most critical geographical regions. This RO retrieval scheme will be further developed focusing on retrieval problems in the troposphere and will serve as retrieval chain for the first real RO based global climatologies which we aim to build starting with RO data from the CHAMP satellite mission, later supplemented with RO data from subsequent missions including METOP/GRAS.

1. INTRODUCTION

Monitoring of climate change over the coming decades is highly relevant since there exists increasing concern and evidence that Earth's climate is significantly influenced by human activities (e.g. IPCC, 2001). A very promising observing system in this context is the Global Navigation Satellite System (GNSS) radio occultation (RO) technique.

The RO technique was originally developed in the early days of interplanetary flight and contributed to the study of the atmospheres of our solar system's planets (e.g. Fjeldbo et al., 1971). This method uses a RADAR transmitter on a spacecraft outside of the respective planet's atmosphere and a receiver on the Earth's surface. As the spacecraft is occulted by the planet's limb (as viewed from Earth's perspective), the electromagnetic rays pass different layers of the planet's atmosphere and get bended and decelerated. This enables the receiver to collect information on the vertical structure of the planet's ionosphere and neutral atmosphere. The application of the RO technique to Earth's atmosphere (see Figure 1 for a schematic depiction of the RO geometry) became possible with the arrival of the U.S. Global Positioning System (GPS) in the early 1980's. Together with the Russian GLONASS system and the emerging European GALILEO

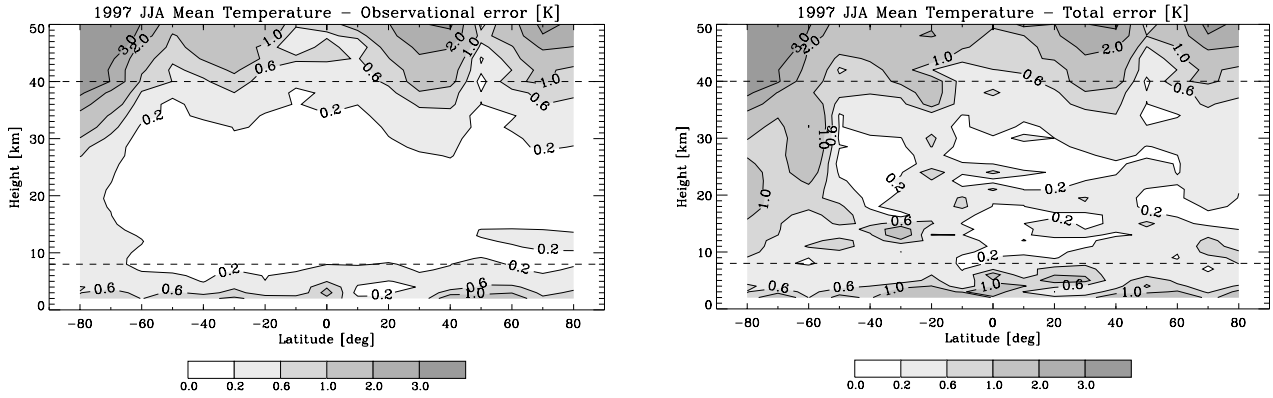


Figure 2: First CLIMATCH-results: Observational error (left panel) and total climatological error for the “tesbed season” (June, July, and August 1997) mean temperature (Foelsche et al., 2002).

We aim at using the complete CHAMP RO data flow for global climate monitoring via temperature, geopotential height, and humidity fields. The climatologies will be built in two modes: (1) *fully background independent* based on interpolation and averaging techniques and (2) *weakly background dependent* but higher resolved. This is done by optimal fusion of RO derived refractivity profiles and suitable time/space averaged ECMWF analysis fields into global climate analyses (3DVAR assimilation). An assimilation scheme tuned for high-vertical/low-horizontal resolution is currently in development (resolution baseline: Gaussian grid, T21L50 i.e. 32 x 64 geographic areas, 50 standard model levels up to ~50 km). To reduce the sampling error of the climatology, the CHAMP data stream may be complemented by RO data from the Argentinean SAC-C satellite (launched in Nov. 2000), providing occultation data since July 2001, and the German GRACE satellite (launched in March, 2002), expected to provide occultation data by end of 2002. These missions will be followed by the upcoming European METOP weather satellite series which will carry the GRAS receiver (GNSS Receiver for Atmosphere Sounding; 1st launch scheduled 2005), the U.S./Taiwan COSMIC mission consisting of six micro-satellites carrying GPS receivers (launch scheduled 2005), and the European ACE+ mission consisting of four micro-satellites carrying advanced GRAS receivers (launches planned 2007/08). The combination of these data will allow to build climatologies with at least the quality described above for the GNSS-CLIMATCH study.

