Final results of the DFG funded project “Development of a tomographic water vapour sounding system based on GNSS data”

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Summary:
Since 2008 a group of scientists of the Leipzig Institute of Meteorology (LIM) and the German Research Centre for Geosciences Potsdam (GFZ) develops a method to derive water vapour profiles out of continuously available GNSS data (Global Navigation Satellite System).
The aim of this project - supported by the Deutsche Forschungsgemeinschaft (DFG) - was to develop a processing system with related scientific algorithms, which uses data of regional GNSS ground networks to derive 3D water vapour distributions above these stations. This systems use the line of sight water vapour information from each ground station to every GNSS satellite in view (slants) as basis of a 3D tomographic reconstruction.
At this time these reconstructions are based on GNSS data of about 330 German or near Germany located groundstations. This leads to a horizontal resolution of the reconstructed 3D water vapour field up to 40km and a vertical resolution of about 0.5km from the upper part of troposphere down to the atmospheric boundary layer (1km height).

Zusammenfassung:
Seit 2008 befasst sich eine Arbeitsgruppe von Wissenschaftlern am LIM und dem GFZ in Potsdam im Rahmen eines DFG-geförderten Projektes mit der Ableitung von dreidimensionalen Wasserdampfverteilungen in der Atmosphäre aus Beobachtungsdaten regionaler GNSS-Bodennetze (Globale NavigationsSatellitenSysteme). Die Wasserdampfverteilungen können aus der atmosphärischen Information entlang der Sichtlinien zwischen den Bodenstationen und den sichtbaren GNSS-Satelliten (sogenannte Slants) berechnet werden. Diese zahlreichen Sichtlinien ermöglichen eine tomographische Verarbeitung der Daten. Der entwickelte tomographische Algorithmus nutzt derzeit bis zu 330 deutsche und nahe Deutschland gelegene GNSS-Stationen, was eine horizontale Auflösung der resultierenden 3D-Felder von 40km und einer vertikalen Auflösung von 0,5km bis hinab zur atmosphärischen Grenzschicht (bis 1 km über dem Boden) ermöglicht.

1. Introduction
1.1. Motivation

The Global Positioning System (GPS) has nowadays many applications used in daily life. An increasing number of GPS applications requires dense networks of GPS ground receivers all over the world and induced the development of the European Galileo programme, the Chinese Compass programme as well as the renewal of the Russian GLONASS. Precise positioning applications of these GNSSs (Global Navigation Satellite Systems) require atmosphere corrections in order to remove the impact of the lower atmosphere and especially the water vapour on the GPS signal and the position. These corrections contain valuable information on the atmospheric state and are the basic input for several applications of theGNSS meteorology or GNSS atmosphere sounding.
The GNSS water vapour tomography makes use of the atmosphere corrections applied to each individual transmitter—receiver link (slant). Each signal path from a GPS satellite to a ground receiver “scans” a different part of the atmosphere and provides information integrated along the signal path. A very large number of such observations can be used to reconstruct the atmospheric state by means of tomographic techniques.
This project was started to set up a continuously running GPS based water vapour sounding system for Germany. Currently, about 270 German and 60 other GPS stations provide ~1.2 millions of observations per day, each covering a different region of the atmosphere. Humidity fields with a spatial resolution of about 40 km horizontally and several hundred meters vertically can be reconstructed from these observations every 15-30 minutes. The tomography system is now in a semi-operational state and can run in near real-time as part of the GPS processing system or be used to reconstruct user defined periods of time with various parameters. GPS slant delays are operationally available since 2007 and this large data set was used to obtain a large number of humidity fields which cover Germany and parts of adjacent countries. The results were validated using independent observations such as radiosonde profiles, the line of sight integrated water vapour observed by water vapour radiometers and analyses of numerical weather models.

1.2 Initial questions and objectives

GNSS observations provide information on the spatial distribution of water vapour in the atmosphere. Such information is essential for high resolution numerical weather models, now-casting or hydrological applications but can currently not be provided by any existing observation system. Therefore, several attempts have recently been made to reconstruct spatially resolved humidity fields from GNSS slant delay data by means of the GNSS tomography. Within this project a GNSS tomography system for Germany was developed which completes the existing GNSS processing system at the GFZ. Utilizing the operationally available slant observations of about 330 stations it was investigated if the quality of the slant data and the information provided by this kind of observations, i.e. quantities integrated along the signal paths, is sufficient to obtain reliable spatially resolved humidity fields for Germany. These questions are closely related to the mathematics of inverse problems as an ill-posed inverse problem needs to be solved.

