Deriving atmospheric water vapor and ozone profiles from active microwave occultation measurements

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ABSTRACT

The GPS/MET experiment was the first active atmospheric microwave occultation experiment using the existing GPS L1 and L2 frequencies to measure the atmospheric refractive index. One major limitation to this technique is that the presence of water vapor in amounts typically found in the lower troposphere (below 5-7 km) causes an ambiguity between the contributions of dry air and moisture to the refractive index. Additionally the profiles of other gases, such as ozone, cannot be measured using the L1 and L2 frequencies.

A new satellite remote sensing technique to independently monitor atmospheric water vapor and ozone is under development. It will include small satellites with both transmitter and receiver capabilities on each. The frequencies will be located around the 22 and 183 GHz water vapor and the 195 GHz ozone absorption lines. The receivers will also have the capability to observe the L1 and L2 GPS frequencies.

Simulation studies show that this new active occultation technique has the potential to provide accurate profiles of water vapor and ozone, as well as refractivity, temperature and pressure.

Keywords: Atmospheric remote sensing, active microwave occultation, water vapor, ozone, temperature, pressure.

1. INTRODUCTION

Studies of planetary atmospheres using the active radio (microwave) occultation technique have had a history of more than 4 decades1. Working together with other observation techniques, radio occultations have greatly enhanced our knowledge of temperature, pressure, and composition of the planetary atmospheres in the solar system2. Recognition that the technique could be applied to the Earth using the Global Positioning System3 (GPS) led to the GPS/MET (GPS/Meteorology), a satellite-to-satellite remote sensing project. GPS/MET was designed to be a proof-of-concept experiment, demonstrating the feasibility of remotely sensing the earth’s atmosphere by means of active microwave occultation using the GPS. This project, sponsored by several U. S. federal agencies, placed a specially designed GPS receiver on-board a small research satellite, Microlab-1, which was launched into a low earth orbit (LEO) in April 1995. Over the next two years, data from about 70,000 globally distributed occultations were collected and archived, from which thousands of accurate and high-resolution profiles of atmospheric refractive index, temperature, pressure, and density have been derived from near the ground to ~40 km height4-7. The vertical resolution of these profiles range from several hundred meters in the lower troposphere to ~1.5 km in the upper stratosphere, and the horizontal resolution is about ~300 km8. With the present 24 GPS satellites, one LEO satellite can, in principle, observe some 500 occultations each day. Given its features, such as high accuracy, all-weather, round-the-clock operation, and long-term stability, GPS occultation remote sensing has the potential to improve weather analyses and to monitor climate and climate change. It is a new and precise sounding technique for the earth’s atmosphere in the 21\textsuperscript{st} century. It is also an important complement for the more conventional passive remote sensing sounders, such as the AIRS/AMSU (Atmospheric Infrared Sounder/Advanced Microwave Sounding Unit) and the MLS (Microwave Limb Sounder).

The major observables in GPS/MET are the phases of the GPS radio signal carriers L1 (1.57542 GHz) and L2 (1.22760 GHz). From the phase measurements it is possible to determine the bending angle of the radio ray because of atmospheric refraction9. In turn, the index of refraction can then be derived from the bending angle under the assumption of a locally spherically symmetric atmosphere10.
The dependence of refractivity on pressure, temperature, and partial pressure of water vapor is given as

\[
N = 77.6 \frac{P_d}{T} + 71.7 \frac{P_w}{T} + 3.73 \times 10^5 \frac{P_w}{T^2},
\]

where \(N\) is the refractivity, and \(P_d\), \(P_w\), and \(T\) denote the dry air pressure, water vapor pressure, and temperature, respectively. By definition, \(N = (\mu - 1) \times 10^6\), where \(\mu\) is the atmospheric index of refraction. In the lower troposphere, the refractivity can have a significant contribution from both the dry air pressure and the water vapor pressure. As a consequence, it is not possible to retrieve atmospheric water vapor from the GPS occultation measurements unless combined with additional observations or Numerical Weather Prediction (NWP) model analysis results\(^{12, 13}\). The accuracy of moisture derived in this manner is limited to about 0.2 g/kg\(^{13}\). Combining the GPS observations with analyzed temperature and moisture fields to improve the accuracy of the analyzed fields within a least-squares optimization framework has been discussed by several authors\(^{14-17}\), and is an active area of research. However, neither of these techniques provides sufficient accuracy to sense the radiatively-important upper tropospheric moisture, nor gives much information in the colder parts of the troposphere in general.