Both, the GNSS-CLIMATCH and CHAMP results clearly show the critical regions of RO based climatologies: The middle and lower troposphere where water vapour and strong horizontal gradients complicate the interpretation of RO data, and the upper stratosphere where the phase-delay signal-to-noise ratio is low and effects from the ionosphere start to dominate the signal. In case of the GNSS-CLIMATCH study, the critical region starts at heights above ~35 km (in the high-latitude winter region at ~25 km), in case of the first CHAMP-retrievals the problems even start as low as 20 km. The remainder of this paper is dedicated to the latter problem: advancement of high altitude RO retrieval.

3. RO RETRIEVAL METHODOLOGY AND HIGH ALTITUDE RETRIEVAL TECHNIQUES

The primary observables of RO measurements are the phase delays of the two GNSS signals L1 and L2 (L1: $f_1 = 1575.42$ MHz, L2: $f_2 = 1227.60$ MHz), i.e. the consequences of deceleration of the electromagnetic wave’s phase velocity by the atmosphere. From phase delays, Doppler shifts and subsequently total bending angles α of the rays are deduced. The refractivity $N (=10^6(n-1)$, n : refractive index) can then be derived via inverse Abel transform (Fieldbo et al., 1971):

$$n(a) = \exp \left[\frac{1}{\pi} \int_a^\infty \frac{\alpha(a')}{\sqrt{a'^2 - a^2}} da' \right], \quad (1)$$

where a is the ray’s impact parameter, which is related to the distance r from the centre of refraction (~Earth’s centre) by: $r(a) = a/N(a)$. Other atmospheric parameters, such as pressure, geopotential height, temperature and water vapour, are derived from refractivity using the Lorentz-Lorenz formula, the ideal gas equation, and the hydrostatic equilibrium. For the retrieval of temperature and humidity in the middle and

lower troposphere, additional a priori information about one of the two parameters is necessary. A detailed treatment of RO retrieval is given, for example, by Kursinski et al. (1997), a sketch of RO retrieval is depicted in Figure 3.

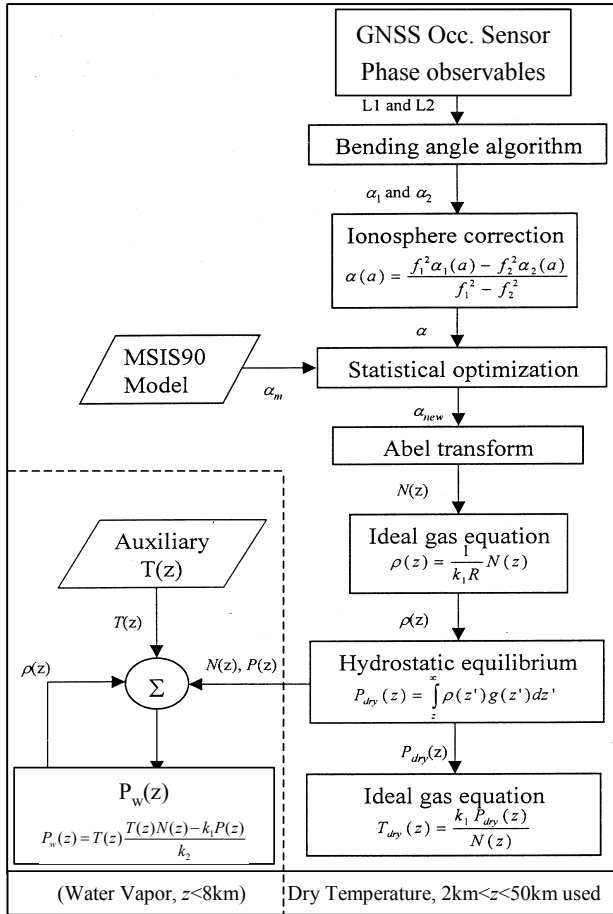


Figure 3: The radio occultation retrieval algorithm - an overview (after Hoeg et al., 1998)