The first part of this project was related to GNSS data processing and quality assessment. The GNSS slant data are estimated by a rather complicated processing chain which provides no reliable error estimates (Gendt et. al, 2004). Validation with independent observation, e.g. from water vapour radiometers or analyses of numerical weather models, was therefore an important task.

In the second part the tomography software was extended in order to combine the slant delays with additional observations and to compare several reconstruction techniques. A large number of tomographic reconstructions with various combinations of parameters was carried out in order to investigate their impact on the results: Initialization, combinations of input data, the reconstruction algorithm, the spatial resolution of the grid, the temporal resolution, etc., can change the results considerably, especially as an inverse problem is solved which is very sensitive to small variations in the input data and the parameters.

The third task was to estimate the quality of the reconstructed humidity fields and to provide error estimates. This was done by comparing the results with radiosonde profiles and model analyses. Complementary information on the inversion quality could be obtained from the resolution matrix which provides a mathematical tool for validation. Reliable tools for quantifying the reconstruction quality would have been required to answer the questions in the previous paragraph.

Altogether, the potential of a future operational GNSS tomography system was to be assessed.

2. Results

2.1. GNSS data processing

The operational GNSS processing system running at the GFZ provides hourly files of zenith total delays (ZTD), the integrated water vapour (IWV), slant total delays (STDs) and other geodetic and meteorological products. An additional tool developed in the first phase of this project separates the slant hydrostatic delay (SHD) and the slant wet delay (SWD) and is also running operationally (Bender et. al, 2010)

Currently, about 330 stations are processed in near real-time (NRT), ~270 of them are located in Germany. These stations provide more than 1000 ZTD/IWV observations and 50000 – 60000 STD/SWD observations per hour. During this project 5 years (2007-2011) of NRT GPS data were processed and are now available for tomographic studies.

In parallel to this project the COPS data reprocessing was finished. The COPS/GOP GPS reprocessing covered the whole year 2007 and is up to now the largest dataset available, containing data from about 450 French and German stations including the densified network in the COPS region. (COPS, Convective and Orographically-induced Precipitation Study and its GOP (Global Observation Period) is reported in Crewell, et al 2008, see also https://www.uni-hohenheim.de/cops/)

The EPOS (Earth Parameter and Orbit Determination System) GNSS processing system is used at the GFZ. EPOS was developed at the GFZ and is continuously updated. The major improvements were described in the progress report (Ge et al., 2005). The quality of the meteorological EPOS products is operationally monitored within the E-GVAP-project (EUMETNET GPS Water Vapour Programme). Comparisons with other processing centers and the HIRLAM weather model (http://www.hirlam.org) can be found on the E-GVAP webpage: http://egvap.dmi.dk.

2.2. Validation of slant delays

The validation of slant delays, i.e. the signal delay along the path from the GPS satellite to the GPS receiver, is a demanding task as very little observations are available: Most observation systems are not aligned to a certain GPS satellite and do not provide slant delays. It is therefore necessary to interpolate or project the available observations on the satellite-receiver axis and to convert between different physical quantities. This has been done in the water vapour radiometer (WVR) validation studies.
Another approach is to use analyses of numerical weather models which provide all information necessary to compute the different contributions to the slant delays:
Of the moisture (Slant Wet Delays, SWD)
Of the hydrostatic dry atmosphere (Slant Hydrostatic Delay, SHD)
Or to the sum of these (Slant Total Delay, STD).
However, the signal path through the model field is not known but must be estimated from the refractivity field between the satellite and receiver position. First studies with COSMO fields (Bender et al, 2008) showed that the slant delays are systematically overestimated at lower elevations if a straight path is assumed. The real bended signal path can be estimated by using Fermat's Principle, e.g. using a variational approach. Such a raytracer (Zus et al., 2012) was applied to ECMWF analyses of several years and used to estimate a huge amount of slant delays for the German GPS stations (Brecht et al., 2011). For COSMO (Consortium for Small-scale Modeling) see http://www.cosmo-model.org.

