

Solar occultation satellite data and derived meteorological products: Sampling issues and comparisons with Aura Microwave Limb Sounder

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[1] Derived Meteorological Products (DMPs, including potential temperature, potential vorticity (PV), equivalent latitude (EqL), horizontal winds and tropopause locations) from several meteorological analyses have been produced for the locations and times of measurements taken by several solar occultation instruments and the Aura Microwave Limb Sounder (MLS). MLS and solar occultation data are analyzed using DMPs to illustrate sampling issues that may affect interpretation and comparison of data sets with diverse sampling patterns and to provide guidance regarding the kinds of studies that benefit most from analyzing satellite data in relation to meteorological conditions using the DMPs. Using EqL or PV as a vortex-centered coordinate does not alleviate all sampling problems, including those in studies using “vortex averages” of solar occultation data and in analyses of localized features (such as polar stratospheric clouds) and other fields that do not correlate well with PV. Using DMPs to view measurements with respect to their air mass characteristics is particularly valuable in studies of transport of long-lived trace gases, polar processing in the winter lower stratosphere, and distributions and transport of O₃ and other trace gases from the upper troposphere through the lower stratosphere. The comparisons shown here demonstrate good agreement between MLS and solar occultation data for O₃, N₂O, H₂O, HNO₃, and HCl; small biases are attributable to sampling effects or are consistent with detailed validation results presented elsewhere in this special section. The DMPs are valuable for many scientific studies and to facilitate validation of noncoincident measurements.

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1. Introduction

[2] The characterization of atmospheric observations by air mass properties, such as location with respect to the

stratospheric polar vortex or the tropopause, is an invaluable tool for research studies and validation. *Butchart and Remsberg* [1986] and *Lait et al.* [1990] mapped atmospheric trace gases with respect to potential vorticity (PV) and equivalent latitude (EqL, the latitude that would enclose

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the same area between it and the pole as a given PV contour, *Butchart and Remsberg* [1986]). This method is especially valuable in studies using solar occultation satellite data, which comprise no more than 15 profiles per day at each of two latitudes. *Manney et al.* [1999] used PV and EqL to enable detailed study of polar vortex dynamics and transport in ATMOS (Atmospheric Trace Molecule Spectroscopy) data from the ATLAS (Atmospheric Laboratory for Applications and Science) space shuttle missions; other studies of ATMOS, Halogen Occultation Experiment (HALOE), Polar Ozone and Aerosol Measurement (POAM) II and III, and Stratospheric Aerosol and Gas Experiment (SAGE) II and III data [*Schoeberl et al.*, 1995; *Randall et al.*, 2005, and references therein] have used EqL or PV to help realize the full “condition space” coverage of the sparse solar occultation data sets. Studies of limb-sounding data sets, such as the Microwave Limb Sounder (MLS) instruments on the Upper Atmosphere Research Satellite (UARS) and Earth Observing System (EOS) Aura missions, and the Michelson Interferometer for Passive Atmospheric Sounding, have also used PV or EqL mapping to study polar vortex dynamics and trace gas evolution [*Manney et al.*, 1995a, 2005a; *Orsolini et al.*, 2005b, and references therein].

[3] Air mass characterization also facilitates comparisons using measurements that are geographically sparse and may not fulfill traditional coincidence criteria based on close matching of time and location. *Santee et al.* [2007] and M. L. Santee et al. (Validation of the Aura Microwave Limb Sounder ClO measurements, submitted to *Journal of Geophysical Research*, 2007, hereinafter referred to as Santee et al., submitted manuscript, 2007) use EqL as a coordinate to compare Aura MLS data with Upper Atmosphere Research Satellite (UARS) MLS measurements taken in the 1990s. EqL and PV mapping have been used in studies of aircraft and ground-based observations [e.g., *Lait et al.*, 1990; *Redaelli et al.*, 1994]. *Manney et al.* [2001] used EqL mapping, standard geographical coincidence criteria augmented by PV matching, and trajectory histories to compare ozone from seven instruments during the November 1994 period of the ATLAS-3 mission, including four solar occultation instruments (ATMOS, HALOE, SAGE II and POAM II). PV or EqL can be valuable for profile comparisons, providing a means to eliminate comparisons of measurements that may be closely spatially coincident but in different air masses, or to maximize the number of coincidences by allowing comparison of spatially distant measurements taken in the same air mass [e.g., *Michelsen et al.*, 2002; *Lumpe et al.*, 2002b; *Chiou et al.*, 2004; *Randall et al.*, 2002].

[4] Several solar occultation data sets are available during the Aura mission, including HALOE, SAGE II and III, POAM III, and the Atmospheric Chemistry Experiment (ACE) Fourier Transform Spectroscopy (ACE-FTS) and Measurements of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation (MAESTRO) instruments. To facilitate noncoincident validation and intercomparison of measurements sorted by air mass characteristics, and for use in research studies combining Aura with solar occultation data sets, a set of “derived meteorological products” (DMPs) has been calculated for these solar occultation data sets; the DMPs consist of fields

derived from the meteorological analyses interpolated to the locations and times of the satellite observations. DMPs have also been calculated for Aura MLS version 1.5 (v1.5) and version 2.2 (v2.2) data sets; as well as contributing to validation and science studies, these are used in producing plots for routine inspection of MLS data, and daily EqL/potential temperature (θ) cross sections that are posted on the MLS Web site (<http://mls.jpl.nasa.gov>). In the following, we document the DMPs for the solar occultation instruments and MLS and use them for comparisons of solar occultation and MLS data. We explore effects of the satellites’ diverse sampling patterns, to provide guidance as to types of comparisons and scientific studies in which DMPs are most valuable. DMPs for MLS and/or solar occultation instruments are used in MLS validation in other papers in this special section [*Santee et al.*, 2007; also submitted manuscript, 2007]; DMPs have been used in several recent studies of solar occultation data, including validation comparisons [e.g., *Chiou et al.*, 2004; *Thomason et al.*, 2007] and scientific analyses [e.g., *Dufour et al.*, 2005; *Nassar et al.*, 2005; *Rinsland et al.*, 2005; *Jin et al.*, 2006b].

2. Data Set Descriptions

2.1. Solar Occultation Data Sets

2.1.1. ACE-FTS

[5] SCISAT-1, also known as ACE, was launched in August 2003 [*Bernath et al.*, 2005]. The primary instrument is the ACE-FTS, a Fourier transform spectrometer featuring high resolution (0.02 cm^{-1} , corresponding to a $\pm 25\text{ km}$ maximum optical path difference) and broad spectral coverage in the infrared ($750\text{--}4400\text{ cm}^{-1}$). ACE-FTS works primarily in the solar occultation mode, collecting atmospheric limb measurements using the sun as a radiation source. Version 2.2 of the ACE-FTS retrievals [*Boone et al.*, 2005] is used here, except for O_3 , for which the ACE-FTS product known as “version 2.2 ozone update” is used. Early validation efforts with the ACE-FTS data identified a roughly 10% low bias for altitudes near the O_3 concentration peak when compared to other satellite measurements, and a $\sim 25\text{--}30\%$ high bias near $45\text{--}50\text{ km}$ [*Walker et al.*, 2005; *Fussen et al.*, 2005; *Petelina et al.*, 2005]. Version 2.2 processing uses microwindows in two spectroscopic regions: $1000\text{--}1150\text{ cm}^{-1}$ and $1800\text{--}2150\text{ cm}^{-1}$. Version 2.2 O_3 update uses microwindows in the $950\text{--}1150\text{ cm}^{-1}$ range and, in preliminary comparisons, exhibits improved agreement with other data sets near the O_3 concentration peak; a comprehensive validation exercise for the ACE-FTS v2.2 O_3 update is being completed (E. Dupuy et al., Validation of ozone measurements from the Atmospheric Chemistry Experiment (ACE), submitted to *Atmospheric Chemistry and Physics*, 2007). ACE-FTS vertical resolution is $\sim 3\text{--}4\text{ km}$. Latitudes of measurements vary over an annual cycle with coverage as high as $\pm 85^\circ$ and an emphasis on the polar regions in winter and spring. Separate files with ACE-FTS geolocation information, primarily latitude and longitude as a function of altitude, are provided for each occultation; for occultations with missing geolocation files, the geolocation information is taken from the headers of the data files, which give 30-km tangent point latitude and longitude values; most differences

are small, but can be up to $\sim 3^\circ$ latitude and $\sim 10^\circ$ longitude for brief periods, depending on the viewing geometry. The data downlink capacity available for ACE early in the mission was ~ 2 Gb/d [Bernath et al., 2005], limiting the number of occultations that could be recorded; the downlink was increased in March 2005, and now almost all available occultations are measured during most of the year.

2.1.2. MAESTRO

[6] The MAESTRO instrument is the secondary instrument on the SCISAT-1 (ACE) payload. It comprises two miniature, photodiode array spectrophotometers designed to cover the wavelength range 285 to 1015 nm. O_3 slant column amounts are determined by spectral fitting of the data between 530 and 755 nm in the version 1.2 (v1.2) data set used here. Slant column amounts are inverted to produce vertical profiles of O_3 mixing ratio [McElroy et al., 2007]. MAESTRO slant column amounts are retrieved using pressure-temperature profile data and tangent height-time information from ACE-FTS. The vertical resolution of MAESTRO O_3 is ~ 1.2 km [Kar et al., 2007]. MAESTRO sunset profiles are very consistent with the ACE-FTS profiles except for a few percent from measurements taken between 2000 and 2400 UT. An analysis of the apparent altitude shift between these MAESTRO and FTS profiles indicates that there is a 1-s time shift during this period. The sunrise profiles have a time error increasing from 0 to 1 s between 0000 and 2400 UT. Since MAESTRO uses the FTS-derived tangent height tables, a time shift between FTS and MAESTRO will introduce an artificial shift in the MAESTRO tangent heights of a few km; this results in mixing ratios that can be significantly low or significantly high, depending on the size of the time shift. While a method to objectively identify and correct these shifts based on MAESTRO internal information is under development, the v1.2 profiles have not been corrected for this artifact. MAESTRO sunrise and sunset O_3 profiles show opposite biases with respect to SAGE III and POAM III, with sunset values in the upper stratosphere being up to $\sim 30\%$ higher than those instruments, and sunrise values up to $\sim 15\%$ lower in most of the stratosphere [Kar et al., 2007].

2.1.3. HALOE

[7] HALOE [Russell et al., 1993] was operational on the Upper Atmosphere Research Satellite (UARS) from October 1991 through November 2005. HALOE observations take approximately one month to cover the full range of latitudes sampled (ranging from $\pm 80^\circ$ to $\pm 50^\circ$, depending on season, reaching highest (lowest) latitudes in summer (winter)). Estimates of uncertainties for the profiles of the retrieved HALOE parameters from its first public release data set (Version 17) are provided in a special UARS Validation Issue in Journal of Geophysical Research, Atmospheres, 101(D6), 1996. The data used here are Version 19. Some updated uncertainty estimates for Version 19 are available for O_3 [Randall et al., 2003], H_2O [Kley et al., 2000], and temperature [Remsberg et al., 2002]. Vertical resolution is ~ 2 km for O_3 and H_2O , ~ 3 – 4 km for temperature, and ~ 4 km for HCl. Temperatures in the HALOE files below 35 km are from the NCEP/CPC meteorological analyses. HALOE latitude and longitude as a function of height are provided on the same 0.3-km grid used for the temperature files.