(Vorob'ev and Krasil'nikova, 1994; Ladreiter and Kirchengast, 1996; Hocke et al., 1997). There are some methods that account for higher order effects of the ionosphere (e.g. Syndergaard, 2000), but they rely on additional a priori knowledge of the ionosphere, which is not easy to obtain. For these reasons, we used the *linear correction of bending angles* in our retrieval scheme. This method relies indirectly, via the definition of the impact parameter, on the assumption of a spherical symmetric atmosphere. Though there are no detailed studies under realistic conditions about this effect, asymmetries in the ionosphere are regarded to be a limiting error source for the retrieval of atmospheric parameters in the upper stratosphere and above (e.g. Kursinski et al., 1997). In section 3 of this paper we present a high-altitude RO retrieval evaluation study which, among other things, systematically tested the ionospheric correction of bending angles.

As described above, even after ionospheric correction, the retrievals at heights above ~30 km are sensitive to residual ionospheric noise (higher order terms, asymmetries in the ionosphere) and measurement noise. This calls for sensible use of the data at high altitudes, in particular above the stratopause, where the phase delay signal-to-noise ratio is low. The simplest way to do so is to select an upper boundary height ("initialisation height") at altitudes between 50 – 70 km, depending on signal-to-noise ratio, above which an extrapolated exponential bending angle profile is used. This traditional approach ("*no optimisation approach*") features several distinct weaknesses, most importantly being the sensitivity of the initialisation height selection and extrapolation quality to the noise in the data and the intrinsic assumption of an isothermal atmosphere above the boundary height. A more advanced approach is the statistical optimisation. It attempts to find the most probable bending angle profile by combining the observed profile with a background profile from climatology in a statistically optimal way. This concept was introduced by Sokolovskiy and Hunt (1996) into the context of GNSS RO retrievals. In general form, the optimisation formula ("*inverse covariance weighting approach*") can be written as:

The transition from bending angles to refractivity is a crucial step in this chain. Eq. (1), the inverse Abel transform, shows that the refractivity at any altitude depends on the bending angles above it, i.e. that errors in the high-altitude bending angle profile propagate to lower levels in the refractivity profile. For this reason, it is vital to use reasonable bending angles even at altitudes above the region of interest. Close to the surface, the bending angle depends mostly on the contribution of the neutral atmosphere, above 45 km the contribution of the ionosphere starts to dominate (e.g. Hocke, 1997). The effect of the ionosphere has to be sorted out before the neutral atmospheric parameters can be calculated. Since the ionosphere, as a dispersive medium, causes different phase delays of the two GNSS signals as well as different L1 and L2 ray paths, ionospheric effects on the signals can be removed to first order by linear combination of the two signals. There are several methods to do so (e.g., Syndergaard, 2000), but in recent applications the method of *linear correction of bending angles* (Eq. (2); Vorob'ev and Krasil'nikova, 1994) has been applied most successfully.

$$\alpha_{LC}(a) = \frac{f_1^2 \alpha_1(a) - f_2^2 \alpha_2(a)}{f_1^2 - f_2^2} \quad (2)$$

where α_{LC} is the ionosphere-corrected bending angle. As shown in several theoretical and simulation studies, the *linear correction of bending angles* provides significantly better results than other correction methods, since it accounts for the different ray paths of L1 and L2 and exploits the fact that most of the total bending angle is accumulated near the ray perigee.

$$\alpha_{opt} = \alpha_b + \mathbf{B}(\mathbf{B} + \mathbf{O})^{-1}(\alpha_o - \alpha_b), \quad (3)$$

where α_{opt} is the optimised bending angle profile, α_b and α_o are the background and observed bending angles, and \mathbf{B} and \mathbf{O} are the background and observation error covariance matrices, respectively. The restrictions of this approach are, that unbiased errors and a linear problem are assumed. The general effect of statistical optimisation is that at higher altitudes, where the observation error exceeds the error of the background profile, α_{opt} is determined by the background. At lower altitudes, where the background error becomes dominant, α_{opt} is determined by the observed data. It should be noted that statistical optimisation does not improve the quality of observed profiles themselves at high altitudes, but rather delivers an improved combined profile, thanks to the climatological information invoked. The most important effect is, however, that the optimisation minimises error propagation downwards to altitudes, where observed data have a good signal-to-noise ratio.

