SH_2OUT

Sensing of H_2O in the Upper Troposphere
A mission concept to improve prediction of climate change

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Summary

We recommend an infrared solar occultation mission to measure simultaneously vertical profiles through the upper troposphere and lower stratosphere of H_2O and HDO in the tropics and subtropics. These measurements will constrain which are the dominant mechanisms regulating the abundance of water in these critical regions of the Earth's atmosphere and improve model parameterizations that are perhaps the biggest source of uncertainty in predicting climate change. This concept will address two of the themes identified in the NRC Decadal Study:

Climate Variability and Change:

Mission Concept and Advances to Earth Science

Understanding the global water cycle is vital to understanding and predicting climate change. In particular, the comparatively small amounts of water in the tropical and sub-tropical upper troposphere (UT) have a disproportionate impact on climate: the vapor phase acts as a strong greenhouse gas while the ice phase (cirrus) can reflect solar radiation. Climate prediction is complicated by competing feedbacks of temperature and water vapor, and the sensitivity of phase changes to the cold temperatures typical of the UT. An accurate understanding and quantification of the transport mechanisms of the UT water cycle are essential to the predictive skill of global change models, but such mechanisms are not well understood, quantified or parameterized. Simultaneous measurement of H_2O and its isotopologue, HDO, is exceptionally sensitive to the cycles of hydration, dehydration and transport as the D/H ratio acts as a "thermodynamic fingerprint" of the different processes controlling water. A properly designed solar occultation mission will capture the spatial and temporal gradients of the isotopic ratios well enough to improve representation of water vapor transport in general circulation and climate models and improve prediction of climate change.

The D/H ratio of water (as found by simultaneous measurement of H_2O and HDO, and usually described as a depletion†) can be an excellent discriminator between competing processes as it has a different sensitivity to temperature depending on phase. For example, in the gradual pseudo-adiabatic uplift of air from the lower to upper troposphere, HDO vapor is precipitated out at a rate proportionally faster than H_2O. In this case, by the time a parcel reaches the TTL, water vapor is nearly depleted in deuterium (some 80% less D in water than that in the ocean, that is, $\delta D \approx -800‰$) On the other hand, if the TTL is hydrated from ice rapidly uplifted in a convective tower, δD is relatively unaffected because the isotopologues are locked in the ice particles. Thus, the δD of water vapor provides a fingerprint of these processes, as suggested by airbourne *in-situ* measurements shown in Figure 1. Co-located measurements of short-lived tropospheric source gases

† Isotopic ratios are generally reported in the standard δ notation, in parts per thousand (‰). For isotope X, $\delta X = 1000*(R/R_0 - 1)$, where R is the measured isotopic ratio in the sample of interest and R_o is that ratio is standard mean ocean water. If a sample had 50% less HDO than mean ocean water, it would be described as $\delta D = -500$ ‰.

such as CO (also in Figure 1), HCN, C_2H_2 and C_2H_6 can provide information on the "age" and mixing history of the air.