2.1.4. POAM

[8] POAM II [Glaccum et al., 1996] and POAM III [Lucke et al., 1999] were visible/near-infrared solar occultation instruments that typically made 14–15 measurements per day in each hemisphere around a circle of latitude with a longitudinal spacing of about 25° . The latitudinal coverage was identical each year, slowly varying between 54 – $71^\circ N$ and 65 – $88^\circ S$. POAM II obtained data from October 1993 until November 1996, when the host satellite failed; POAM III obtained data from late April 1998 through early December 2005. POAM II provided measurements of O_3 , aerosol extinction, and NO_2 ; POAM III provided H_2O in addition to these. The POAM III Version 4 ozone retrievals differ little from the Version 3 retrievals described by Lumpe et al. [2002a], and validated by Lumpe et al. [2002b] and Randall et al. [2003]. At 15 km and above, the O_3 retrievals have a vertical resolution of ~ 1 km and an estimated precision of 5% [Lumpe et al., 2002a]. The H_2O retrievals extend from 5 to 50 km with 5–7% precision and a vertical resolution ranging from 1 km in the lower stratosphere to 3 km in the upper stratosphere. The H_2O retrievals have been validated by Lumpe et al. [2006]. Geolocation information (latitude, longitude and line-of-sight (LOS) angle) for POAM III were calculated on an 8-km grid, and interpolated linearly to the POAM 1-km measurement grid.

2.1.5. SAGE II

[9] SAGE II (http://science.hq.nasa.gov/missions/satellite_45.htm) used radiances at 600 nm to derive O_3 and at 940 nm to derive H_2O ; it took measurements from October 1984 through August 2005. The instrument and earlier versions of the retrieval algorithm, as well as O_3 validation, are discussed by Chu et al. [1989], Cunnold et al. [1989], and McCormick et al. [1989]. SAGE II data used here are Version 6.2. O_3 data have ~ 1 km or better vertical resolution, and H_2O data no better than ~ 1 km. Validation of v6.1 O_3 is discussed by Wang et al. [2002]; Wang et al. [2006b] show some correlative data comparisons with v6.2 O_3 . H_2O validation is discussed by Chiou et al. [2004] and Taha et al. [2004]. The precision of SAGE II O_3 is estimated to be $\sim 2\%$ [Borchi and Pommereau, 2006] and no credible estimates of the precision of H_2O measurements exist. The SAGE II coverage follows a pattern similar to that of HALOE. Geolocation information, including line-of-sight (LOS) angle, was provided on the measurement grid in separate files.

2.1.6. Sage III

[10] The SAGE III instrument (http://science.hq.nasa.gov/missions/satellite_8.htm) used radiances from several channels in the 570 to 600 nm region to derive O_3 and at several more in the 925 to 960 nm region to derive H_2O (though H_2O retrievals are not yet available); it took measurements from May 2002 through December 2005. The instrument and the retrieval algorithm, as well as O_3 validation, are discussed by Mauldin et al. [1985], McCormick et al. [2002], and Wang et al. [2006a]. SAGE III data used here are Version 3 “MLR” O_3 , which has a vertical resolution of ~ 1 km. The precision of SAGE III O_3 has not been objectively estimated but should be comparable to SAGE II. SAGE III solar measurement coverage from the sun synchronous orbit is confined to mid to high latitudes with

Table 1. Derived Meteorological Product (DMP) Fields and Units for Solar Occultation Instruments

Field	Units	Description
<i>Geolocation (From Instrument Geometry)</i>		
Alt	km	(2D ^a) altitudes
Lat	deg	(2D) latitudes as a function of altitude
Lon	deg	(2D) longitudes as a function of altitude
Sun dir ^b	deg cw from N	(2D) line-of-sight angle (LOS)
<i>Interpolated From Meteorological Data</i>		
Temperature	K	(2D) temperature from meteorological data
Geop hgt	m	(2D) geopotential height
Zonal wind	m/s	(2D) zonal wind
Merid wind	m/s	(2D) meridional wind
<i>Calculated From Meteorological Data</i>		
θ	K	(2D) potential temperature from met data
PV ^c	$10^{-4} \text{ K m}^2 \text{ kg}^{-1} \text{ s}^{-1}$	(2D) potential vorticity (PV)
Scaled PV	10^{-4} s^{-1}	(2D) scaled PV, in "vorticity units" ^d
EqL	deg	(2D) equivalent latitude (EqL)
Hor PV grad	–	(2D) normalized horizontal PV gradient
Hor T grad	K/km	(2D) horizontal temperature gradient
LOS T grad ^b	K/km	(2D) temperature gradient along LOS
LOS PV grad ^b	$(10^{-4} \text{ K m}^2 \text{ kg}^{-1} \text{ s}^{-1})/\text{km}$	(2D) PV gradient along LOS
EqL–VEC	deg	(2D) distance (EqL) from vortex edge center
EqL–VEI	deg	(2D) distance (EqL) from inner vortex edge
EqL–VEO	deg	(2D) distance (EqL) from outer vortex edge
Dyn tropopause	km	(1D ^a) dynamical tropopause altitude ^e
TG tropopause	km	(1D) WMO tropopause altitude

^a2D indicates profile information, and 1D indicates a single value for each occultation.

^bNot Available for ACE or HALOE DMPs.

^cInterpolated directly from provided data set for DMPs derived from GEOS-4.

^d*Dunkerton and Delisi* [1986] and *Manney et al.* [1994b].

^e3.5 PVU joined to 380 K θ in tropics, see text.

sunrise events in the southern hemisphere ($\sim 30\text{--}50^\circ\text{S}$) and sunset events in the north ($\sim 50\text{--}80^\circ\text{N}$). Geolocation information is included in the SAGE III data files every 10 km in the vertical; this is interpolated linearly to the 0.5-km data grid.

2.2. Aura MLS Data Set

[11] MLS measures millimeter- and submillimeter-wavelength thermal emission from the limb of Earth's atmosphere. Detailed information on the measurement technique and the MLS instrument on the EOS Aura satellite is given by *Waters et al.* [2006]. The Aura MLS fields of view point in the direction of orbital motion and vertically scan the limb in the orbit plane, leading to data coverage from 82°S to 82°N latitude on every orbit. Vertical profiles are measured every 165 km along the suborbital track and have a horizontal resolution of $\sim 200\text{--}300$ km along-track and $\sim 3\text{--}9$ km across-track. Vertical resolution of the Aura MLS data is typically $\sim 3\text{--}4$ km in the stratosphere, depending on the product. *Livesey et al.* [2007b], as well as papers on individual MLS products (listed below), provide detailed precision and resolution information for v2.2 MLS data.

[12] Examples using DMPs to compare many of the species retrieved from MLS measurements with solar occultation data are presented here. Comprehensive validation of these species for v2.2, including detailed precision and resolution information, is done in papers in this special section: *Lambert et al.* [2007] (N_2O and H_2O), *L. Froidevaux et al.* (Validation of EOS MLS stratospheric ozone measurements, submitted to *Journal of Geophysical Research*, 2007, hereinafter referred to as *Froidevaux et al.*, submitted

manuscript, 2007), *Jiang et al.* [2007], *Livesey et al.* [2007a, and references therein] (O_3), *Froidevaux et al.* [2007] (HCl), *Santee et al.* [2007] (HNO_3), *Pumphrey et al.* [2007] and *Livesey et al.* [2007a] (CO), and M. J. Schwartz et al. (Validation of the Aura Microwave Limb Sounder temperature and geopotential height measurements, submitted to *Journal of Geophysical Research*, 2007, hereinafter referred to as *Schwartz et al.*, submitted manuscript, 2007) (temperature). Initial validation comparisons of v1.5 MLS data are given by *Froidevaux et al.* [2006] and *Barrett et al.* [2006]. Reprocessing with MLS v2.2 is ongoing at the time of writing, and will be complete by mid-2008; the comparisons shown here use v2.2 data, except one example that uses v1.5 data to illustrate sampling effects over a full season (section 3.2).

2.3. Meteorological Analyses

[13] DMPs are currently calculated from the Met Office (MetO) data set for each of the instruments, from the NASA Global Modeling and Assimilation Office's (GMAO) Goddard Earth Observing System (GEOS) data sets (4 and/or 5) for MLS and ACE-FTS, and from the NCEP/CPC (National Centers for Environmental Prediction/Climate Prediction Center) analyses for SAGE II. A brief description of these data sets follows; further information is given by *Manney et al.* [2005b, and references therein], which also provide comparisons between these and other meteorological data sets.

[14] The MetO data through 12 March 2006 are from the stratosphere-troposphere (STT) data assimilation system first developed for the Upper Atmosphere Research Satellite

Table 2. Derived Meteorological Product (DMP) Fields for MLS

Field	Units	Description
<i>On Standard Pressure Surfaces</i>		
Pressure	hPa	standard pressure level values
θ	K	potential temperature from met data
Geop hgt	m	geopotential height
<i>On Standard Potential Temperature Surfaces</i>		
θ	K	standard θ level values
Pressure	hPa	pressure on θ surfaces
Zonal wind	m/s	zonal wind
Merid wind	m/s	meridional wind
PV	$10^{-4} \text{ K m}^2 \text{ kg}^{-1} \text{ s}^{-1}$	potential vorticity (PV)
EqL	deg	equivalent latitude (EqL)
Hor PV grad	–	normalized horizontal PV gradient
EqL–VEC	deg	distance (EqL) from vortex edge center
EqL–VEI	deg	distance (EqL) from inner vortex edge
EqL–VEO	deg	distance (EqL) from outer vortex edge
<i>Single-Level Fields</i>		
Latitude	deg	MLS Level 2 reported latitude
Longitude	deg	MLS Level 2 reported longitude
Dyn tropopause	hPa	dynamical tropopause pressure
TG tropopause	hPa	WMO tropopause pressure

(UARS) project [Swinbank and O'Neill, 1994], and have been produced since October 1991. The assimilation used an analysis-correction scheme as described by Lorenc *et al.* [1991] until late 2000, when a three-dimensional variational (3D-Var) scheme was implemented [Lorenc *et al.*, 2000]. In late 2003, a new dynamical core [Davies *et al.*, 2005] was implemented in the assimilation system [Swinbank *et al.*, 2002, 2003]. The MetO-STT data (three-dimensional winds, temperature, and geopotential height) are supplied once daily at 1200 UT on a 2.5° latitude by 3.75° longitude grid, and at UARS pressure levels (6 levels per decade in pressure) between 1000 and 0.3 hPa (0.1 hPa after late 2003). After 12 March 2006, the stratospheric analyses are provided from the same numerical weather prediction (NWP) model system as operational forecasts from the Met Office (D. Walters *et al.*, Enhancing vertical and horizontal resolution in the Met Office Global NWP (Unified) Model, manuscript in preparation, 2007); the same fields are provided, but on a 0.375° latitude by 0.5625° longitude grid, at 27 levels from 1000 to 0.4 hPa (to 0.1 hPa starting in May 2007). When there is a need to distinguish, the recent MetO analyses are referred to as MetO-NWP and the original ones developed for UARS as MetO-STT. DMPs are calculated for all instruments from the MetO data.

[15] The GEOS-4 analyses are described by Bloom *et al.* [2005]; a Physical Space Statistical Analysis Scheme is used. The GEOS-4 data used here are provided on 55 hybrid (σ /pressure) model levels from the surface to 0.01 hPa. The horizontal grid is 1.0° latitude by 1.25° longitude. Six-hourly average fields are provided centered at 0000, 0600, 1200 and 1800 UT. Besides the standard meteorological variables, GEOS-4 products include an extensive set of fields from the model and assimilation system, including PV calculated internally in the model. DMPs for ACE-FTS and for MLS v1.5 data are calculated from GEOS-4.