Since the *inverse covariance weighting approach*, Eq. (3), faces the difficulty of requiring accurate covariance matrices, which are not so easy to define properly, Sokolovskiy and Hunt (1996) demonstrated this technique by using a simpler form, assuming vertically uncorrelated errors (i.e., all non-diagonal elements of the error covariance matrices set to zero). Healy (2001) suggested to use the full *inverse covariance weighting approach* with a simplified analytical background error covariance matrix formulated as:

$$\mathbf{B}_{ij} = \sigma_i \sigma_j \exp\left(-\frac{(a_i - a_j)^2}{l^2}\right) \quad (4)$$

where σ_i and σ_j are the standard deviations of the i^{th} and j^{th} background bending angles, a_i and a_j are the corresponding impact parameter values. l is the error correlation length (usually $l = 6$ km). The observed bending angle errors have still been assumed to be vertically uncorrelated. Since observation errors mainly contain noise, this assumption is valid to a much higher degree than for the errors in the climatology. An advanced optimisation concept has been discussed by Rieder and Kirchengast (2001). This general treatment is not specifically focused on bending angle optimisation but the background information can be fused in at any retrieval product level. Syndergaard (priv. communications, 1999) suggested to perform background bending angle profile search prior to statistical optimisation, i.e., to fit the available background bending angle profiles to the observed profile and subsequently use the best-fit instead of the geographically co-located profile as the background in the statistical optimisation process. The latter concept was implemented into the statistical optimisation algorithm described by Rieder and Kirchengast (2001) and used in this study. As applied here, it uses bending angles, i.e. it is comparable to the approach by Healy (2001), though it includes vertically correlated observation errors (correlation length $l=1$ km), which represents the effect of smoothing of the phase delays in a prior step of the retrieval. For each occultation event the observation error is estimated from the observed profile between 70 – 80 km where the signal is very weak and ionospheric residuals and measurement noise dominate. As background we use the MSIS90 climatology (Hedin, 1991). The background errors are assumed to amount to 20% of the background bending angle, which is a relatively arbitrary and rather conservative estimation. It was chosen by Sokolovskiy and Hunt (1996) as representing the stratopause/mesosphere rms deviation of the climatology. The retrieval scheme, as described here, was also applied in the GNSS-CLIMATCH study (see section 2).

4. EVALUATION OF HIGH-ALTITUDE RETRIEVAL

In this section we present a systematic case study aimed at the evaluation and enhancement of high-altitude RO retrieval. A detailed description of this study is given by Gobiet and Kirchengast (2002). In order to study the residual errors from ionospheric correction and the effects of statistical optimisation as a function of ionospheric state, we chose three occultation events as base scenarios, each of them being representative for one type of symmetry (or asymmetry) of the electron density distribution in the ionosphere (see Figure 4). We simulated the propagation of the GNSS signal through the atmosphere (“forward modelling”) both without ionosphere (“no ionosphere” case) and at three different ionisation levels, represented by the radio flux at 10.7 cm ($F_{10.7}$ -index) ranging from $F_{10.7} = 70$ to $F_{10.7} = 210$. Additionally, two different receiving systems were modelled: an idealised, where observation system related errors were neglected and a “realistic” one which is based on the error specifications of the GRAS receiver. Subsequently, we performed the retrieval using different statistical optimisation approaches. In this paper we show results for *no optimisation* (with observed profile exponentially extrapolated) and *inverse covariance weighting optimisation* (with and without background profile search in MSIS90). The complete study was realised by means of a modified version of the EGOPS software tool (End-to-end GNSS Occultation Performance Simulator; Kirchengast et al., 2001).