Today, monitoring of the global distribution of atmospheric water vapor from the surface through the tropopause remains one of the outstanding problems in atmospheric remote sensing. This is a top priority for climate and global change research, meteorology, and the study of the global water and energy cycles. Another outstanding issue is the distribution of global ozone, particularly the tropospheric ozone distribution. Ozone is not only an important greenhouse gas but also the only atmospheric constituent that can effectively absorb soft ultraviolet solar radiation, thereby protecting terrestrial life on the earth. At present, remote sensing techniques for observing tropospheric ozone are inadequate.

In the mid-1990s, groups at the University of Arizona and Jet Propulsion Laboratory (JPL) began looking to extend the radio occultation technique to address these issues by utilizing higher frequencies that are partially absorbed by certain atmospheric constituents. With frequencies between 10 GHz and 23 GHz and around 183 GHz, it would be possible to accurately retrieve water vapor from the lower stratosphere down to the ground. With additional frequencies near 195 GHz, accurate profiles of tropospheric and stratospheric ozone can also be obtained.

In early 1999, ATOMS (Active Tropospheric Ozone and Moisture Sounder) was selected as one of the NASA’s Instrument Incubator Programs (IIP). Besides utilizing the existing GPS frequencies, ATOMS will develop technologies for frequencies up to 200 GHz for moisture and ozone soundings using the occultation technique. It will provide important new atmospheric data sets for use in climate, climate change, meteorology, and a variety of other earth science disciplines.

2. ATOMS – THE ACTIVE TROPOSPHERIC OZONE AND MOISTURE SOUNDER

2.1 ATOMS Science Objectives

ATOMS’ main products are: (1) water vapor profiles throughout the troposphere and lower stratosphere, (2) ozone profiles between ~8 km and ~40 km, (3) atmospheric refractivity, temperature, pressure, and geopotential heights. Combining nearby occultation measurements, the gradient wind field may also be derived from the horizontal gradients of the geopotential height field. The GPS occultation observations will also provide measurements of the satellite-to-satellite total electron content from which it is possible to retrieve the electron density in the ionosphere.

These data may be useful to characterize the present climate, study processes in the climate system, and detect the climate system’s response to a variety of external forcings, such as increased greenhouse gas concentrations, variations in solar irradiance, and forcings-of-opportunity including volcanic eruptions and large scale fires. The data will also have broad applications in meteorology, space weather, and geodesy. The potential of these data for improving weather prediction may, in turn, lead to the long-term continuation and expansion of the constellation by operational weather services.

2.2 The ATOMS Constellation

The concept of the ATOMS cross-link occultation experiment for global profiles of atmospheric ozone and moisture is outlined in Fig. 1. The ATOMS baseline mission calls for 12 small LEOs in two nested arrays of six planes each (Fig. 2). The satellites, in circular orbits at 700 and 850 km altitudes, will have both transmitting and receiving capabilities and will
make two kinds of observations: (1) GPS L-band signal phases and amplitudes; (2) LEO-to-LEO cross-link signal phases and amplitudes.

Assuming a 12-microsatellite constellation, approximately 6,000 GPS occultations and 1,500 cross-link occultations could be realized each day. Fig 3 shows the global distribution of the 1,500 cross-link occultations. The uniformity of the distribution depends on the different altitudes and phasing of the two sub-arrays.

2.3 ATOMS Measurements

As mentioned, ATOMS observes both the phases and amplitudes at the cross-link frequencies. The LEO-to-LEO cross-link amplitude measurements are drawn schematically in Fig. 4. Radio signals at these cross-link frequencies are partially absorbed by atmospheric water vapor and ozone. The fractional reduction of amplitude after passing through the atmosphere is directly related to the water vapor pressure or ozone concentration along the signal paths. Consequently, water vapor and ozone profiles can be obtained from the cross-link amplitude measurements.

2.4 Selection of the ATOMS Cross-Link Frequencies

The correct choice of cross-link frequencies is of crucial importance for ATOMS. Below 200 GHz, there are two water vapor absorption lines at 22.235 and 183.310 GHz and many ozone lines with the strongest at 195.430 GHz. Radio signals at these frequencies experience a certain amount of absorption when they pass through the atmosphere at different heights. After taking many factors into consideration, we preliminarily selected several frequencies in the ranges 179.0–182.0 GHz, 22.20–22.21 GHz, and 9.5–17.3 GHz for upper, middle, and lower tropospheric water vapor retrievals, respectively. For stratospheric and tropospheric ozone, frequencies in the range 192.0–195.42 GHz have been tentatively selected.