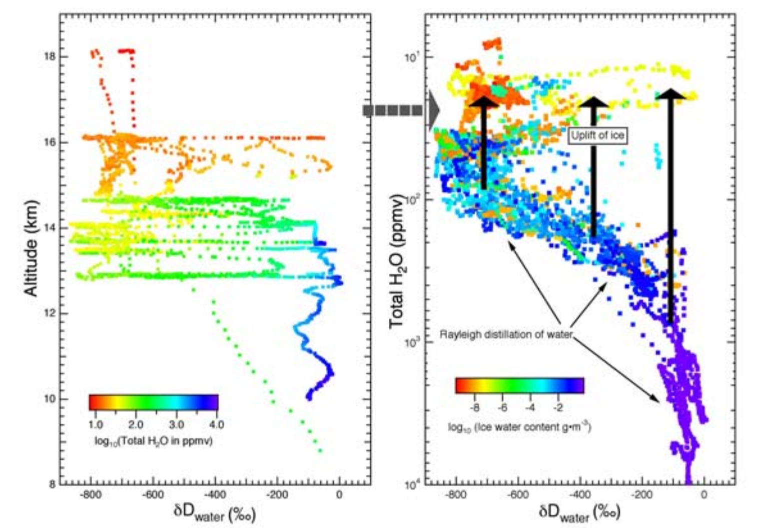


Figure 1: δD results from JPL ALIAS measurements (Chris Webster, P.I.) on board the WB-57 aircraft during flights of July 26 and 28, 2002 [*Webster and Heymsfield*, 2003]. The left panel shows δD on the horizontal axis as a function of altitude, while the right panel shows δD as a function of total water. The color scale represents measurements of CO by M. Lowenstein.

A variety of mechanisms may be responsible for the mixing of moisture between altitudes, and across latitudes to the subtropics, greatly impacting the radiative balance. Mechanisms include formation/evaporation of liquid and ice particles, convective updrafts and fallout, and lateral transport; these can leave different signatures on δD depending on their temperature regimes and phase changes. In addition, there are intraseasonal and interannual variations in UT δD, and these variations will provide insight into variations in hydrology, and thus climate. Measurements of the isotopic makeup of water can therefore provide strict tests for current and future hydrology and climate models: a successful model must not only quantify H_2O properly, it must also do so for HDO.

Current state of knowledge

No global (or even tropical) survey of upper tropospheric HDO currently exists, although there have been numerous measurements from a variety of platforms from the 1970's until the present, including balloon, rocket, aircraft, and remote sensing measurements from the Space Shuttle. The ACE instrument, on board the Canadian SCISAT platform, can measure HDO, but is in an orbit optimized for measurement at high latitudes where seasonal variation is believed to be minimal (see below). Recent aircraft measurements discussed in *Webster and Heymsfield* [2003] as well as *Gettelman and Webster* [submitted, 2005] have shown a wide dynamic range in UT δD, but the limited spatial and temporal extent of these observations do not allow constraints on the relative importance of convection and large scale motions in controlling the water vapor concentration of the tropical tropopause layer.

A number of two- and three-dimensional models now include water vapor isotopes. The GISS GCM, ECHAM GCM, and other include these important isotopes. Figure 2 illustrates three-month averages at 14.5 km from a year's run from the GISS GCM, provided by Gavin Schmidt of NASS GISS. Significant regional and seasonal variation in δD can be seen throughout the tropics and subtropics. Noting that small changes to entrainment rates in convective plumes may have a small impact on the climate simulation, but a

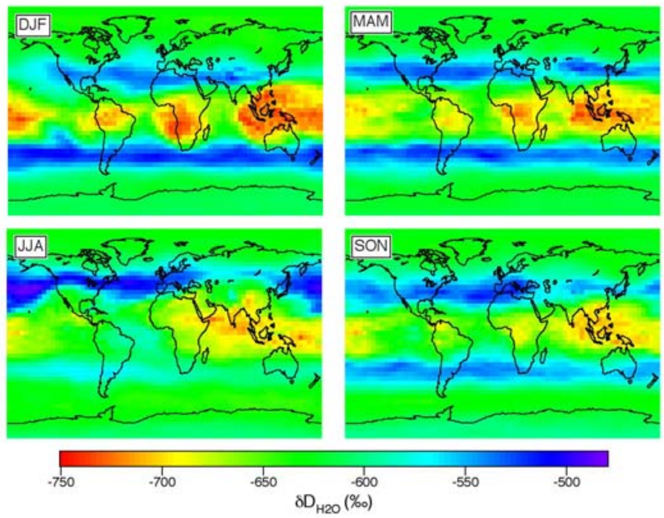


Figure 2: Seasonal averages for δD from GISS GCM control run at 14.5 km.

significant effect on the isotopes, *Schmidt et al.* [2005, submitted] argued that that water isotope measurements can aid in the validation of model parameterizations.