[16] GEOS-5 analyses [Reinecker *et al.*, 2007] have been produced for the full period of the Aura mission, and have replaced GEOS-4 as the operational system. GEOS-5 uses

the Grid Point Statistical Analysis method of Wu *et al.* [2002], a 3D-Var system, with a six-hour analysis window. Analyses are produced for surface pressure, temperature, winds, moisture and ozone. Along with operational meteorological products, infrared radiances from AIRS on EOS-Aqua were assimilated, as described in detail by Stajner *et al.* [2007]. The interface between the observations and the GCM is performed using the incremental analysis update (IAU) approach [Bloom *et al.*, 1996], which avoids shocking the model, thus producing smoother analyses. GEOS-5 analyses are provided on 72 model levels from the surface to 0.01 hPa, and a 0.5° latitude by $2/3^\circ$ longitude grid. DMPs for ACE-FTS and for MLS v2.2 data are calculated from GEOS-5.

[17] NCEP/CPC analyses (used for SAGE II DMPs) are from an objective analysis at levels above 10 hPa (above 100 hPa prior to April 2001) [Finger *et al.*, 1965, 1993; Gelman *et al.*, 1986, 1994]; these analyses have been available since June 1979. Analyses at and below 100 hPa are from the tropospheric analysis and forecast cycle [e.g., Derber and Wu, 1998; McNally *et al.*, 2000]. The NCEP data are provided once a day at 1200 UT on a 65×65 point polar stereographic grid for each hemisphere; the fields used here are interpolated to a $2.5^\circ \times 5^\circ$ latitude/longitude grid. Only temperature and geopotential height are provided in the stratosphere, so horizontal winds are calculated from the NCEP geopotential heights using a form of the primitive equations that neglects the vertical advection and time tendency terms [Randel, 1987; Newman *et al.*, 1989].

3. DMP Field Description

[18] Table 1 lists the DMPs calculated for the solar occultation instruments; these DMPs are produced on the vertical grids used for the solar occultation instruments' data. Table 2 lists the DMPs provided for the MLS instrument. MLS records over 100 times more profiles per day than the solar occultation instruments, so calculating the

DMPs is computationally intensive. To make the calculations feasible, and since the MLS positions are not altitude-dependent, MLS DMPs are calculated and output on standard θ or pressure levels, allowing the calculations to be done in advance on the gridded meteorological analysis fields once for each analysis time, and then interpolated to the MLS times and positions. File formats and access to the DMPs are described in Appendix A; the DMP calculations are described in more detail below.

3.1. Description of Calculations and Interpolations

[19] Interpolation of fields provided in the meteorological analyses (horizontal winds, temperature, geopotential height, PV from GEOS-4 and GEOS-5 analyses) is done linearly in time (between six-hourly fields for the GEOS analyses, daily fields for the MetO analyses) and bilinearly in latitude and longitude. Vertical interpolations are linear in $\log(\theta)$ for PV or $\log(\text{pressure})$ for the other products. EqL is calculated on isentropic surfaces and interpolated linearly in $\log(\theta)$. For the MetO and NCEP DMPs, PV is calculated as described by *Manney et al.* [1996b], based on the algorithm of *Newman et al.* [1989]; PV is provided from the assimilation model in the GEOS data sets, and these PV fields are used in the DMP files, as they are more fully consistent with the analyzed fields than an offline calculation. Scaled PV (sPV) is in “vorticity units” (10^{-4} s^{-1}) [*Dunkerton and Delisi*, 1986; *Manney et al.*, 1994b], giving a similar range of values at levels throughout the stratosphere.

[20] Horizontal PV gradients are calculated on isentropic surfaces and normalized to the hemispheric average; the calculation is strongly dependent on the resolution of the meteorological analysis used. The magnitudes of gradients calculated from different meteorological analyses are thus not directly comparable. Horizontal temperature gradients are calculated on pressure levels. LOS PV and temperature gradients are also provided for several of the solar occultation instruments for which the LOS angle information is available. These are potentially useful for validation and data quality studies in assessing the homogeneity of atmospheric conditions along the LOS.

[21] Knowledge of the position of measurements with respect to the vortex edge frequently aids in interpretation, and can be valuable for selecting observations from the same air mass [e.g., *Nassar et al.*, 2005; *Sica et al.*, 2007]. To provide this information in the DMP files, the vortex edge “center” is defined as the EqL of the maximum of the wind speed times the PV gradient. The “inner” and “outer” vortex edges are EqL on vortex and extravortex sides, respectively, where that vortex definition function changes curvature [e.g., *Nash et al.*, 1996]. The vortex is undefined if $\theta < 34 \text{ K}$, or if the EqL of the vortex edge center is greater than 80° (vortex too small [e.g., *Manney et al.*, 1994a]), the wind speed is less than 15.2 m/s (polar night jet is too weak [e.g., *Nash et al.*, 1996]), or the normalized PV gradient is less than 1.1 (not significantly above average).

[22] Figure 1 shows the wind speed, PV gradient, and position in relation to the vortex edge center from MLS GEOS-4 DMPs during northern hemisphere (NH) winter and spring. Only those days on which a vortex edge is defined can be included in the averages for the position relative to the vortex edge; thus, in some cases (e.g., SH lower stratosphere in March, when vortex is just starting to

develop and does so substantially over the month) a vortex edge is defined when the plotted PV gradients and wind speeds do not show an obvious transport barrier. The vortex appears to be defined in the SH at the lowest levels in January in Figure 1, a misidentification of the top of the upper tropospheric subtropical jet as the vortex edge; this is a common occurrence, but setting the lower θ limit to a higher value would eliminate much of the SH subvortex region in winter and spring. In the upper stratosphere, and near the stratopause, the jet/PV gradient structure is much more complex, and thus misidentification (e.g., January in SH) is common; in fact, there is often not a single most appropriate definition of the upper stratospheric vortex edge, even in winter.

[23] The inclusion of wind speed in the definition reduces the likelihood of spurious maxima in the PV gradient at high EqL being identified as the vortex edge, and the use of the combined function provides a means for choosing which of multiple peaks in the PV gradient (common in fall [e.g., *Manney et al.*, 2002]) are selected. Automated vortex edge identification is most robust under conditions for which the vortex is simply defined, i.e., when there is a single region of strong PV gradients associated with a sharply peaked polar night jet. This is the case in the middle to lower stratosphere during SH winter and many NH winters; in these cases, results from the algorithm used for the DMPs agree closely with those using the criteria of *Nash et al.* [1996] and other methods of determining the vortex edge. Our comparisons suggest that the algorithm used for the DMPs can give more desirable results than the *Nash et al.* [1996] method in complex situations such as that in the upper stratosphere.

[24] Figure 2 shows the vortex edge as a function of time, versus sPV and ACE-FTS CH_4 , for December 2004 through March 2005, in the upper and lower stratosphere; since CH_4 is a long-lived tracer with strong gradients across the vortex boundary, it is strongly negatively correlated with sPV throughout the stratosphere [*Manney et al.*, 1999, and references therein]. In the lower stratosphere (through the middle stratosphere, not shown), the vortex edge is marked by a very well defined region in sPV and CH_4 (and other trace gases and dynamical markers, not shown) in January through late March, becoming slightly less distinct only after mid-March during the early final warming. In the upper stratosphere, however, the region of the vortex edge is much less well defined throughout the winter because of its complex structure, and Figure 2 shows a less distinct transition in CH_4 and sPV. These results demonstrate that caution should be used in applying automated vortex edge identification methods, and their appropriateness should be checked against the physical conditions. For individual profile comparisons, or other studies where it is critical to correctly identify the air mass properties of each measurement, it is suggested that the vortex edge criteria be compared with sPV, PV gradients, and wind speeds; where DMPs are available from different meteorological analyses, comparison of these fields can also aid in assessing the robustness of identification of position with respect to the vortex.

[25] The conditions under which any automated vortex edge identification is robust are exactly those under which any reasonable definition of the vortex edge (including, e.g.,

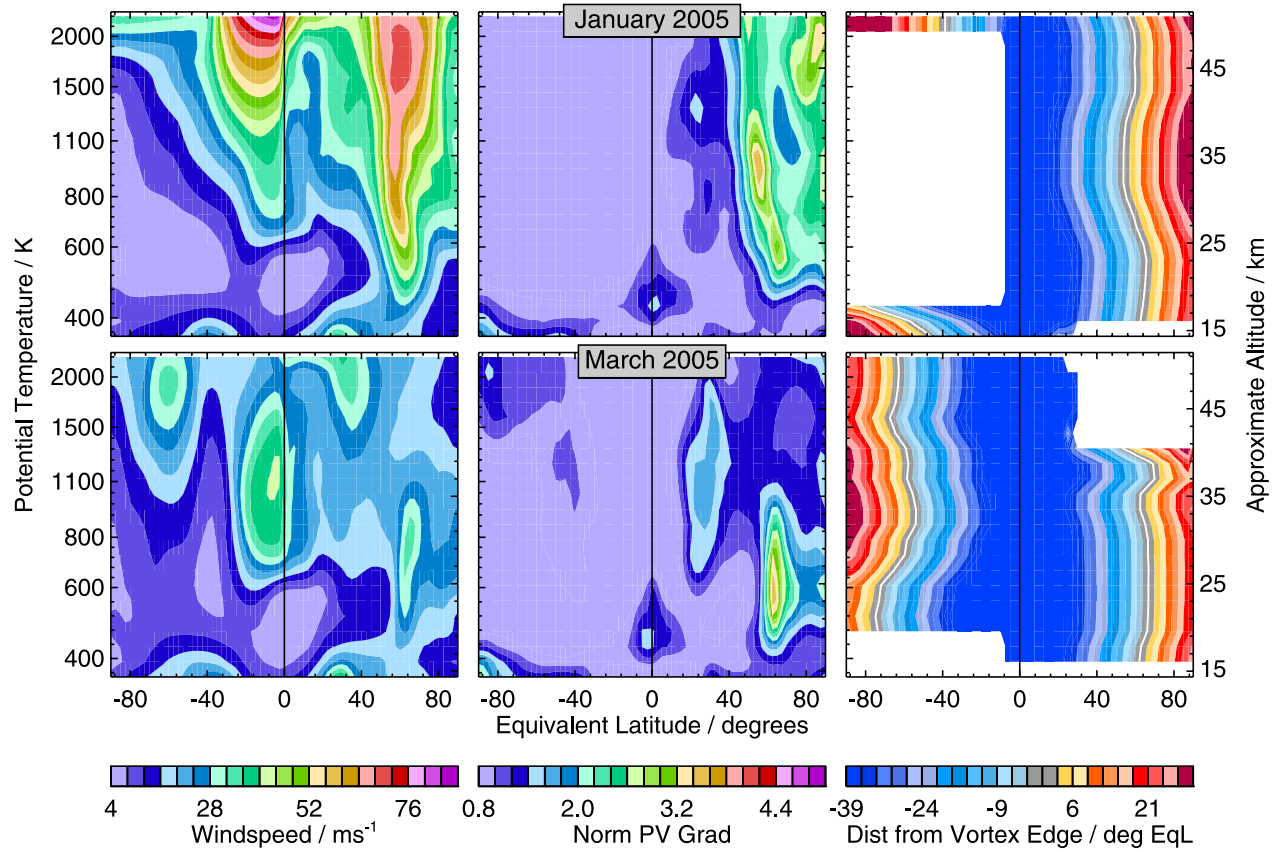


Figure 1. Monthly averages of equivalent latitude (EqL)/potential temperature (θ)-mapped (left) wind speed (m s^{-1}), (middle) normalized (see text) horizontal PV gradient, and (right) distance in EqL from the vortex edge center ($^{\circ}\text{EqL}$, see text). EqL/ θ mapping is from derived meteorological products (DMPs) calculated from GEOS-4 data for MLS locations, during (top) January 2005 and (bottom) March 2005. White space in EqL from vortex edge plots indicates that the vortex is not defined anytime during the month in these regions.