Occultation transmittances at several frequencies are plotted in Figs. 5 and 6 using the MODTRAN standard atmospheric model. In these figures, altitude refers to the tangent height (or perigee) of the ray path. Fig. 5 is for ozone transmittances, while Fig. 6 is for water vapor transmittances. Fig. 6 illustrates that one cannot use a single frequency, say 182.0 GHz, to cover water vapor distribution from the upper troposphere to the lower troposphere, because below ~10 km the atmosphere is virtually opaque at this higher frequency. Kinks on the water vapor transmittance curves in Fig. 6 at 1.5 km and 3.5 km are caused by a cloud layer added to the atmosphere model used here.

3. SOUNDING ATMOSPHERIC MOISTURE AND OZONE FROM ACTIVE CROSS-LINK OCCULTATION

Retrieval of the atmospheric refractive index and related parameters using the radio occultation technique has previously been described in detail by many authors. We describe here the principles of the cross-link ozone and moisture retrievals, assuming the index of refraction profile $\mu(r)$ has already been derived from the cross-link phase measurements. As in the refractivity retrieval, a spherically symmetric atmosphere is assumed.

3.1 Occultation Optical Depth from the Cross-Link Amplitude Measurements

Let $I_0$ denote the (hypothetical) intensity at the cross-link frequency $f_i$ received by the receiving satellite in the absence of the atmosphere, and let $I_i$ denote the actual intensity received at the same frequency. Then

$$\tau_i = -\ln\left(\frac{I_i}{I_0}\right)$$

(2)

where $\tau_i$ is the occultation optical depth at frequency $f_i$. This optical depth can be further decomposed as

$$\tau_i = \tau_{ai} + \tau_{ci} + \tau_{ui} + \tau_{di}$$

(3)

where $\tau_{ai}$, $\tau_{ci}$, $\tau_{ui}$, and $\tau_{di}$ are the component optical depths at frequency $f_i$ due to the absorption agent (water vapor or ozone), clouds, atmospheric aerosols, and the atmospheric defocusing effect, respectively. ATOMS will measure cross-link signal
amplitudes at two closely adjacent frequencies, \( f_i \) and \( f_j \), so that to a good approximation, \( \tau_{\omega i} = \tau_{\omega j} \) and \( \tau_{\omega u} = \tau_{\omega v} \). On the other hand, by the choice of the frequencies close to an absorption line—where the absorption strongly varies with frequency—we in general have \( \tau_{\omega i} \neq \tau_{\omega j} \) and \( \tau_{\omega u} \neq \tau_{\omega v} \). Therefore, after rationing the intensities of the signals at such two adjacent frequencies, \( \tau_{\omega i}, \tau_{\omega j}, \tau_{\omega u}, \) and \( \tau_{\omega v} \) cancel out, leaving

\[
\Delta \tau = \tau_i - \tau_j = \ln \left( \frac{I_j / I_{\omega j}}{I_j / I_{\omega j}} \right) = (\tau_{\omega u} + \tau_{\omega v}) - (\tau_{\omega u} + \tau_{\omega v}).
\]

(4)

The optical depth difference \( \Delta \tau \) is then used in the following water vapor or ozone retrieval computations.

### 3.2 Derivation of Water Vapor and Ozone Volume Absorption Coefficients

We define the atmospheric volume absorption coefficient \( k_i \) at frequency \( f_i \) as the optical depth per km, such that

\[
\tau_i = \int_{path} k_i \, ds,
\]

where \( ds \) is an element of length along the curved ray path, and \( \tau_i \) is the total optical depth along this path. For water vapor the volume absorption coefficient is generally a function of temperature \( T \), dry air pressure \( P_d \), water vapor pressure \( P_w \), and cloud liquid water content \( C_w \), while for ozone it is related to the temperature, total atmospheric pressure \( P = P_d + P_w \), and ozone number density \( n_o \). If the difference in absorption coefficients at adjacent frequencies \( f_i \) and \( f_j \) is \( \Delta k = k_i - k_j \), the corresponding optical depth difference is \( \Delta \tau = \tau_i - \tau_j \) via eq. (5). Using the Abel transform 23, \( \Delta k \) can now be computed from \( \Delta \tau \),

\[
\Delta k(r_p) = \Delta k(x_p) = \frac{\pi}{dx} \int_{x_p}^{\infty} \frac{d\Delta \tau}{dx} \frac{dx}{\sqrt{x^2 - x_p^2}},
\]