Mission Concept

A mission of solar occultation measurements with a high-spectral resolution Fourier transform infrared (FTIR) spectrometer is well-suited for measuring vertical profiles of water and its isotopologues, and provide significant data for the development of GCMs and climate models. Furthermore, such a mission can measure short-lived tracers of boundary-layer origin which, as described below, can help in determining the origin and age of air masses, again aiding model development. FTIR technology is a flight-proven technique for monitoring trace gases, and we discuss the design of a solar occultation mission that could meet science requirements.

The required features of a measurement valuable for understanding water vapor in the TTL are high precision and accuracy, vertical resolution of 1 to 2 km, and sufficient sampling to capture the spatial and temporal features in HDO appropriate for comparison with GCMs. While a variety of remote sensing techniques have some capability for measuring the HDO/H_2O ratio, their sensitivity, cooling requirements, and calibration differences present different challenges or limitations. Nadir measurement techniques tend to have overly broad vertical resolution, or lack sensitivity in the near-tropopause region. Limb viewing in emission has significant tradeoffs between integration times, signal-to-noise and vertical resolution. While solar occultation instruments will not have as many viewing opportunities within an orbit as emission instruments, it uniquely allows for high vertical resolution (on the order of 1 to 2 km) along with high precision on HDO measurements. A cartoon of the observation geometry is shown in Figure 3. Calibration is easier as telluric spectra can be ratioed to exo-atmospheric spectra, removing instrument and solar residuals, thus producing pure atmospheric absorption spectra. With a carefully selected orbit, sampling could be focused on the climatologically important water vapor in the tropics and subtropics, with enough measurements to provide comparative data to GCMs.

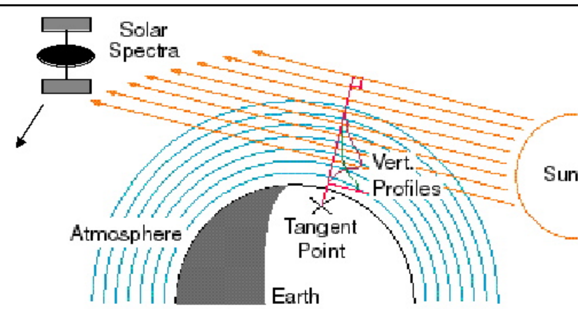


Figure 3: Geometry of solar occultation remote observation.

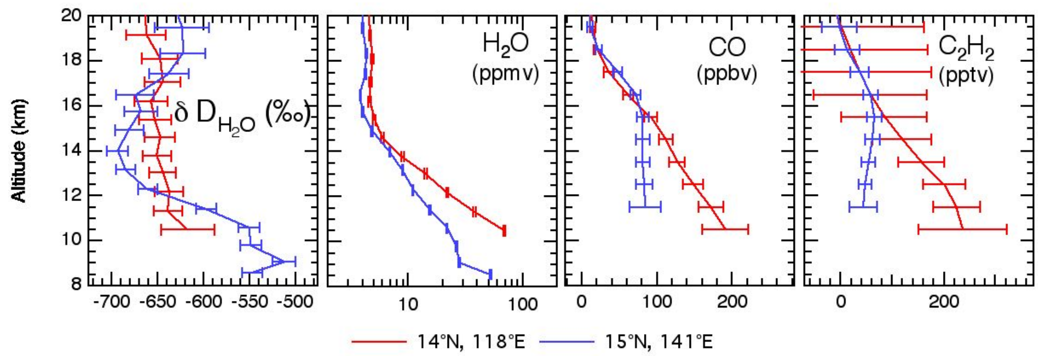


Figure 4: ATMOS tropical observations near the Intertropical Convergence Zone from the ATLAS-3 shuttle flight of November, 1994. The left panel shows depletion of D in water while the others are retrievals of gas mixing ratios. These observations were made using different spectral filters, which affect their error bars. Note that as the scan time of ATMOS was ~2.2 seconds, these measurements have a vertical resolution of ~4km. Depletion and H_2O data are from *Kuang et al.* [2003]. CO and C_2H_2 data are from *Irion et al.* [2002].