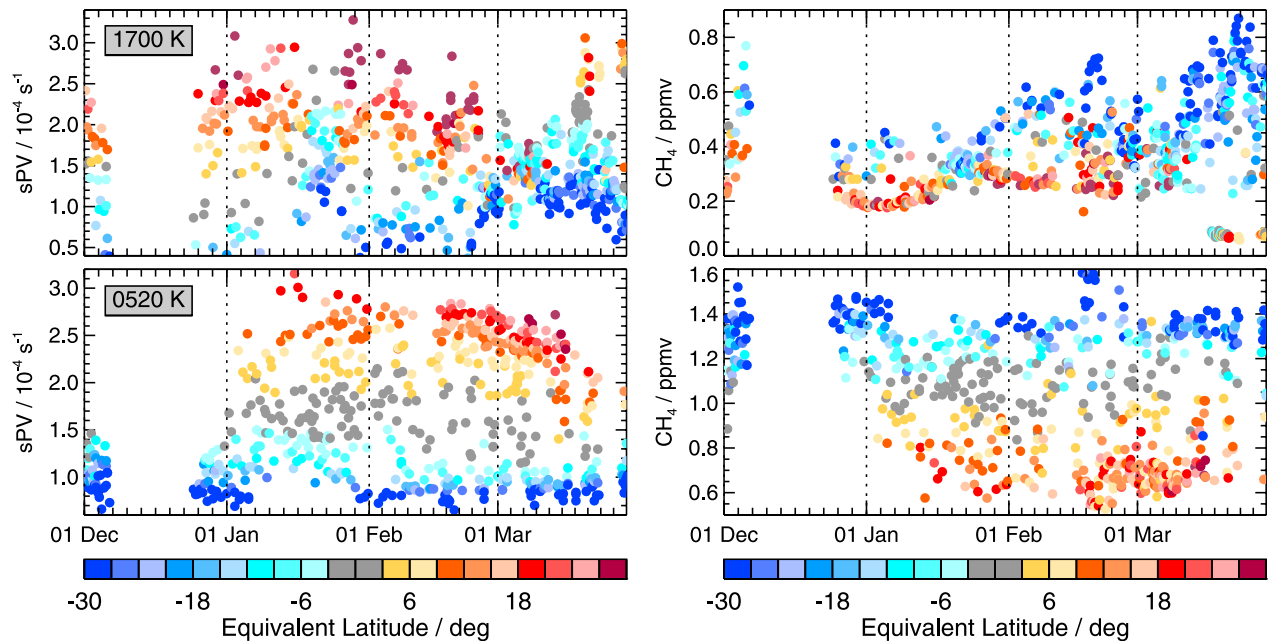


Figure 2. Time series of distance in EqL from vortex edge center (colors, $^{\circ}\text{EqL}$) as a function of (left) sPV (10^{-4} s^{-1}) and (right) ACE-FTS CH_4 (ppmv) at (top) 1700 K and (bottom) 520 K, for ACE measurement locations during December 2004 through March 2005. Vortex edge location values are from GEOS-4 DMPs.

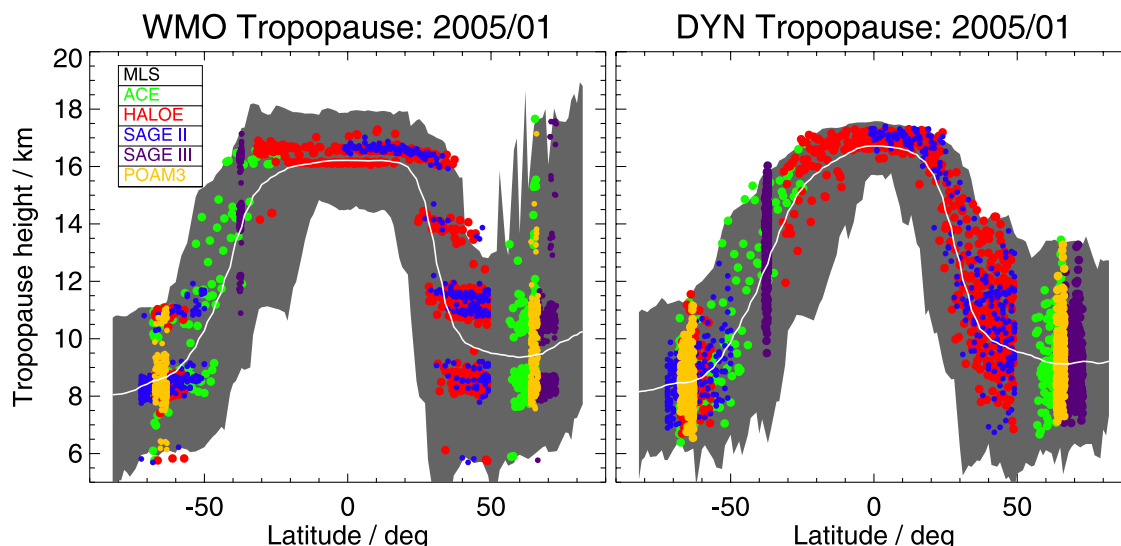


Figure 3. (left) WMO and (right) dynamical (see text) tropopause altitudes from MetO DMPs for MLS (range shown as grey shading, white line average), ACE (green), HALOE (red), SAGE II (blue), SAGE III (purple) and POAM III (gold) for all measurements in January 2005. Tropopause pressures from MLS DMPs are converted to altitude using a scale height of 7.0 km.

a specific sPV contour) will provide a comparable value. For the vortex averages shown below (section 3.2), an sPV contour ($1.4 \times 10^{-4} \text{ s}^{-1}$) is used, chosen by visual inspection to be within the region of strong PV gradients throughout the stratosphere; this definition, or nearby sPV values, has been used extensively in previous studies [e.g., Manney *et al.*, 1994a, 1994b, 2003a; Jin *et al.*, 2006b]; similar results are obtained using the EqL from the vortex edge center, though these depend more strongly on which meteorological analyses is used for the vortex edge calculation.

[26] The WMO (temperature gradient) tropopause height is defined as the lowest altitude where the temperature lapse rate drops below 2 K/km and remains below that for at least 2 km. The WMO tropopause is calculated using the algorithm of Reichler *et al.* [2003]. For the solar occultation instruments, it is calculated from the meteorological analyses' temperatures after they have been interpolated to the solar occultation instrument's measurement location and vertical grid; for MLS it is calculated on the native grid of the meteorological analysis before interpolating to the MLS times/positions. The "dynamical" tropopause is defined by the $3.5 \times 10^{-6} \text{ K m}^2 \text{ kg}^{-1} \text{ s}^{-1}$ PV contour in the extratropics (found to be an appropriate value by, e.g., Highwood and Berrisford [2000] and Schoeberl [2004]), joined to the 380 K isentropic surface in the tropics or subtropics where that PV contour rises above this level. Tropopause altitude is saved for the solar occultation instruments, and tropopause pressure for MLS, consistent with the native vertical grid of each satellite data set. Because of the limited vertical resolution of the meteorological analyses, the calculations used here (especially the WMO tropopause where the calculation of vertical gradient changes depends on resolution) are not expected to be able to capture very fine vertical structure that often exists near the tropopause and can alter local tropopause levels [e.g., Birner *et al.*, 2002]. Figure 3 shows the WMO and dynamical tropopause altitude for MLS and the five solar

occultation instruments during January 2005. The WMO and dynamical tropopause calculations agree quite well in the summer hemisphere through midlatitudes in the winter hemisphere; as noted previously [Highwood and Berrisford, 2000, and references therein], there is often a deep, nearly isothermal layer in the polar winter where the WMO tropopause is not well defined. At the latitudes covered by the solar occultation instruments, the range of tropopause values sampled is typically similar to that sampled by MLS; more MLS values in the low end of the range may simply reflect inaccuracy in the conversion of the MLS tropopause location from pressure to altitude.

3.2. Sampling Issues

[27] The DMPs help us to explore the effects of sampling and coverage on a variety of comparisons and analyses of the satellite data by providing versions of the same fields as sampled by different instruments.

[28] An example of how the MLS sampling may affect our perception of atmospheric conditions is given in Figure 4, showing PV from the $1 \times 1.25^\circ$ GEOS-4 analyses in the lower and upper stratosphere, and maps of the same fields gridded from the MLS GEOS-4 DMPs. (MLS fields are mapped on a $2 \times 5^\circ$ grid using a weighted average of all the points in a day within a specified distance of the grid points.) The day shown is a case where the MLS sampling captures some small-scale features quite well, e.g., the intrusion into the vortex near 30°E at 490 K, and the very narrow double filament drawn off the vortex near $120\text{--}180^\circ\text{E}$, 30°N at 1700 K. However, much of the small-scale structure inside the vortex at 1700 K is either distorted or not apparent in the MLS DMP fields, and other small-scale features are smeared out (e.g., the small high/low PV dipole near 310°E , 30°N at 490 K). When comparing features in PV with MLS trace gas observations, viewing the PV fields as sampled by MLS can help assess whether features in the full PV fields may be missed or distorted by the MLS sampling.

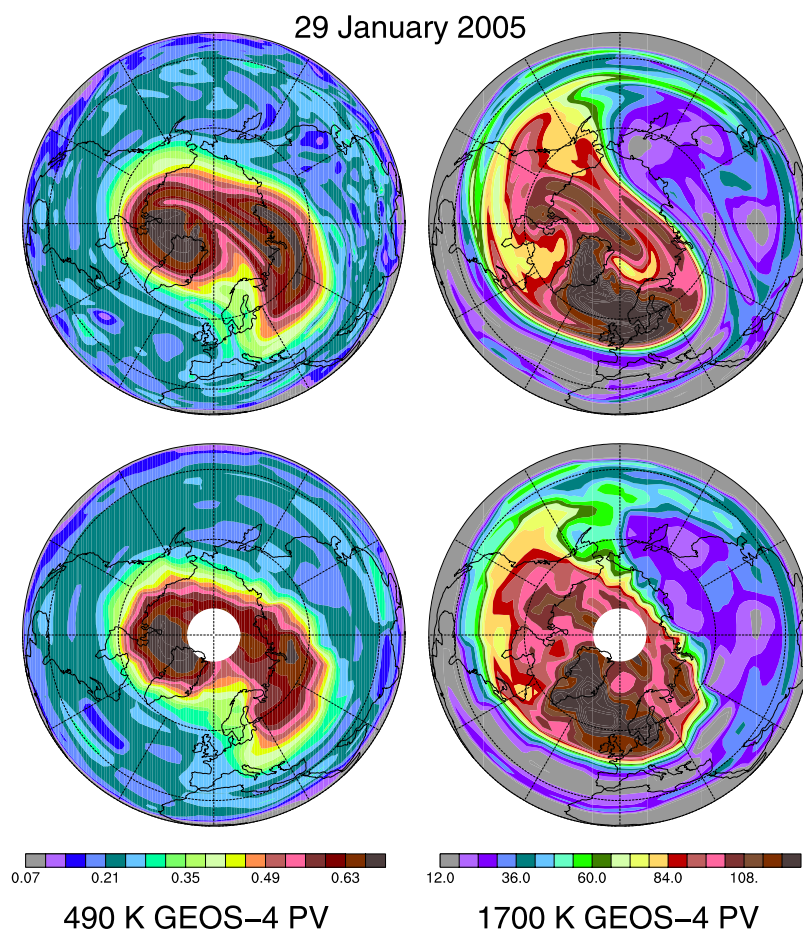


Figure 4. PV ($10^{-4} \text{ K m}^2 \text{ kg}^{-1} \text{ s}^{-1}$) maps (top) from GEOS-4 analyses and (bottom) gridded (see text) from the MLS GEOS-4 DMP PV field, at (left) 490 K and (right) 1700 K. Projection is orthographic, with 0° longitude at the bottom and 90°E to the right; latitude range is from 0° to 90°N ; fine dashed lines show a 30° latitude/longitude grid. White space above $\sim 82^\circ\text{N}$ in Figure 4 (bottom) is region not sampled by MLS.