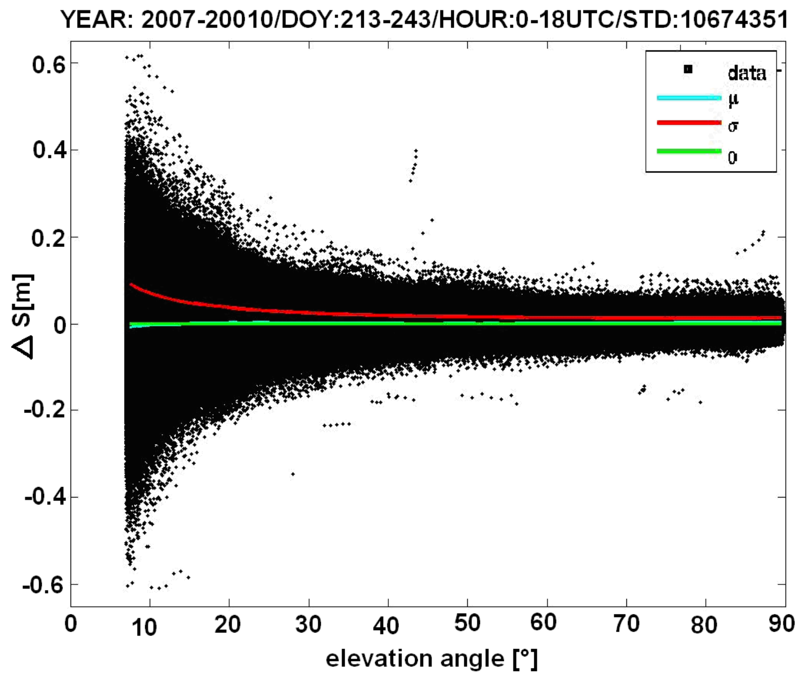
2.3. Validation using water vapour radiometers

A WVR with satellite tracking capabilities was acquired by the GFZ in order to obtain WVR observations exactly along the satellite-receiver axes. The radiometer is now available but, unfortunately, it was not possible to take a sufficient number of observations and to analyse the data before the end of this project.
Therefore, the analysis of the COPS observations provided by the University of Cologne was used.
In the first part of the project (Progress Report, 2009) GPS and WVR observations were compared only if they coincide both in time and direction, i.e. azimuth and elevation. With these criteria only between ~4000 and ~10000 SWV observations could be compared within three months, i.e. 30-100 observations per day at different elevations. Another approach was therefore chosen which utilizes the information provided by the continuous radiometer hemisphere scans. Assuming that the atmosphere does not change significantly within the 10 minutes required to perform a full hemisphere scan the WVR observations can be interpolated on the GPS SIWV (Slant Integrated Water Vapour). Using a linear interpolation within observations neighbored in time, azimuth and elevation, about 230000 SIWV observations could be compared which is approximately 50 % of all GPS observations available. This large

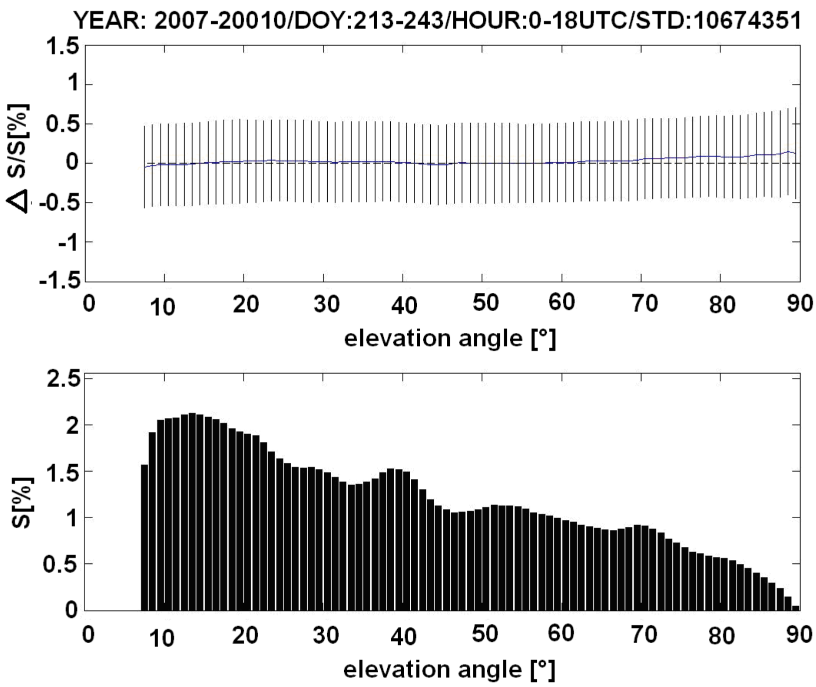
data set was analysed in order to identify possible deficiencies in the GPS slant processing strategy. The GPS and WVR data agree in general very well: Regarding all data a bias of 0.4 kg m^{-2} was found indicating that the WVR detects somewhat more humidity than GPS. The standard deviation is 1.9 kg m^{-2}, increasing from 1.3 kg m^{-2} near the zenith up to 3.0 kg m^{-2} at lower elevations between 14.4° and 25.2°. The relative difference is almost constant with a slightly falling trend at lower elevations. Regarding the uncertainties due to the STD→SIWV conversion and the interpolation of the WVR data which add to the original STD observation error this indicates that the quality of the GPS observations is increasing with decreasing elevations.
The comparison described above was repeated for different methods to separate the SWD from the STD in order to find the best strategy. It turned out that the method suggested by Runge et al. 1996 leads to the best agreement for the whole period.
In further studies the correlation of the GPS-WVR differences with the atmospheric humidity and atmospheric gradients as detected by the WVR azimuth scans was investigated. No such correlations could be found. However, the time series of GPS and WVR observations show periods of nearly identical observations followed by periods of large and almost constant differences. So far no correlations with pressure, temperature or relative humidity could be found and further investigations would be required.