Fourier transform infrared (FTIR) spectroscopy is well suited to capture the wide dynamic range of H_2O and HDO lines and absorption depths throughout the mid- to upper-troposphere, where concentrations of vary by orders of magnitude. In addition, FTIR spectrometry can detect "dynamic tracers" which can be brought to middle and upper tropospheric levels from the boundary layer by convective events (see, for example, *Thompson et al* [1997]). Measurement of species such as C_2H_2, C_2H_6 and CO can be quite useful in analyses as these molecules have short but differentiated atmospheric lifetimes. For example, C_2H_2 has a shorter lifetime than CO; a low ratio of C_2H_2/CO generally indicates "old" air, while a high ratio indicates younger air recently brought up from the boundary layer. FTIR remote spectroscopic measurement of H_2O, HDO and dynamic tracers has been achieved in flight using the Atmospheric Trace Molecule Spectoscopy (ATMOS) instrument on the Space Shuttle. Figure 4 illustrates some retrievals of δD_{H2O}, H_2O, CO and C_2H_2 by ATMOS.

Measurement requirements and capabilities of solar occultation

A flowchart showing the science drivers for technical choices is given in Figure 5. A study has been performed assuming the following instrument and mission characteristics:

(1) Medium inclination orbit (~38°) to maximize observation in the tropics and subtropics.
(2) 440 km circular orbit. This altitude is low enough to provide adequate time for enough scans during a sunrise or sunset (as seen from the satellite), but not so low as to seriously decay the orbit because of drag.
(3) 0.8 second spacing between scans. This is amenable to a flight-qualified 800 Mhz analog-to-digital converter for a 500K point interferogram and provide tangent observations less than 2 km apart–less than the scale height of water in the upper troposphere.

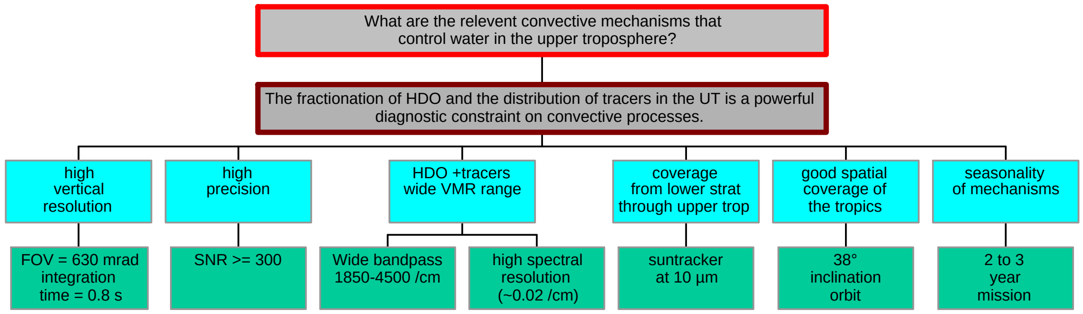


Figure 5: Flow chart of science and technical considerations for FTIR solar occultation measurement of δD in water.

(4) Signal-to-noise ratio of 300 and spectral resolution of 0.3 cm-1. This is reasonable considering current experience with solar occulation FTIR spectrometers and detector technology.

(5) 630 mrad field-of-view (equivalent to a ~1.5 km vertical footprint at the tangent point).

(6) A single InSb detector system (1850–4500 cm^{-1}). Note that expanding the bandpass by employing a two-detector system (say, by including a HgCdTe detector for the 600–1850 cm^{-1} range) would need a mechanical cooler to reduce the HgCdTe temperature to a required ~77 K and effectively double the telemetry load.