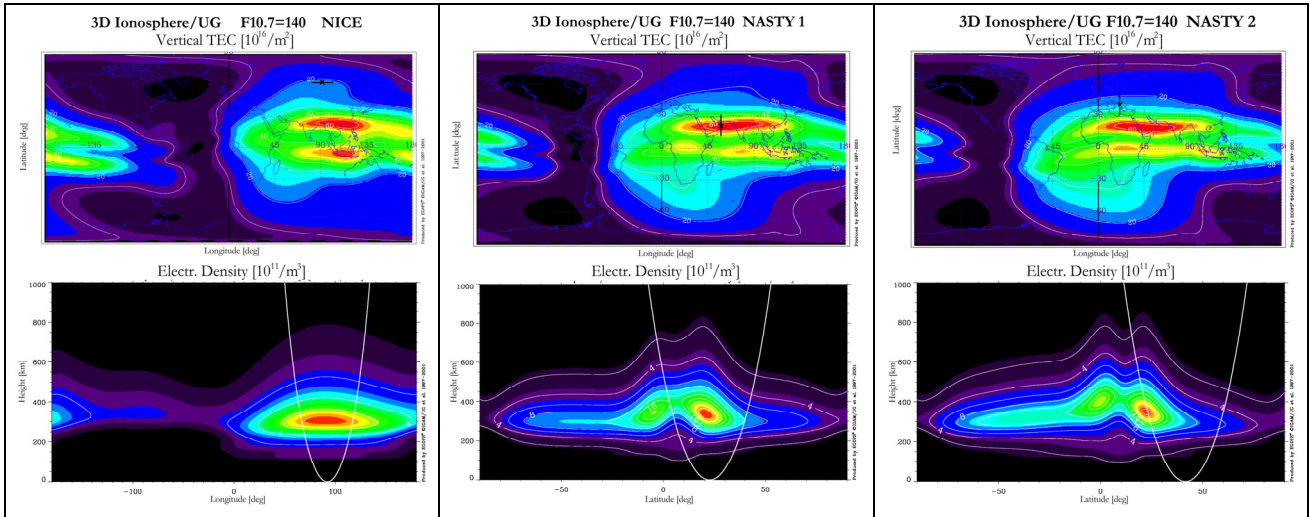


Figure 4: Ionospheric conditions during the three base scenarios. “Nice” event (left): Vertical total electron content above tangent point: $\sim 20 \cdot 10^{16} \text{ m}^{-2}$; electron density varies $< 1.5 \cdot 10^{11} \text{ m}^{-3}$ between inbound and outbound of the lowermost ray. “Nasty 1” event (middle): Vert. TEC above tangent point: $\sim 60 \cdot 10^{16} \text{ m}^{-2}$; electron dens. varies $\sim 12 \cdot 10^{11} \text{ m}^{-3}$ between inbound and outbound of lowermost ray; electron dens. max. above tangent point. “Nasty 2” event (right): Vert. TEC above tangent point: $\sim 25 \cdot 10^{16} \text{ m}^{-2}$; electron dens. varies $\sim 18 \cdot 10^{11} \text{ m}^{-3}$ between inbound and outbound of lowermost ray; electron dens. max. at outbound of lowermost ray.