(6)

where the integration variable \( x(r) = \mu(r) \times r \). The variables \( \mu \) and \( r \) are the index of refraction and the radial distance from the local center of curvature of the earth. The subscript \( p \) indicates the variable is to be evaluated at the ray perigee point. Equation (6) is similar to the formula employed by Jenkins et al. 24, except that we use the differences of the absorption coefficients and the optical depths rather than the absorption coefficient and optical depth themselves.

As mentioned earlier, the absorption coefficients are known functions of \( T, P_d, P_w, C_w, n_o, \) and \( f_i \). For water vapor,

\[
k_i = F(T, P_d, P_w, f_i) \quad \text{(clear sky case)},
\]

(7a)

and for ozone,

\[
k_i = F(T, P_d, P_w, C_w, f_i) \quad \text{(cloudy sky case)},
\]

(7b)

In eq. (8), \( A_1 \) and \( A_2 \) are constants depending on the ozone absorption line, and \( f_{ic} \) is the line center frequency such as 195.430 GHz for ozone’s \( \text{14}_1 \rightarrow \text{14}_0 \) transition 18. The pressure broadening is \( \Delta f = W P T^{-0.5} \), and \( W \) is a constant that may be experimentally determined 25, 26. For accurate retrieval of water vapor, we need to take into account water vapor and oxygen absorption as well as background absorption. The explicit forms for eqs. (7a) and (7b) are therefore rather lengthy and complicated, and will not be given here. The detailed description for the absorption due to water vapor and oxygen for frequencies below 1000 GHz is given by Liebe (1989) 27.

### 3.3 Retrieval of Water Vapor
For the water vapor retrievals, we distinguish the clear sky case (no clouds) from the cloudy sky case. In the clear sky case there are 3 unknowns, i.e., temperature $T$, dry air pressure $P_d$, and water vapor pressure $P_w$. In the cloudy case, we have one additional unknown, the cloud liquid water content, $C_w$.

In the clear sky case, generally ~183 GHz and ~22 GHz are used to cover the 12-18 km altitude range and the 7-12 km range, respectively. With the already known refractivity $N$ and the volume absorption coefficient difference $\Delta k$ we now solve for $T$, $P_d$, and $P_w$, using eqs. (1), (7a) (with frequencies $f_i$ and $f_j$), and the hydrostatic equation,

$$\frac{d(P_d + P_w)}{(P_d + P_w)} = - \frac{g dz}{RT}.$$  \hspace{1cm} (9)

Here $g$ and $z$ are the gravitational acceleration and the altitude, respectively, and $R$ is the gas “constant” for moist air, which changes with height due to the variation in water vapor content.

In the lower troposphere frequencies between 10 and 17 GHz are used. Because of the possible cloud liquid water content, $C_w$, three frequencies must be used in order to generate two absorption coefficient differences. Then we solve for $T$, $P_d$, $P_w$, and $C_w$, using eqs. (1), (9), and (7b) written separately for each frequency.

3.4 Retrieval of Ozone

For ozone retrievals, two slightly different frequency pairs near the 195 GHz ozone line are employed: one pair for profiles in the upper stratosphere, and another for profiles in the lower stratosphere and upper troposphere. The ozone retrievals are relatively simpler than the water vapor retrievals because after the water vapor retrievals have been completed, $T$ and $P$ become known. Thus, one may directly solve eq. (8) for the ozone concentration $n_o$.

4. SIMULATED RETRIEVAL RESULTS

Simulation studies with and without measurement errors have been conducted for 6 atmospheric models. Using the MODTRAN atmospheric model, a refractivity profile is first computed and optical depth data is then simulated by integration of eq. (5) at the cross-link frequencies under the assumption of spherical symmetry. The retrievals are then performed as described in the previous section. Without random noise and measurement errors, the simulated retrieval results are virtually perfect. Adding noise to the simulated data results in errors in the retrievals shown in Fig.7-10. We display these using only the MODTRAN standard atmospheric water vapor and ozone models. A cloud layer between 1.5 and 3.5 km was added to the water vapor model. Results using other MODTRAN models look similar to those presented here. In all figures, 0.5% Gaussian random noise was added into the refractivity data and 0.4% Gaussian random noise was added into the optical depth data.