The study evaluated the potential of H_2O and HDO retrievals from such a mission to provide adequate validation to GCM climate analyses. Put another way, would such an instrument provide adequate coverage, precision and resolution to substantively validate and/or "tune" a GCM?

To assess the scientific value of potential year-round vertical profiles of the HDO/H_2O ratio, we sampled model data as a remote sensing measurement would. Year-long model runs were created by Gavin Schmidt of NASA GISS for this study [*Schmidt et al.,* submitted 2005]. The first, CONT, is a control model run using "non-entraining" plumes, acting as pure Rayleigh distillation columns. The other model run, ENT10, allows plumes to retain 10% of their mass. The GCM model data are on a 4° latitude by 5° longitude bins. Variables were converted to water mixing ratio and parts-per-mil depletion for HDO, and regridded to 1 km layers by assuming a 7km vertical scale height. Three-month average maps were created (DJF, MAM, JJA, and SON), with one set averaging all data in a grid box ("Cloudy" data), the second averaging only those grid-boxes above regions that had *any* cloud optical depth ("Cloud-filtered" data.) Note that this creates a pessimistic scenario for the observations a solar absorption IR spectrometer could potentially make, however a thin optical depth in the vertical (as in the model) can be much higher in the limb.

Considering that, in general, remote measurements are best suited for large-scale evaluations of UT moisture, several questions can be posed:

(a) Will the horizontal coverage and sampling frequency be adequate for comparison to GCM results?

(b) What are the vertical and horizontal resolutions and will they be adequate as well?

(c) Will the precision of the measurements be high enough to differentiate between different convective schemes?
(d) How will cloud-cover limit the observations and/or bias the comparison to GCM results?

We address these issues with feasibility study results in conjunction with results of the GISS GCM model.

Horizontal coverage and sampling frequency

Figure 5 illustrates seasonal averages for "control" results of the GISS GCM at 14.5 km. Overall, one expects significant seasonal and large-scale variability of HDO, as different convection mechanisms predominate depending on region and season. The tangent points for the occultations, shown for the March-April-May period in Figure 6, argue that the low inclination orbit is adequate to provide coverage to the parts of the globe that show varied δD throughout the year.

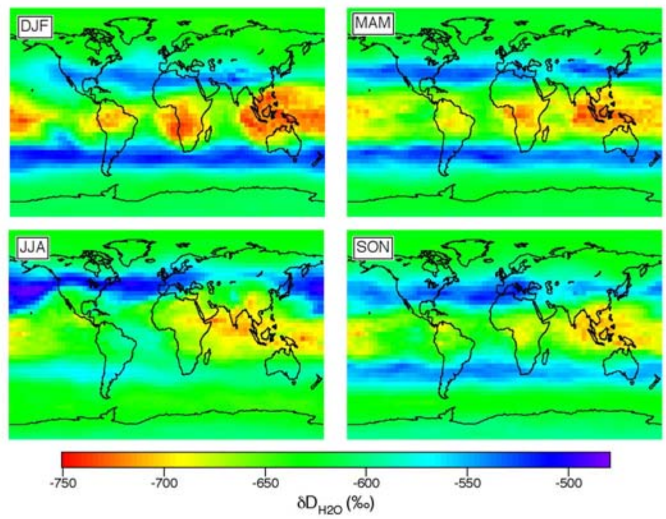


Figure 5: Seasonal averages for δD from GISS GCM control run at 14.5 km.

As solar occultation measurements are limited to 2 measurements per orbit, then for a 440 km orbit, 32 measurements per day could be achieved. In addition, when thick clouds are present, the sun tracker loses the ability to stay locked on the sun, and an occultation measurement may end. (We discuss the biasing this may cause below.) Figure 7 compares cloud-filtered "occultation sampled" results to model δD distributions over tropical Pacific during the different seasons over one year. The red lines show the distribution of δD for two model runs (discussed in detail below), while the blue lines illustrate results sampled from the model data as though they were sampled during a mission. In each case, the sampling is enough to capture the expected mean and standard deviation of the model results.