[29] With the sparse coverage and varying views of the solar occultation instruments, sampling effects are always an important consideration. Figure 5 shows the latitude and sPV sampled by each of the solar occultation instruments as a function of EqL in the lower stratosphere during the 2004–2005 NH winter. The broad range of EqL covered each day based on measurements at a single geographic latitude demonstrates the power of an EqL view in describing the full range of atmospheric conditions using solar occultation data; however, differences in sampling still argue for continued caution in interpretation of these measurements. The vortex edge is near $1.3\text{--}1.5 \times 10^{-4} \text{ s}^{-1}$ sPV at this time and level (region of strong sPV and tracer gradients, see Figure 2). HALOE and SAGE II sampled very little vortex air during the winter; SAGE II coverage moved into the vortex in late February, when variability in vortex shape and position increased [e.g., Manney *et al.*, 2006]. Its measurements in late March reached the highest EqLs; despite being taken at much lower geographical latitudes than those of the other instruments sampling the vortex at this time ($\sim 55\text{--}65^\circ$ as opposed to $\sim 68\text{--}85^\circ$), the highest sPV values sampled by SAGE II were comparable to those seen by ACE, POAM III, and SAGE III, suggesting that at this time the geographical latitude should not be a

large factor in comparing fields that are well correlated with the vortex. The four instruments that measured primarily at high latitudes (ACE (ACE-FTS and MAESTRO), POAM III, SAGE III) also covered high EqLs with measurements at quite different geographic latitudes. In January and February, SAGE III's denser coverage (resulting from reduced sampling for POAM III and limited data downlink time for ACE, section 2.1) and higher-latitude sampling result in measurements at higher sPV values and more complete coverage of the regions of very strong sPV gradients than provided by ACE and POAM III. These differences can be a significant factor in some comparisons. Different coverage will also, of course, be a large factor in comparisons of fields that do not correlate well with the vortex, e.g., temperature (section 4.3), O_3 in some regions (section 4.2), and some trace gases affected by polar processing (section 4.3).

[30] The wide variation in density and completeness of vortex coverage (Figure 5) strongly influences interpretation of vortex averages from different instruments. Figure 6 shows the average latitude of all measurements inside the vortex (defined by the $1.4 \times 10^{-4} \text{ s}^{-1}$ sPV contour, see Figure 2, section 3.1) during the NH 2004–2005 fall and winter, from MLS and ACE measurements. As expected,

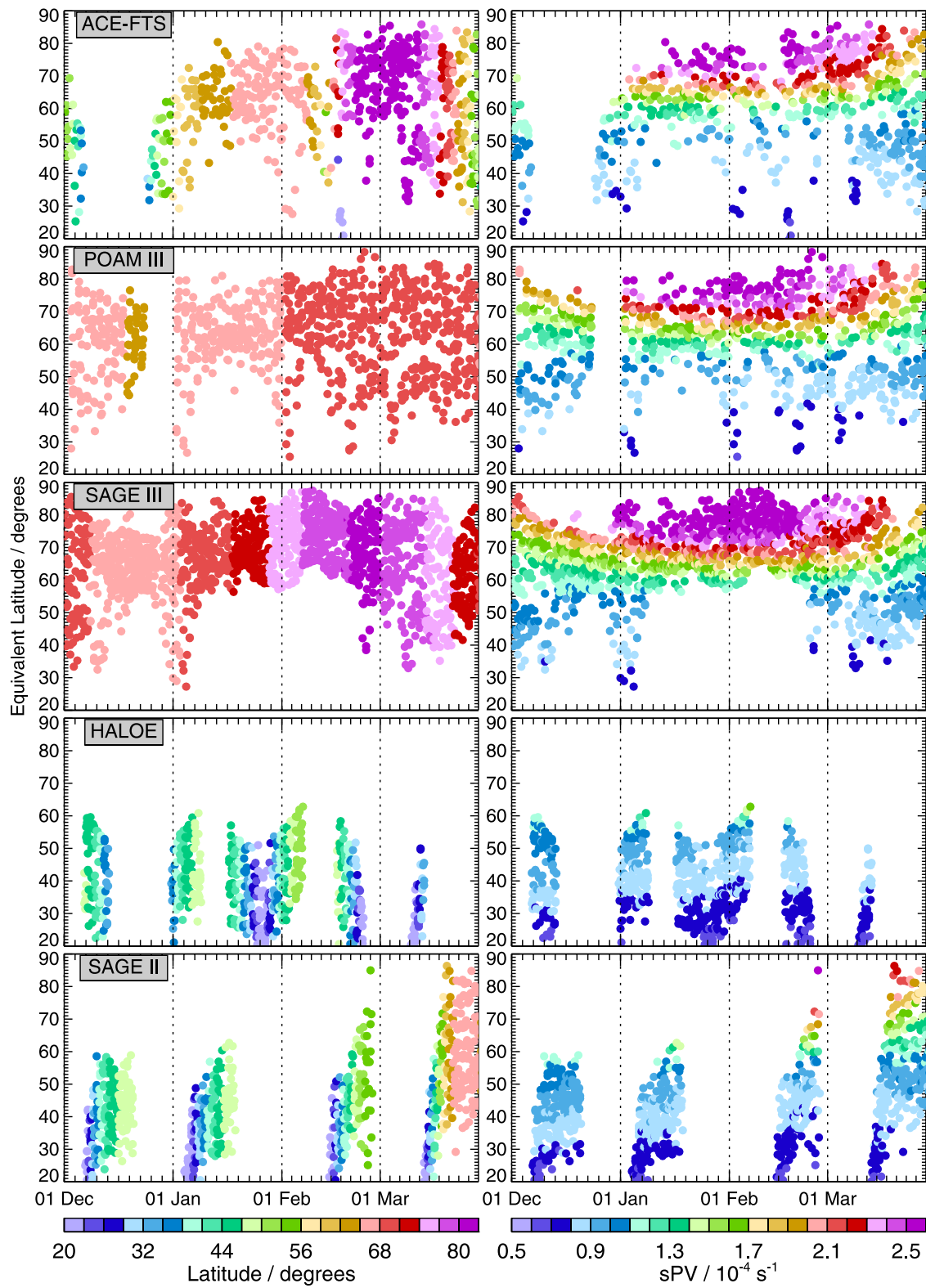


Figure 5. EqL/time plots of (left) latitude ($^{\circ}$) and (right) sPV (10^{-4} s^{-1}) sampled by (top to bottom) ACE, POAM III, SAGE III, HALOE, and SAGE II during December 2004 through March 2005 EqL on the 490 K isentropic surface.

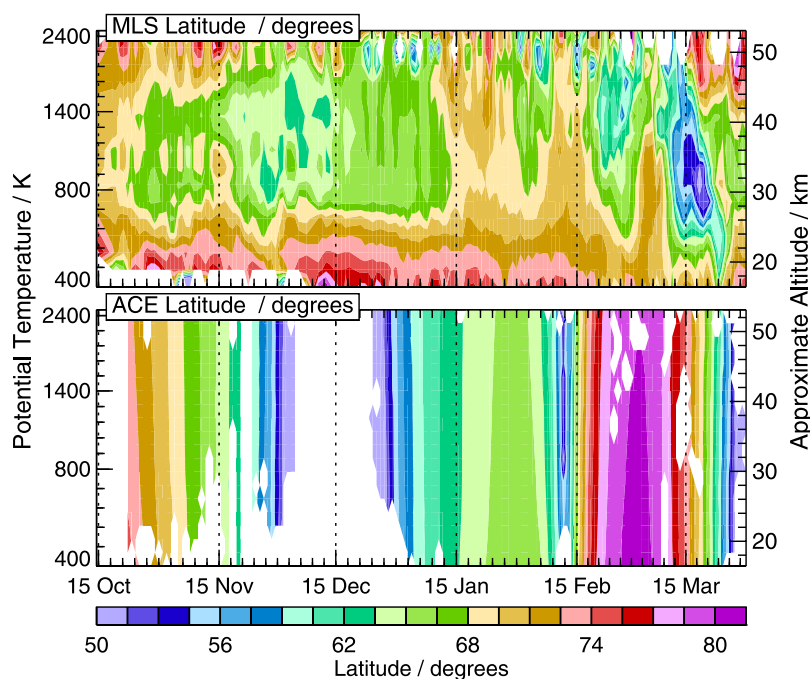


Figure 6. Vortex-averaged (within the $1.4 \times 10^{-4} \text{ s}^{-1}$ sPV contour, see text, from GEOS-4 DMPs) latitude ($^{\circ}$) sampled by (top) MLS and (bottom) ACE from 15 October 2004 through 31 March 2005.

MLS average latitudes are typically from $\sim 65^{\circ}$ to $\sim 72^{\circ}\text{N}$ (except at lowest levels where vortex is smaller); they decrease dramatically during the vortex breakup starting in early March as the vortex and its remnants move away from the pole. In contrast, the latitude from solar occultation instruments (represented here by ACE) is determined solely by their measurement patterns. Figure 7 shows how these sampling differences can affect interpretation of vortex averages of trace gases. Vortex averages of the long-lived species N_2O , H_2O , and CO are shown in the 2004–2005 NH fall and winter from ACE-FTS and MLS v1.5 (v1.5 is used to show the time evolution throughout the season, including periods when v2.2 MLS data are not yet available) data, along with similar averages using only those MLS measurements that are coincident with ACE observation locations. For the “colocated” MLS averages, coincidence criteria are $\pm 1^{\circ}$ latitude, $\pm 8^{\circ}$ longitude, and 12 hours, similar to values used in traditional coincident comparisons in other papers in this special section; results do not depend strongly on the exact coincidence criteria, and depend especially weakly on the longitude criterion.