Figs. 7 and 8 are water vapor and temperature retrieval errors. For the water vapor retrieval, several frequencies were used: ~182 GHz for 9.5 – 18 km, ~22 GHz for 4 – 9.5 km, and 10-17 GHz for 0 – 4 km. The sudden changes of the retrieval errors at the transition altitudes can be attributed to the frequency switching at these heights. Above ~14 km altitude the water vapor retrieval error rapidly increases with altitude. This is because above this altitude water vapor pressure is very low (see Fig. 9) resulting in very little water vapor absorption even at 182 GHz. Below ~3.5 km the errors become larger again because, at far off-center frequencies (~10 GHz), the ratio of dry air absorption to water vapor absorption gets larger and the water vapor absorption spectrum gets rather flat. The r.m.s. water vapor retrieval errors are about 5.7% from 0 to 3.5 km and about 4.9% from 4 to 14 km. Temperature retrieval errors plotted in Fig. 8 are generally less 0.5% except below 3.5 km. The (standard) models and retrieved water vapor and temperature profiles are plotted in Figs. 9 and 10 for direct comparison.

The ozone simulation results are shown in Figs. 11 and 12. Two frequency pairs around the 195 GHz ozone line were employed: a pair near 195.4 GHz for 30 – 45 km and a pair near 195.3 GHz for 8 – 30 km. Below 10 km, the ozone retrieval error quickly increases as altitude decreases. This is because the ratio of ozone density to air density, related to the ratio of ozone absorption to air absorption, is rapidly reduced, resulting in a much weaker signal. The model and retrieved ozone profiles are plotted in Fig. 12 for comparison.
The retrieval results described in the previous section seem promising and demonstrate that the principles, the selected cross-link frequencies, and the data analysis procedures of ATOMS work well under the conditions assumed here. These simulation studies, however, should be considered preliminary because they did not include all aspects of the ATOMS cross-link sounding technique. More research, involving theoretical studies as well as software and hardware development is needed and is now in progress at the University of Arizona and JPL.

The ATOMS Instrument Incubator Program will take technology development through breadboarding and possibly limited field-testing. We are looking towards balloon and perhaps orbiting satellite opportunities for real and complete validation of the technique. Our eventual goal is to attain the full science potential of an ATOMS-based mission with a dozen or so micro-satellites. Such a system may be dedicated for this purpose or perhaps piggy-backed onto another satellite constellation such as SBIRS-Low (Space-Based Infrared System-Low), or onto scientific systems like COSMIC (Constellation Observing System for Meteorology, Ionosphere and Climate). One concept under evaluation for NASA’s Post-2002 Basic Measurement Set is the “OP-3” radio occultation mission whose baseline consists of 8-16 micro-satellites carrying both GPS and cross-link sounders. Although we cannot say now how these developments will play out, the prospects for a suitable array of host platforms in the foreseeable future are rich indeed.

REFERENCES


Fig. 1  The concept of ATOMS radio cross-link occultation at 10 – 200 GHz for obtaining precise global profiles of atmospheric ozone and water vapor by observing signal attenuation and phase. All satellites are identical and have both transmitting and receiving capabilities.

Fig. 2  ATOMS’ two 6-satellite arrays at 700 and 850 km with 65° inclination make up the constellation.
Fig. 3  Typical one-day cross-link occultation coverage with a 12-satellite constellation.

Fig. 4.  ATOMS observes amplitude changes caused by signal absorption to sense ozone and moisture.
Fig. 5 Occultation transmissions around the 195 GHz ozone line.

Fig. 6 Occultation transmissions between 10–182 GHz.

Fig. 7 Simulated ATOMS crosslink water vapor retrieval error (%)

Fig. 8 Simulated ATOMS crosslink temperature retrieval error (%)
Fig. 9  Water vapor profiles: model and retrieved.

Fig. 10  Temperature profiles: model and retrieved.

Fig. 11  Simulated ATOMS crosslink ozone retrieval error (%).

Fig. 12  Ozone profiles: model and retrieved.