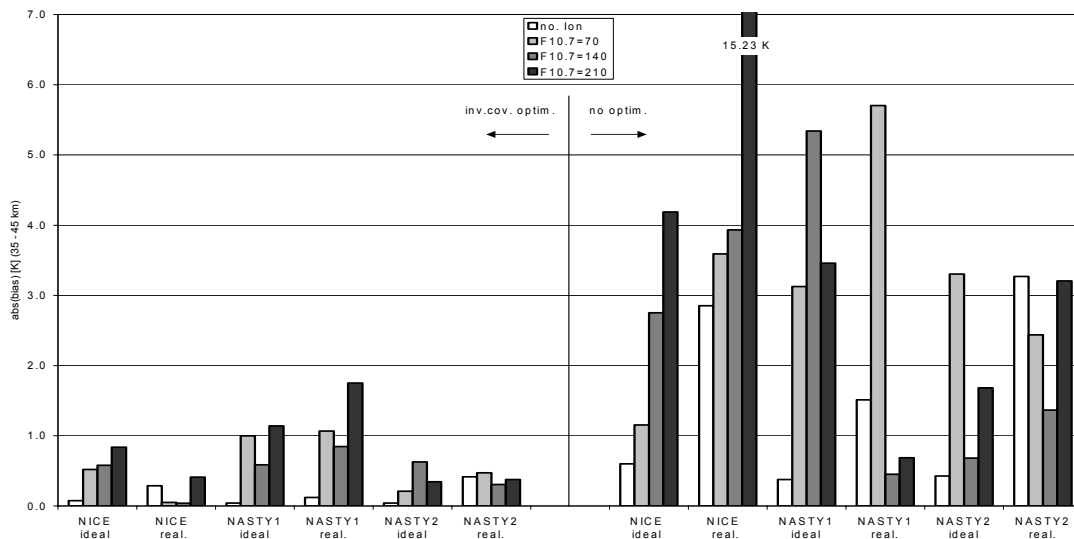


Figure 5: Bias of the retrieved temperature in the 35 – 45 km interval (“upper stratosphere bias”) for all simulated occultation events at different ionospheric conditions and with different simulated receiving systems (ideal and quasi-realistic receiving system). Left: retrieval with inverse *covariance weighting optimisation* and background search. Right: *no optimisation*.

Figure 5 gives an overview of the retrieval results: It depicts the mean temperature bias between 35 – 45 km altitude (“upper stratosphere bias”) for all three base scenarios, each simulated with ideal and realistic receiving system, and for 4 different ionisation-levels. In the right panel the *no optimisation* retrieval and in the left panel the *inverse covariance weighting optimisation* with background search in the MSIS90 climatology is shown. The most apparent result is the strong mitigation of the upper stratosphere bias by statistical optimisation. This is also demonstrated for one selected error profile (“nasty 1” event, realistic receiver, $F_{10.7}=70$) in Figure 6 (leftmost and rightmost panel). Figure 6 shows that errors due to deficient high-altitude initialisation can propagate down to below 20 km in the temperature profile. This is an extreme example we chose for demonstration, in average the error propagates to ~ 30 km. Furthermore, the results in Figure 5 indicate that the applied linear ionosphere correction of bending angles is remarkably robust against the violation of the ionospheric spherical symmetry assumption. We found no convincing evidence for both, highly asymmetric ionospheric conditions and high ionisation levels, that these do systematically degrade the RO retrieval performance, especially if *inverse covariance weighting optimisation* with prior background profile search is applied.

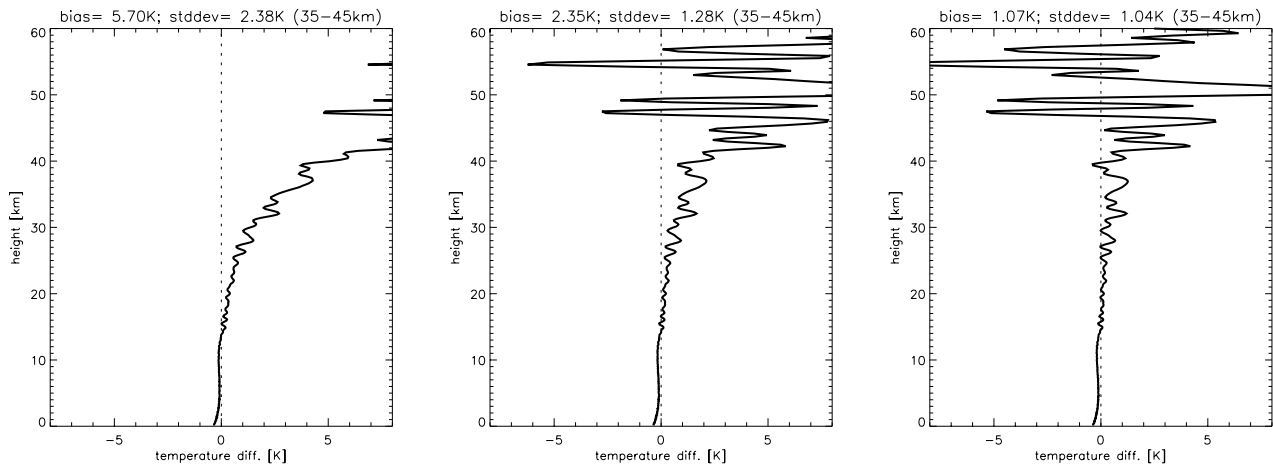


Figure 6: Temperature error of the “nasty 1” occultation event. $F_{10.7}=70$; quasi-realistic receiving system. Left: *no optimisation*. Middle: *inverse covariance weighting optimisation* with co-located background. Right: *inverse covariance weighting optimisation* with background search. At the top of each panel, the upper ionosphere bias and standard deviation is quoted.