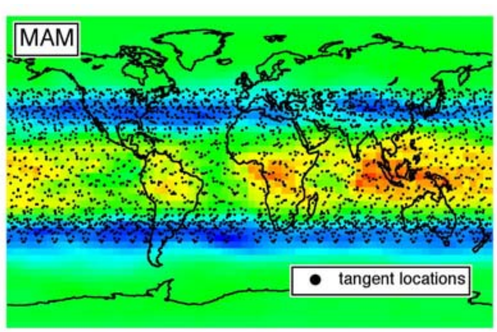
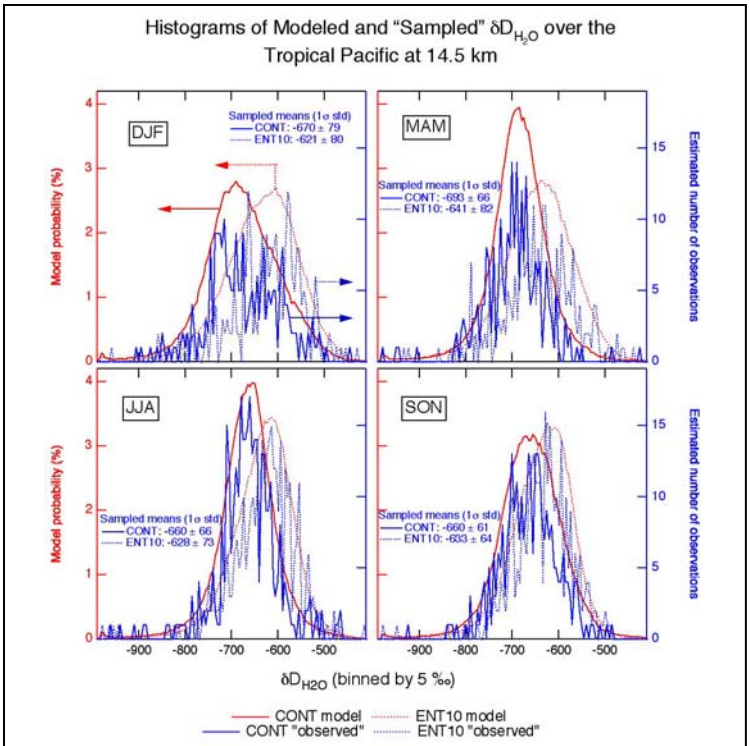


Figure 6: Occultation locations for the March-April-May timeframe.

Horizontal and vertical resolution

As the horizontal gradients in upper tropospheric water can be quite high, horizontal resolution is a key consideration in evaluating the utility of limb sounding for measuring water. As one sees through the atmosphere from the instrument through the tangent layer to the sun (see Figure 3), the horizontal resolution of a single measurement is tied to the vertical scale height of the gas concentration (which may not be the same as air.) Thus, for H_2O and HDO, the horizontal resolution improves below the tropopause because the vertical gradient in water concentration is steeper than that of air. Analyses of the limited aircraft "straight-leg" data available (not shown) indicate that reasonable agreement between limb sounding and in situ δD observation can be achieved provided the horizontal resolution of the limb sounder is better than 200 km. Calculations of the orbital slant paths indicate that the horizontal resolution for the proposed mission would be about to ~200 km at 17.5 km altitude decreasing to ~100 km at 10.5 km. These are roughly the same order-of-magnitude as horizontal resolutions in many current GCMs.



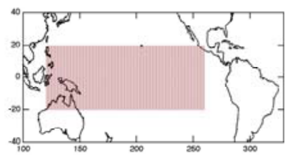


Figure 7: Modeled and "sampled" δD over the Tropical Pacific (right). The model probabilities (red lines) are on the left axis while the number of samples (blue lines) are on the right axis.