2.4. Validation using weather model analyses

The European Centre for Medium-Range Weather Forecasts (ECMWF) provides model analyses every 6 hours at 0, 6, 12, 18 UTC. Four years (2007-2010) of these analyses were used to validate the corresponding STD observations from the German GPS stations. A raytracer was used to estimate the bended signal path through the model atmosphere for each observed STD (Zus et al., 2012) and the model STD was computed by integrating the refractivity along this curve. The differences between the observed and model STDs were analysed in various ways: Statistics for each whole year, seasonal statistics, day-night comparisons, daily and monthly statistics, etc., were computed. A typical result for the month August is shown in Fig. 2. The bias between model and observations is small and almost independent from the elevation, the standard deviation σ increases with decreasing elevations but the relative σ is almost constant. The latter is a very important result for the GPS tomography: The error per unit length or the error per grid cell is almost constant if the relative σ is not varying with elevation and the uncertainty of the tomographic reconstruction is not affected by using STDs at low elevations. The absolute numbers of the bias and σ vary somewhat for different months or days but in general model and observations agree very well (Zus et al., 2012, Deng et al., 2011).
These results also indicate that the assimilation of STDs into numerical weather models could have a positive impact on weather forecasts. Especially slants at low elevations should provide information on the vertical humidity structure.



a)



b)

Fig. 1: *Differences between observed and computed STDs for the month August in the years 2007-2010. The absolute STD differences in meters for about* $10{\cdot}10^6$ *slants observed within the 4 months (a) show an almost constant bias for all elevations and a standard deviation increasing from ~10 mm near the zenith up to ~80 mm at an elevation of 7°. The relative standard deviation in % (b, top) is almost constant 0.5 % at all elevations. The GPS satellite constellation leads to very few STDs near the zenith but an increasing number of observations at lower elevations (b, bottom).*