[31] Strong descent from the mesosphere through the middle stratosphere is generally represented well in both data sets, with the ACE-FTS capturing the extent and timing of CO and H_2O changes. After ~ 15 January, the magnitude of changes in N_2O and H_2O in the lower to middle stratosphere is correctly estimated by ACE-FTS. However, during November through early January (across the gap in ACE data), ACE-FTS and MLS vortex averages do not agree well. At this time, mixing into the vortex resulting from strong wave activity led to increases (decreases) in vortex-averaged N_2O (H_2O) in the middle and lower stratosphere, and a pause in the descent of high CO /low H_2O contours in the upper stratosphere. When MLS is sampled

like ACE, a significant overestimate of the N_2O and H_2O changes in the middle and lower stratosphere results because ACE sampled near the edge of the vortex at this time, where N_2O (H_2O) is higher (lower) and mixing in of extravortex air is greater. The colocated MLS averages agree very well with those from ACE-FTS. ACE-FTS vortex-averaged values converge with those from MLS when ACE sampling moves farther into the vortex in late January. In late November, ACE-FTS and the colocated MLS averages also show a decrease (rather than just a pause in the increase in full MLS averages) in CO in the upper stratosphere, resulting from the same sampling effects. “Vortex averages” from solar occultation instruments are often used to estimate descent rates for polar processing and O_3 loss studies [e.g., Nassar *et al.*, 2005; Jin *et al.*, 2006b]; situations such as this could lead to a substantial overestimate of descent from ACE-FTS measurements after the period of strong mixing.

[32] The vortex averages shown above illustrate a type of analysis for which a vortex-centered view is still highly dependent on the latitude sampling of the individual instruments. For other types of analyses, using DMP products to analyze measurements taken in similar air masses can facilitate more comprehensive comparisons and detailed scientific studies as a function of the meteorological conditions under which the measurements were taken. In the following section, we provide examples of comparisons of MLS and solar occultation data using the DMPs during polar winter. These examples illustrate situations in which the degree of correlation with the vortex of atmospheric processes affecting various species determines how robust the comparisons between instruments with different sampling are. Our aim is neither to present a comprehensive validation of MLS versus solar occultation data (though our examples complement

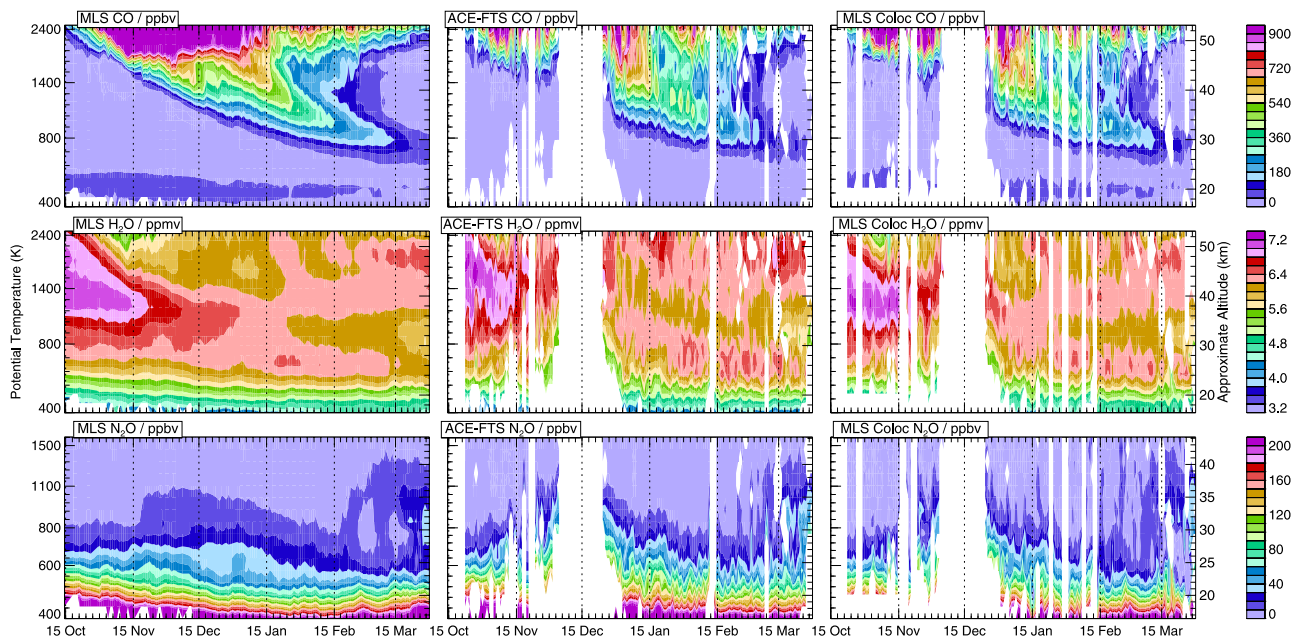


Figure 7. Vortex averages (within $1.4 \times 10^{-4} \text{ s}^{-1}$ sPV contour, see text, from GEOS-4 DMPs) for 3 October 2004 through 31 March 2005 of (top) CO (ppbv), (middle) H₂O (ppmv), and (bottom) N₂O (ppbv) from (left) MLS v1.5, (middle) ACE-FTS, and (right) MLS v1.5 measurements coincident with ACE (see text). Vertical range is 400 to 2500 K for CO and H₂O, 400 to 1600 K for N₂O.

detailed analyses given in other papers for this special section), nor to provide detailed scientific analysis, but rather to illustrate the value of the DMPs as well as precautions that still need to be taken to ensure consistent analyses when combining data sets with disparate sampling patterns.

4. Comparisons of MLS With Solar Occultation Data Using DMPs

[33] In the following subsections, we compare EqL/time series and EqL/ θ vertical sections of MLS v2.2 and solar occultation data. Comparisons that involve only ACE-FTS and MLS use EqL and θ from the GEOS-5 DMPs, others use MetO DMPs. EqL/ θ plots are produced by taking weighted averages around each grid point in EqL, θ and uncertainty, as described by Manney *et al.* [1999, 2001]. The EqL grid spacing used is 5° , so many MLS points are included in the average for each grid point. The θ grid corresponds to an ~ 3 -km spacing, comparable to the vertical resolution of many of the instruments, and coarser than the data grids. EqL/ θ plots are for data from continuous 7–8 day (d) periods. MLS/ACE-FTS comparisons are shown to the higher altitudes allowed by the GEOS-5 DMPs (section 2.3).

[34] EqL/time plots are produced in the same way, but are gridded in time instead of θ . Time grid points are at 1200 UT each day. Plots for the solar occultation instruments have a 5° latitude half-width and 3 d time half-width; 2.5° latitude and 1.5 d time half-widths are used for MLS to more fully illustrate potential sampling effects on the representation of time evolution.

4.1. Long-Lived Tracers

[35] Three species measured by MLS that are commonly used as tracers of transport are N₂O, H₂O, and CO. The

vortex averages in Figure 7 (section 3.2) showed good agreement of ACE-FTS with coincident MLS v1.5 measurements of CO and H₂O in most regions, but slightly lower MLS H₂O near the stratopause. N₂O showed excellent qualitative agreement in time evolution, but a slight low bias in MLS with respect to ACE-FTS, as was noted for NH means of coincident profiles by Froidevaux *et al.* [2006]. V2.2 MLS N₂O is on average about 10% higher than v1.5 between 46 and 2 hPa [Lambert *et al.*, 2007], which reduces (though does not eliminate, see below) that bias.

[36] Figure 8 shows times series as a function of EqL at 490 K (~ 18 km, in the lower stratosphere) of MLS v2.2 and ACE-FTS N₂O and H₂O. Very good qualitative agreement is seen in the time evolution of both species. Both species show slightly weaker PV gradients across the vortex edge (region of strongest gradients, solid sPV contours and contour just below them) in ACE-FTS than in MLS, leading to slightly lower (higher) N₂O (H₂O) values outside the vortex. This results primarily from the incomplete sampling of ACE in that region (e.g., Figure 5, section 3.2), though MLS v2.2 N₂O does show a small high bias with respect to ACE-FTS throughout the lower stratosphere [Lambert *et al.*, 2007]. MLS H₂O and N₂O are both substantially lower in the vortex core than ACE-FTS values. Since both the horizontal and vertical gradients of the two species are opposite, dependence on sampling in either coordinate would tend to produce opposite biases in H₂O and N₂O, suggesting that the vortex-core difference results from real biases between the instruments. The slight low bias in the MLS N₂O in the lower stratosphere is consistent the results of Lambert *et al.* [2007]. In the middle stratosphere (not shown), MLS and ACE-FTS H₂O and N₂O time evolution agrees well quantitatively. POAM III H₂O (not shown) is noisier than MLS and ACE-FTS, and displays some arti-

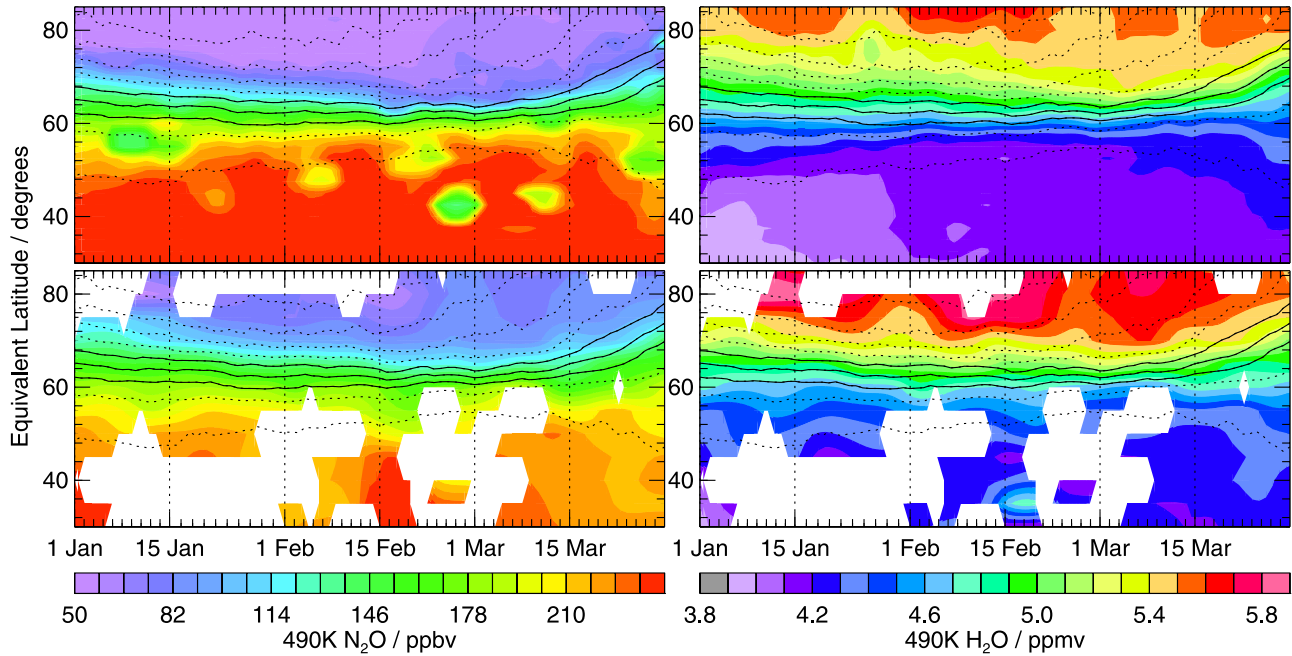


Figure 8. EqL/time series for 1 January through 31 March 2005 of (top) MLS v2.2 and (bottom) ACE-FTS (left) N₂O (ppbv) and (right) H₂O (ppmv) at 490 K, using GEOS-4 DMPs.

facts; nevertheless, very similar time evolution is seen in the middle and lower stratosphere, but with values biased high with respect to MLS and ACE-FTS.