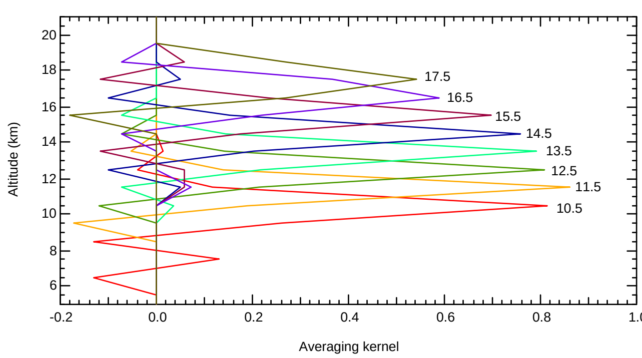


Figure 8: Averaging kernels for a synthetic HDO retrieval in the tropical troposphere. Altitudes for central layers are noted on the right. The kernels for H_2O would be similar.

Figure 8 illustrates averaging kernels for HDO assuming the instrument and mission parameters given earlier. Vertical resolutions are ~1.5 km at 10.5 km altitude increasing to ~ 2 km at 17.5 km. Thus 2 to 3 measurements may be made within the TTL for each occultation, clouds permitting. Again, these vertical resolutions are within the resolutions of current GCMs.

Measurement precision

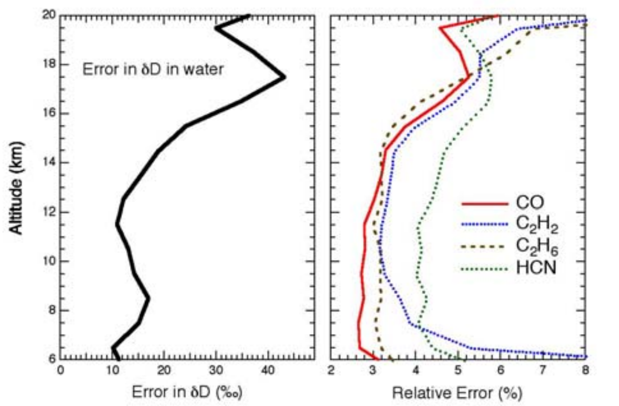


Figure 9: **Estimated retrieval errors.** Left panel – estimated per-mil error in δD assuming a signal-to-noise ratio of 300. Right panel – estimated relative error in CO, C_2H_2, C_2H_6 and HCN.

Figure 9 illustrates estimated retrieval errors for δD and the gas tracers using instrument parameters given earlier. Under clear sky conditions, for the InSb range, the expected precision for δD retrievals is ~20‰ at 10.5 km altitude, increasing to ~ 40‰ at 17.5 km. Decreasing the signal-to-noise ratio from 300 to 150 increases these errors by 10 to 20‰ HCN, C_2H_2, C_2H_6 and CO mixing ratios can be measured to a precision of about 3–6%.

Cloud-cover biasing

Figure 10 shows the effects of removing cloud-occluded data. The left panels show the (cloudy) CONT averages for DJF showing significant regional differences in the HDO depletion in the tropical regions from 10 to 16 km. The middle panels show significant, but localized, loss of observations due to clouds in the tropics at 10 and 12 km (regions of deep, convective clouds), losses of 0 – 60% at 14 km, and minor losses at 16 km. This is roughly consistent with experience with the ATMOS instrument on the ATLAS-3 shuttle mission, where about 90% of the occultations reached below 16 km, and about 50% of the occultations reached 10 km or lower. The right hand panels of Figure 6 are the difference of cloud-filtered to cloudy results, showing biasing at 10 km of –50 to 0 ‰ in the tropics, and 0 to +20 ‰ at mid-latitudes. Minor to negligible biasing is seen at 14 and 16 km. Thus, there is an expected observational bias compared to model results, mostly at altitudes below 14 km, so model results should be filtered for clouds when comparing with observations.