2.5. Tomography

During this project a quasi-operational GPS tomography system was developed and tested (Bender et al., 2011). The tomography system was designed to reconstruct spatially resolved fields of the refractivity N, the wet refractivity Nwet (shown also in Fig. 2) or the absolute humidity from a large number of STDs, SWDs or SIWVs, respectively. The numerical solution requires a spatial grid which can be adapted to dimensions of the GPS network and defines the spatial resolution of the reconstruction. Several techniques were implemented to solve the ill-posed inverse problem: Several modifications of the algebraic reconstruction techniques (ART) are available to solve the large set of linear equations iteratively, e.g. MART, DART, SIRT (Subbaro et al., 1997). A damped weighted least-squares solution (Tarantola, 2005) was implemented which is basically matrix algebra but is complicated by the large sparse matrices which have to be inverted. A third option is a Kalman filter. Additional observations can be used to stabilize the inversion: Point observations such as synoptic data, profiles provided e. g. from water vapour radiometers or radiosondes or integrated observations like WVR-SIWV data or GPS-IWV data. The tomography can be initialized in different ways: Simple exponential profiles, standard atmospheres, horizontally interpolated and vertically extrapolated synoptic data (Troller et al., 2006), COSMO analyses/forecasts or the previous inverted field can be loaded. The tomography software was supplemented with several tools for visualizing the STD data entering the tomography and the reconstructed humidity fields, for monitoring the reconstruction process and for simulating STD data based on satellite orbits, station coordinates and fields provided by numerical weather models (COSMO, ECMWF).
The above mentioned reconstruction techniques can be used with different parameters: The initialization, different combinations of input data, the reconstruction algorithm, the spatial resolution of the grid, the temporal resolution, etc., was varied systematically. A large number of reconstructions was carried out for the subsequent validation studies. One set of reconstructions was based on a limited number of reference data and epochs resulting in one humidity field for each parameter set. These humidity fields should be rather similar and can easily be compared. Another set was computed for long time series up to one month consisting of 700 – 3000 single fields. These data were used to investigate the temporal variations of the reconstruction quality and to test the behavior of a future operational tomography system. The results were investigated carefully: After a first visual inspection a validation with radiosonde (RS) profiles was started.
Almost all results belong to two categories:
1) The inversion process is divergent and the results are obviously useless.
2) The inversion converges and leads to reasonable humidity fields with some artifacts.
Unfortunately, no results were found which were clearly superior. In the 2. case it was very difficult to quantify the reconstruction quality of the whole 3D fields. Lots of different parameters lead to results of comparable quality and it was almost impossible to identify an optimal combination of parameters. A simulation study (Bender et al., 2011) was started in order to eliminate the impact of observation errors and to have a reference field for the validation. Furthermore, GLONASS and Galileo observations

were also simulated for investigating the impact of additional GNSS. Even with the reference field being available it was difficult to estimate the reconstruction quality.
A different approach was to compute the resolution matrix which provides more insight to the inversion process. The approximate data resolution matrix (influence matrix, hat matrix) could be computed from the intermediate results of the ART algorithms. This matrix describes the impact of individual observations on the result. Some influence matrix properties could be computed, e.g. the global observation influence which describes the impact of the observations with respect to the background impact (background = initialization). It was found that the impact of the observations is between 80% and 90%. More interesting would be the model resolution matrix which describes how a hypothetical true state is mapped to the estimated state by the kernel matrix. The estimated state parameters are a weighted function of the true state parameters and the model resolution matrix describes what can be expected in an ideal case if a certain kernel matrix is given. To compute the model resolution matrix the generalized inverse is required. Unfortunately, this is not computed by the inversion algorithms and approximate solutions are required. It turned out that this task is equally demanding as the inversion itself. Attempts were made to obtain approximate solutions but the results were rather instable and much more work would be required to finish this task.

2.6. Validation of tomographically reconstructed humidity fields

The validation of tomographically reconstructed humidity fields with independent observations is not only required to estimate the errors of the results: To decide which set of parameters leads to the best tomographic reconstruction it is necessary to quantify the quality of different results. Therefore a set of radiosonde (RS) profiles observed by the 12 operational German RS stations in 2007 was compared with the corresponding tomographically reconstructed profiles. Tomographic reconstructions were generated for each day of the year at 0:00 UTC and 12:00 UTC in order to provide tomographically reconstructed data for each RS profile. As the spatial grid used by the tomography had a rather small horizontal resolution of 30 – 50 km the grid columns were interpolated to the RS station coordinates. In total two sets of 6803 profiles at 12 stations were available for the comparison. The details of the validation study can be found in Shangguan, et al., 2013.

2.6. Complexity of quality assessment

After a first analysis of different comparisons it turned out that the quality of the humidity fields could not be quantified in a consistent manner. A standard statistical analysis providing, e.g., mean differences and their standard deviations, leads to rather meaningless results. These quantities look rather promising if a sufficiently large number of profiles are compared but they are not really significant if the observations are taken from profiles which do not represent the real vertical structure of the atmosphere. The same is true for error estimates computed for specific altitude intervals.

It was therefore necessary to compare entire profiles instead of isolated observations at different altitudes. Several parameters were defined to identify similar profiles and to quantify the degree of similarity. With this strategy it was possible to identify a subset of rather similar profiles and another subset of obviously deviating profiles. Unfortunately, there remains a majority of profiles which show sequences of good agreement together with severe discrepancies. A visual inspection of the profiles shows at least two types of problems:

1) The tomography tries to modify the initial profiles in order to minimize the discrepancies but the STD observations are insufficient to finish this process. The result is a combination of the initial profile and partial distortions by the observations.