[37] EqL/ θ sections of MLS and ACE-FTS N₂O are shown in Figure 9 for the NH in March. These show the persistent low bias of MLS in the polar vortex, and in the summer polar lower stratosphere. Similar plots using only the MLS data coincident with ACE-FTS (not shown) have only slightly smaller biases in the lower stratosphere, indicating that sampling differences are not the primary factor producing this pattern. Lambert *et al.* [2007] also show a low bias in this region in hemispheric averages of

differences between MLS and ACE-FTS coincident profiles. Elsewhere, localized differences are up to ~ 15 ppbv, but most areas are within ~ 5 ppbv, with ACE-FTS slightly lower than MLS.

[38] Figure 10 shows EqL/ θ comparisons of MLS v2.2 H₂O with ACE-FTS and HALOE during March 2005. MLS and ACE-FTS agree extremely well throughout the range, with differences typically under 0.2 ppmv (less than 5%) and maximum localized differences up to 15%. MLS is higher than HALOE by ~ 0.2 – 1.0 ppmv (~ 5 – 25%) throughout the range shown, consistent with HALOE H₂O biases reported elsewhere [e.g., Kley *et al.*, 2000; Lambert

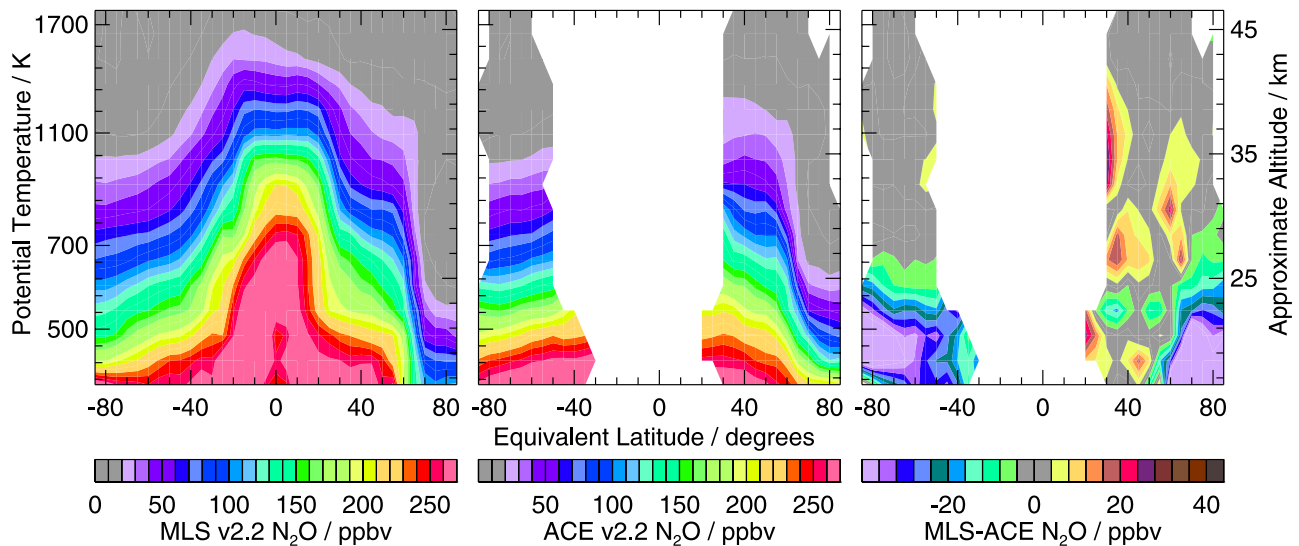


Figure 9. Global EqL/ θ cross sections for 10–16 March 2005 comparing MLS v2.2 with ACE-FTS N₂O. (left) MLS v2.2 N₂O, (middle) ACE-FTS v2.2 N₂O, and (right) the MLS-ACE-FTS N₂O difference (ppbv). GEOS-5 DMPs are used for EqL/ θ mapping. Vertical range is 400 through 1800 K.

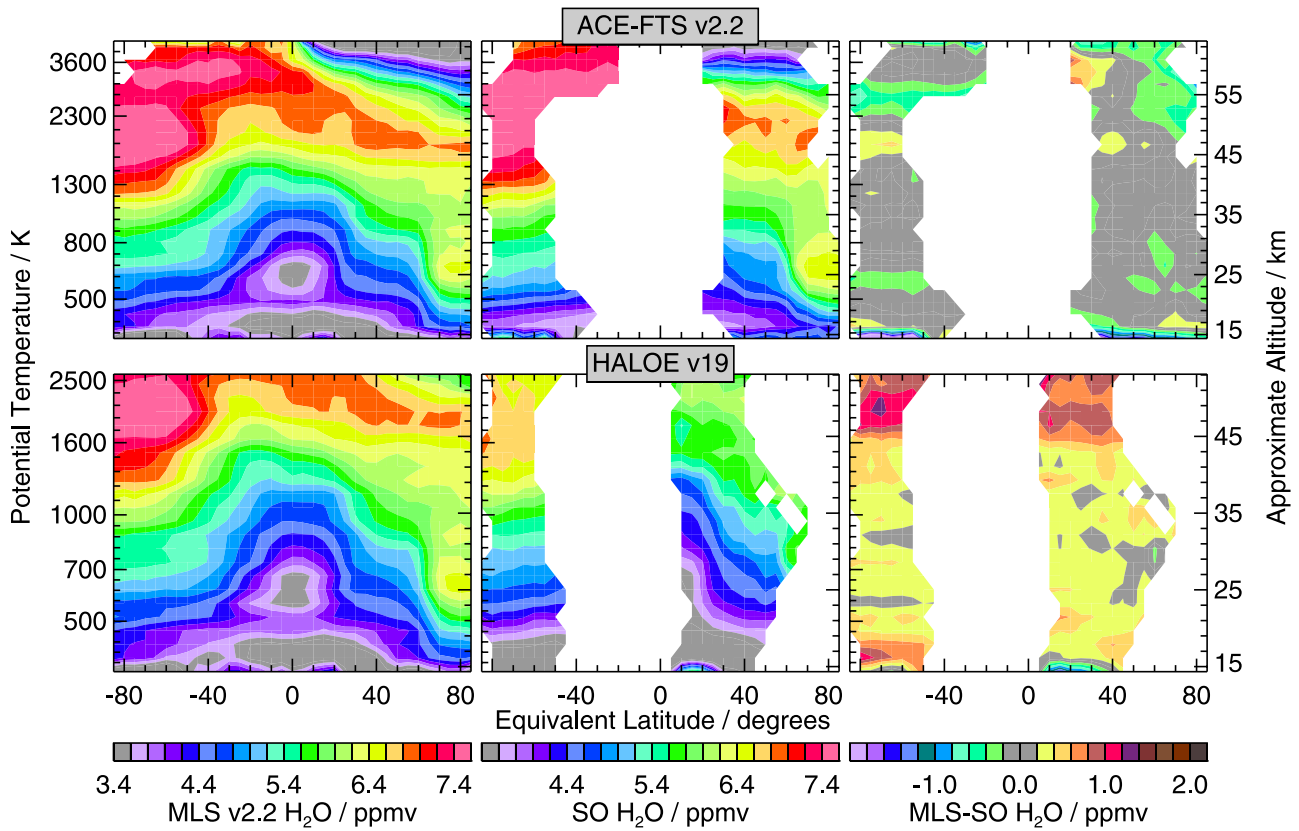


Figure 10. As in Figure 9 but for MLS v2.2 H₂O (ppmv) compared with (top) ACE-FTS and (bottom) HALOE. GEOS-5 DMPs are used for ACE-FTS comparison and MetO for HALOE comparison. Vertical range for ACE-FTS comparison is 360–4300 K, for HALOE comparison, 360–2500 K.

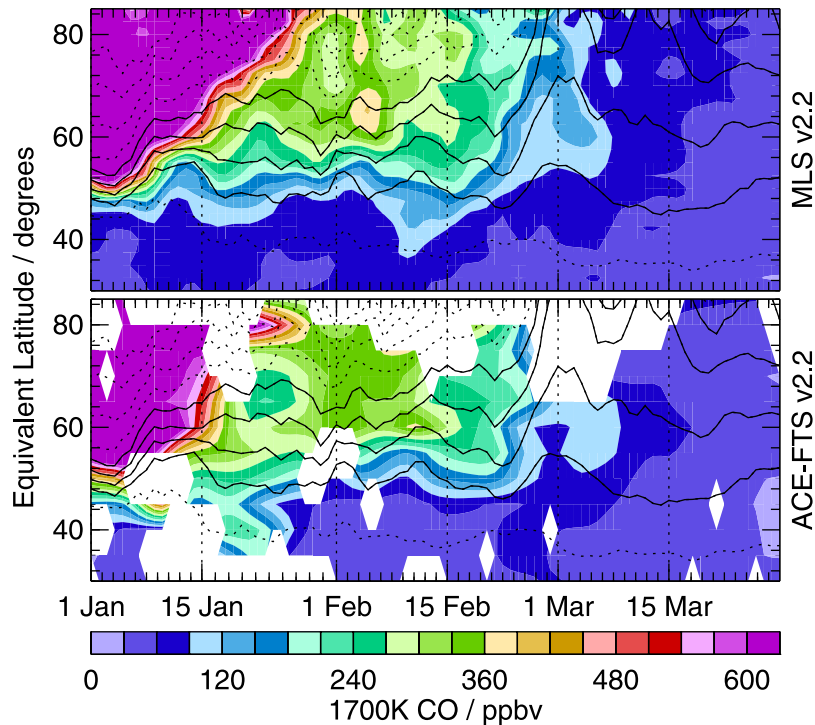


Figure 11. As in Figure 8 but for (top) MLS v2.2 and (bottom) ACE-FTS CO (ppbv) at 1700 K, using GEOS-4 DMPs.

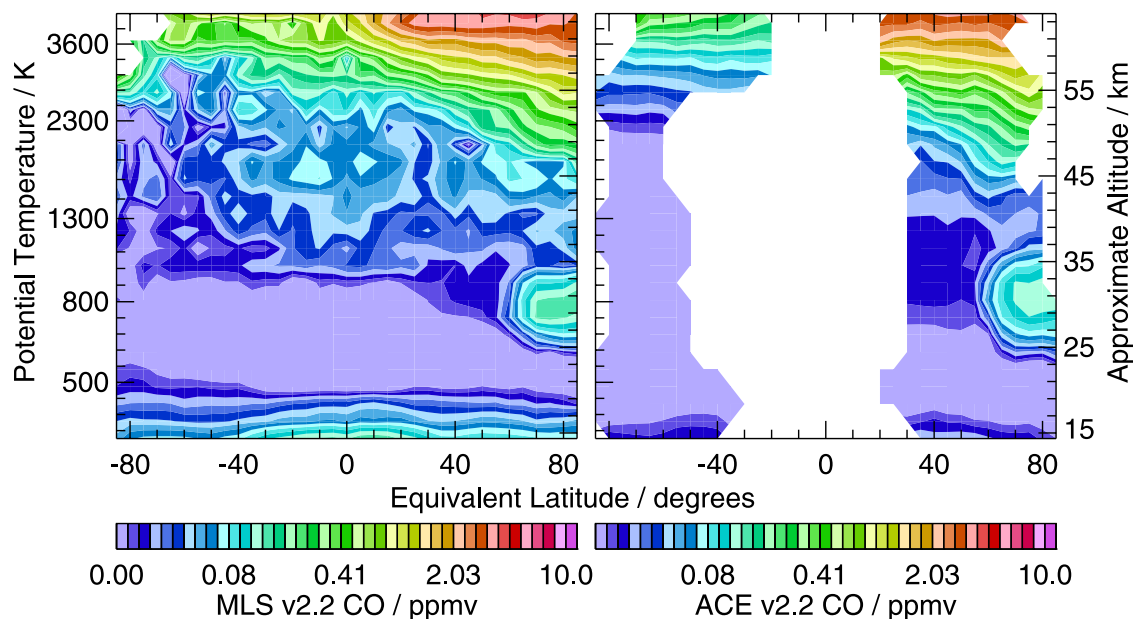


Figure 12. As in Figure 9 (with difference panel omitted) but for MLS v2.2 CO (ppbv) compared with ACE-FTS, using GEOS-5 DMPs. Vertical range is 360–4300 K. CO contour interval is on a log scale, from 20 to 10,000 ppbv.

et al., 2007]. SAGE II and POAM III H₂O EqL/ θ -mapped fields for this period (not shown) are noisy, but comparisons indicate that SAGE II is ~ 5 –15% lower than MLS between 500 and 1600 K, and POAM III is ~ 5 –15% higher than MLS between 400 and 1600 K. Each of these biases is consistent with hemispheric biases with respect to v1.5 H₂O data given by Froidevaux *et al.* [2006]; Lambert *et al.* [2007] show little overall bias between v1.5 and v2.2 H₂O in the stratosphere.