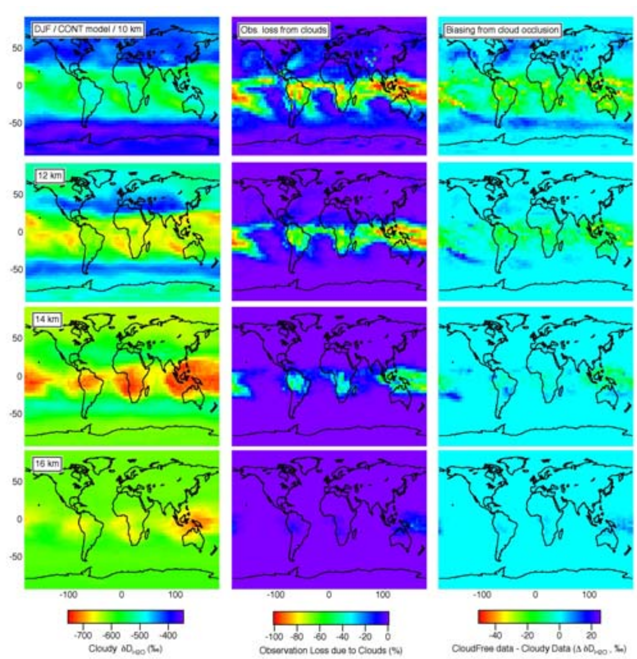


Figure 10: Average DJF control model results. The left panels show δD for a series of 1km thick altitude bins, middle panels show the fractional loss due to cloud occlusion, while the right panels show the expected observation biasing due to clouds.

Figure 7 shows histograms of the model and "observed" data for four seasons at one altitude in the tropical Pacific region. The ENT10 model run is in dashed red while the CONT model runs is shown in a solid red line. The blue lines show the distribution of depletions that would be observed by the candidate solar occultation mission, accounting for both frequency of sampling and the obscuring impacts of clouds. The difference in the average δD between the two models is greater than the expected error of the candidate solar occultation measurements, and the distribution of the solar occultation measurement is very similar to the model data, showing that the sampling of solar occultation is sufficient to capture the important isotope features. While the CONT and ENT10 "samplings" have overlapping standard deviations, the difference in the averages is statistically significant.

1. Rough estimate of total cost:

It is estimated that this would be a small mission, to build, launch, and operate for two to three years. The mission should cost less than 200M, with approximately 25% for launch, 25% for the instrument, 25% for flight system/spacecraft, and 25% for other aspects (science, ground data software, management, operations, etc). This estimate allows for 30% reserves on all aspects.

2. Criteria

This mission meets four of the prioritization criteria: contributes to important Earth science questions, identification as a high priority, is affordable, and uses flight proven technology and has a high degree of readiness.

The scientific contribution of this mission is to make global observations of upper tropospheric water vapor isotope mixing ratios, which are essential for quantifying the mechanisms for transporting water vapor to the upper troposphere, an important greenhouse gas.

The Implementation Plan For The Global Observing System For Climate has identified isotopes of water as an emerging essential climate variable for climate monitoring. Water vapor isotopes are not yet widely measured, but they are recognized as important variables in an area of emerging climate analysis.

This mission is affordable. The mission should cost on the order of 200M, with approximately 25% for launch, 25% for the instrument, 25% for flight system/spacecraft, and 25% for other aspects (science, ground data software, management, operations, etc). This estimate allows for 30% reserves on all aspects.

There is a high degree of readiness, as this mission builds on flight proven technology. The heritage of ATMOS, MkIV, and ACE contribute strongly to this concept. The new features of this mission are the use of higher speed ADCs and the selection of orbit that will allow for a focus on water vapor transport and climate. This mission concept has been thoroughly thought through and has a team of active supporters.

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