2) Another class of profiles shows rather strong artifacts at different altitudes leading to unreliable profiles.

Both problems are related to the sparse observations which are used to solve an ill-posed inverse problem. To summarize, it was not possible to develop a validation tool which was sensitive and reliable enough to distinguish between tomographic reconstructions obtained with different parameter sets.

First tests with profiles or horizontal layers taken from numerical weather models (COSMO, ECMWF) lead to similar or even more severe problems as more observations were available. It was therefore decided to concentrate on the RS validation study.

Detailed results of the quality assessment with RS observations are given in Shangguan et al., 2013. To summarize, the results of this validation study show that the tomographic inversion is able to provide reliable profiles with some minor artifacts as long as sufficient STD observations are available. In cases of insufficient observations the results become unpredictable and are in many cases worse than the initial profiles. It must be pointed out that the observations regarded here as „sufficient“ are in general not anywhere near the quality usually required by tomographic methods. In general each voxel must be observed from a wide angular range but in case of GPS tomography even the best profiles are based on very incomplete data with lots of empty voxels and other voxels observed only from very few narrow angles.

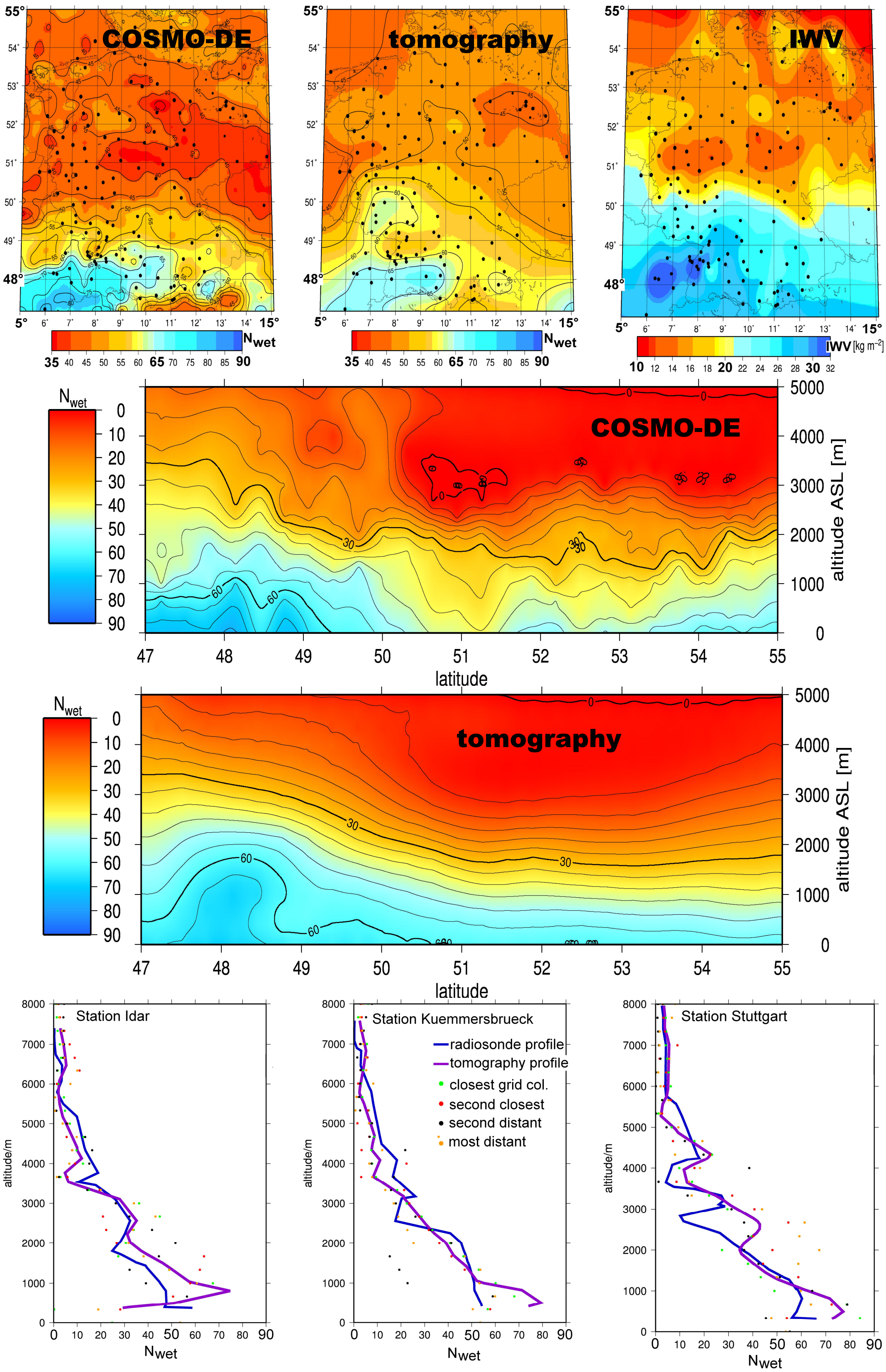


Fig. 2: *8.7.2007, 12:00 UTC – Results of the tomographic reconstruction (using N_{wet}), horizontal layer at 676 m (top), vertical slice (center) and comparison with radiosonde profiles (bottom). COSMO-DE fields and radiosonde profiles are shown.*

Regarding the rather limited number of observations which already leads to profiles of good quality the results of this study are very promising. These results are based on parts of the humidity fields which are really a result of the tomography. Regions with no observations or very few STD data were separated and not used in the validation study. The criteria defining regions with almost no observations, regions of insufficient data and regions of presumably sufficient data can later be extended to confidence parameters which can be provided together with the tomographically reconstructed humidity fields.

3. Outlook

The results of this project demonstrate that slant total delays (STDs) provided by GNSS processing systems contain valuable information about the spatial water vapour distribution in the atmosphere. The realized STD validation studies show that GNSS STDs and similar observations from other observation systems correspond within the errors of both systems. However, regarding specific stations or special periods of time there are also discrepancies and the processing of STDs could be improved.

The validation showed that the GPS observations present sufficient information to reconstruct 3D humidity fields of good quality as long as all parts of the atmosphere are “scanned” by GPS signal paths. Currently, this is the case only for limited regions and periods. The number and distribution of GPS observations does not yet cover all parts of Germany at all times. Rather large unobserved regions affect the quality of the results and more stations and satellites would be required by an operational GPS tomography system.