Figure 6 also demonstrates the effect of the search algorithm: The middle panel shows the temperature error profile for the *inverse covariance weighting* retrieval without search, while the right panel shows the same retrieval with search. The discrepancy between the two error profiles exemplifies the importance of good quality background data: Though the error of the background profile used in the middle panel, compared to the “true” profile (which we know from the forward model), is $< 8\%$ in the stratosphere and mesosphere (i.e. clearly within the assumed uncertainty of 20%), the effect is a marked degradation of retrieval performance in the upper stratosphere, compared to the optimisation case with search. This is due to the fact that the background error is not, as theoretically assumed, bias-free. The no-search approach yields an upper stratosphere bias of 2.35 K , while the search-approach reduces the bias to the 1 K level.

5. ADVANCEMENTS IN STATISTICAL OPTIMISATION

As mentioned above, the statistical optimisation approach is limited to bias-free observation and background data. This assumption is more or less valid for the observation (due to the self-calibrating nature of RO measurements), but frequently violated by the background data. The search algorithm, as presented in section 4, is a first step of empirical bias correction, but rigorous testing of this algorithm showed that there are some geographical regions where no unbiased background profiles can be found in the MSIS90 climatology (see, e.g., Figure 2; observational error south of 60°S latitude). One way to cope with this problem is further sophistication of the background bias correction. (Another pathway would be to look for different background data. We will briefly address this topic in the concluding section 7.) Following the considerations above, we designed an advanced background bias correction scheme:

- 1) Optimisation and stabilisation of the search algorithm by smoothing (0.4 km sliding average) the observed bending angle profile prior to the search. This is done since it can be assumed that the ionospheric correction works well for the broadband-features of the bending angle profile. Search interval: $45 - 65\text{ km}$.
- 2) Additional bias correction by linearly fitting the searched background to the smoothed observation between $55 - 75\text{ km}$. Empirical tests showed that this region is especially sensitive for detecting remaining background biases. A similar approach was suggested by Gorbunov (2002), though that approach uses a different height interval and no background search.
- 3) Considering the reduced background bias, the background error was set to 15% (instead of 20%) of the background bending angle profile. Different relative errors from 5% to 20% were also tested empirically resulting in an optimal value of 15% .

6. RESULTS

The enhanced RO retrieval algorithm as described in section 5 was tested using a large sample of quasi-realistically simulated occultation events. For sake of simplicity and comparability with prior results, we

utilised the GNSS-CLIMATCH sample, (i.e. ECHAM4 fields in the forward model, see section 2). This sample consists of ~ 1000 occultation events that characterise the summer season 1997 (June, July, and August) and are evenly distributed in time and space. The whole sample was separated according to latitude resulting in 17 equal area bins, each extending over 10° and containing 50 – 60 occultation events. Figure 7 shows a latitude-height plot of the temperature observational error E^{obs} which is defined as:

$$E^{obs} = \left[\left(E^{bias} \right)^2 + \left(E^{stddev} / \sqrt{N} \right)^2 \right]^{1/2} \quad (5)$$

where E^{bias} is the mean error, E^{stddev} is the standard deviation and N is the number of observations for each grid point (17 latitude bins). The left panel shows the retrieval results of the basic algorithm as described in section 3 (*inverse covariance weighting approach* with background search, this algorithm was also applied in the GNSS-CLIMATCH study), the right panel shows the result of the enhanced *background bias correction algorithm* as described in section 5. (The better results of the basic algorithm as compared to the GNSS-CLIMATCH results (see Figure 2) in the troposphere are due to a more exact treatment of the satellite orbits in the forward model and not related to the retrieval; this topic is not discussed here.)