The number of satellites is already increasing as GLONASS, Compass and Galileo will soon be available. Beyond that attempts must be made to densify the GNSS networks as the resolution of the reconstructed humidity fields is limited by the interstation distances.

The validation of the tomographically reconstructed humidity fields shows that the currently available STD data and inversion algorithms are not yet sufficient to guarantee stable and reliable results. None of the techniques so far used in the field of GNSS tomography leads to superior results. Equally important as the reconstruction algorithm is the exact form of the forward operator. The results could be improved by replacing a simple operator based on voxels of constant refractivity by a smoothing operator which interpolates the refractivity on the signal path. The smoothing operator does not only lead to better humidity fields but has also a stabilizing effect on the whole inversion procedure.

The reasons for the somewhat ambiguous results are obvious: A visualization of the slant paths in the atmosphere clearly shows that there are at all times large parts of the atmosphere which are not covered by any observations. For geometrical reasons this is especially true for parts of the lower atmosphere up to altitudes of ~3 km. The basic requirements of a stable tomographic reconstruction are therefore not satisfied and the quality shows considerable temporal and spatial variations. Under these conditions the results are surprisingly good.

To improve the results two different strategies should be followed:
1) More data are required which cover all parts of the atmosphere more homogeneously.
2) Advanced adaptive inversion strategies need to be developed which can deal with the highly variable GNSS observations.
More GNSS satellites will be available in near future: GLONASS observations are already available, Compass and Galileo observations will follow in the next 5 years, leading to more than 100 GNSS satellites. However, more dense GNSS networks would also be required, especially to improve the situation in the lower part of the atmosphere but also to increase the resolution of the reconstructed fields which is limited to approximately the mean station distance. Within this project the data available from existing geodetic stations were utilized. In order to obtain nationwide 3D humidity fields with a quality comparable to existing humidity profilers or radiosondes efforts must be made to extend the GNSS networks for meteorological applications. This could lead to a unique humidity observation system with a much higher spatial resolution than any existing system and with real-time capabilities.
Advanced inversion strategies to retrieve optimal information from the available STD data and to provide reliable error estimates need to be developed in cooperation with mathematicians specialized on inverse problems. Adaptive techniques have been proposed which transform the given inverse problem into an optimal form which can be solved in the best way.

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