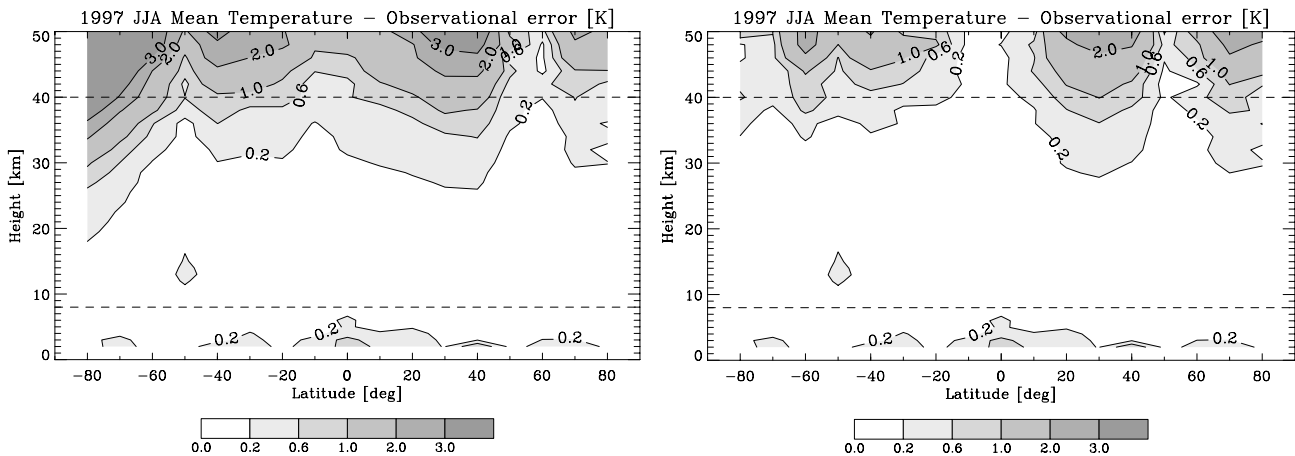


Figure 7: Observational error of the mean temperature in the 1997 summer season (June, July, August). Left: *Inverse covariance weighting retrieval* with background search. Right panel: *Inverse covariance weighting retrieval with enhanced background bias correction*.

The most prominent achievement of the enhanced background bias correction algorithm is the drastic error reduction in the so far most problematic regions, i.e. the southern high latitudes. This is due to the additional bias correction by linear fitting, which can be regarded as an emergency reserve of the algorithm: In most cases the fit yields a very small coefficient and the amount of the background bias correction stays below 1% of the original profile. However, in some cases when no unbiased background is available, the correction can amount to 10%. This is a rather drastic correction, but it is necessary to compensate for biases in the background climatology. A less eye-catching but nevertheless existing further benefit is the general improvement of the retrieval above 30 km in almost all cases.

7. SUMMARY, CONCLUSIONS AND OUTLOOK

The ability of RO measurements to provide valuable data for climate monitoring is claimed frequently, but has not been tested in a rigorous way yet. First results of the GNSS-CLIMATCH study, which is especially designed to do such test, are encouraging (total temperature error < 0.6 K in most regions) but also show a lack of retrieval performance in high altitudes (above ~ 35 km) and in the polar winter region. Concerning the high altitude problem, first results from the CHAMP mission, where the retrieved temperature bias exceeds 1 K above ~ 20 km, point to the same direction. The results of a study designed to evaluate high altitude RO retrieval performance showed that the retrieval biases are correlated to biases in the background data used by the statistical optimisation approach (which is vital to obtain good-quality RO data at high altitudes), while the ionospheric correction of bending angles is remarkably robust under varying and extreme ionospheric conditions. Considering this, we developed a method of background bias correction that proved to be very effective, especially in the so far most critical regions. We currently prefer this enhanced background bias correction scheme using an independent climatology (MSIS90) to the use of NWP analysis fields since we safely avoid to introduce an eventual high altitude bias of the analysis fields into RO observation. Moreover,

the validation of RO retrievals using analysis fields as background needs care to ensure independency of these background from validation analyses. We aim at further developing the presented RO retrieval scheme focusing on problems in the lower troposphere and at using it to realise RO based global climatologies of temperature, humidity, and geopotential height, starting with RO data from CHAMP.

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