[39] The chemical lifetime of CO varies from a few weeks to many months, making it a useful tracer of transport [e.g., Solomon *et al.*, 1985; Allen *et al.*, 1999] in many situations. As shown in Figure 7 (section 3.2), starting in fall very high CO descends from the mesosphere into the winter stratospheric vortex. Figure 11 shows the time evolution of MLS v2.2 and ACE-FTS CO in the upper stratosphere. Quantitative agreement between ACE-FTS and MLS is good, as is also the case in the middle stratosphere (not shown). The combination of sparse sampling and longer time averaging used in the EqL/time gridding for ACE-FTS are the primary factors responsible for the small qualitative differences in short-lived features near the vortex edge in late January and early February. Consistent with the good agreement shown here, Pumphrey *et al.* [2007] show little overall bias between ACE-FTS and MLS stratospheric CO, but some remaining vertical oscillations in MLS CO in the stratosphere that can result in biases at individual levels.

[40] Figure 12 shows an EqL/ θ comparison of MLS v2.2 and ACE-FTS CO for March 2005. The MLS CO measurement is noisy, as seen in the variations in mid-EqLs in the upper stratosphere, and v2.2 still shows some remaining vertical oscillations in the stratosphere [Pumphrey *et al.*, 2007]; because of this, and the extremely large range of CO values, difference plots (not shown) are difficult to interpret. However, qualitative agreement is good throughout the range. Quantitative agreement is best in the Arctic lower

mesosphere, above about 2000 K (50 km). A high bias of MLS with respect to ACE-FTS in most regions, but low bias from ~ 600 to 800 K, is consistent with profile comparisons shown by Pumphrey *et al.* [2007]. MLS is strongly biased high with respect to ACE-FTS at the lowest levels shown, in the upper troposphere/lower stratosphere, consistent with the results of Livesey *et al.* [2007a].

[41] The effects of disparate sampling on interpretation of these long-lived tracer fields are minimal, and easily assessed using the DMPs (e.g., using sPV fields to diagnose the representation of gradients across the vortex edge). Using DMPs for mapping in EqL to provide a vortex-centered view is thus a powerful method for combining data sets with different sampling patterns to enhance validation and scientific studies; for the latter, EqL mapping can be used to analyze long-lived tracers that are not measured by MLS (e.g., CH₄ from ACE-FTS) in a consistent framework with the species shown here.

[42] In the following subsections, we examine other species for which chemical and other processes not correlated with the vortex may make some analyses in EqL coordinates more challenging.

4.2. Ozone

[43] In the lower stratosphere, the chemical lifetime of O₃ is long, except in the cold polar winter when heterogeneous chemical processing occurs [e.g., Solomon, 1999]. Figure 13 shows a comparison of lower stratospheric O₃ from MLS and solar occultation instruments with good coverage of the vortex during the 2004–2005 NH winter. 2004–2005 was arguably the winter with the largest lower stratospheric chemical O₃ loss of any NH winter [World Meteorological Organization (WMO), 2007, and references therein]. The morphology of O₃ was also complex, being highest near the vortex edge even before chemical loss began; this distribution complicates separation of dynamical and chemical

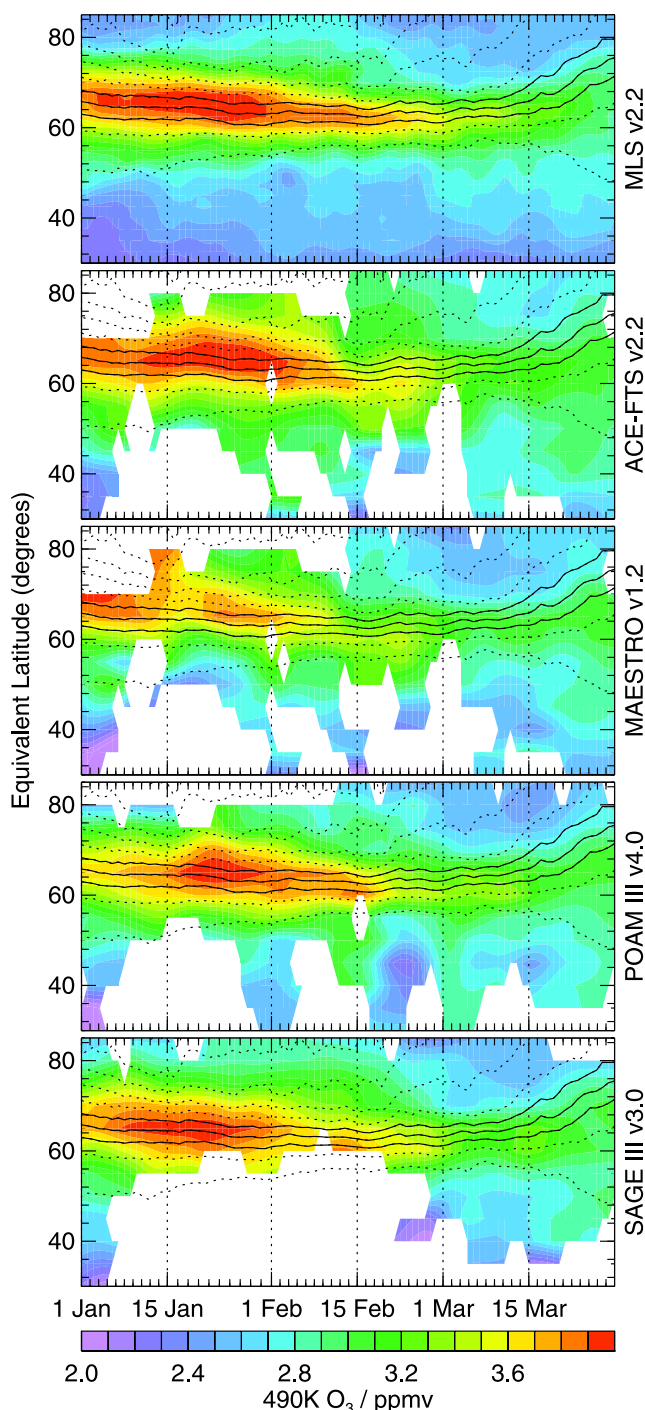


Figure 13. EqL/time series for 1 January through 31 March 2005 of O_3 (ppmv) at 490 K from (top to bottom) MLS (v2.2), ACE-FTS, MAESTRO, POAM III, and SAGE III. EqL mapping is done with MetO DMPs. Overlaid contours are MetO sPV (10^{-4} s^{-1}), with three contours in the vortex edge region shown as solid lines.

effects and makes assessment of chemical O_3 loss more problematic [e.g., Manney *et al.*, 2006]. O_3 evolution in the vortex and along its edge agrees quite well between MLS, ACE-FTS, MAESTRO, POAM III, and SAGE III. The discontinuity in MAESTRO O_3 between ~ 10 and 20 January (seen most strongly near the vortex edge) is an artifact related

to the time offset from ACE-FTS at specific measurement times (section 2.1.2). POAM III and SAGE III show slightly higher values at $40\text{--}60^\circ\text{EqL}$ than MLS, SAGE II and HALOE; this may be related to sampling, as the POAM III and SAGE III measurements are all taken at higher latitudes (Figure 5) where high O_3 values are not completely aligned with the vortex (see, e.g., maps given by Manney *et al.* [2006]). ACE-FTS vortex interior values are slightly higher overall (0.2 ppmv) than those from the other instruments, but with very similar time evolution. Examination of late-January/mid-March differences as a function of EqL and θ (not shown) from solar occultation instruments and MLS v2.2 data indicates very similar amounts of decrease in the lower stratospheric vortex (a signature of chemical loss), a maximum of $\sim 1.0 \pm 0.1 \text{ ppmv}$, for each instrument, near 70°EqL and 490 K. Detailed calculations [Singleton *et al.*, 2007] using MLS v1.5 for this winter showed very good agreement in O_3 loss estimated from these instruments, especially when MLS v1.5 data were sampled similarly to the solar occultation instruments; values for chemical O_3 loss were larger than the observed changes reported here because of replenishment of O_3 by diabatic descent [WMO, 2007, and references therein].

[44] O_3 at tropopause level is also primarily controlled by dynamics; since O_3 gradients across the tropopause are extremely strong, O_3 is sometimes used to identify the tropopause [e.g., Bethan *et al.*, 1996]. Figure 14 shows O_3 at the tropopause from MLS v2.2 data and five solar occultation instruments for 18 d periods in January–February and September 2005. Given the strong O_3 gradients, this is a very sensitive comparison; also, in this region of very low O_3 and increasing possibility of clouds, the retrievals are difficult. Overall, the values agree remarkably well, especially considering that measurements at the same latitude from different instruments may have been taken several days apart. Most of the instruments show some points with negative O_3 , reflecting the difficulty of retrieving such low O_3 values (negative MLS values represent a very small fraction, $\sim 1.7\text{--}4.2\%$, of the total number of MLS values, and are concentrated in the tropics for the WMO tropopause (where O_3 is lowest and clouds most likely to affect the retrievals) and in the polar winter (where atmospheric variability is greatest) for the dynamical tropopause). The vast majority of O_3 values at the dynamical tropopause from all instruments are ~ 0.1 to 0.4 ppmv , consistent with previous estimates [e.g., Bethan *et al.*, 1996; Pan *et al.*, 1997]. The MLS average at the dynamical tropopause, near 0.15 ppmv , agrees well with the center of the distributions for ACE-FTS, POAM III and SAGE III, and is slightly higher than that for HALOE and MAESTRO. O_3 varies more at the WMO tropopause, and shows a very large scatter in the winter polar regions, where that definition of the tropopause is most ambiguous (e.g., Figure 3); MLS, ACE-FTS, MAESTRO, and SAGE III all show large ($\sim 2.0 \text{ ppmv}$) values at high northern latitudes in January/February, when the temperatures and tropopause height were highly variable [e.g., Schoeberl *et al.*, 2006]; a similar plot for March 2005 (not shown), when the WMO tropopause is better defined, shows much lower, more typical, values in the Arctic. A very similar pattern is seen in the Antarctic winter, but with less scatter in the O_3 values for all instruments, likely because of more

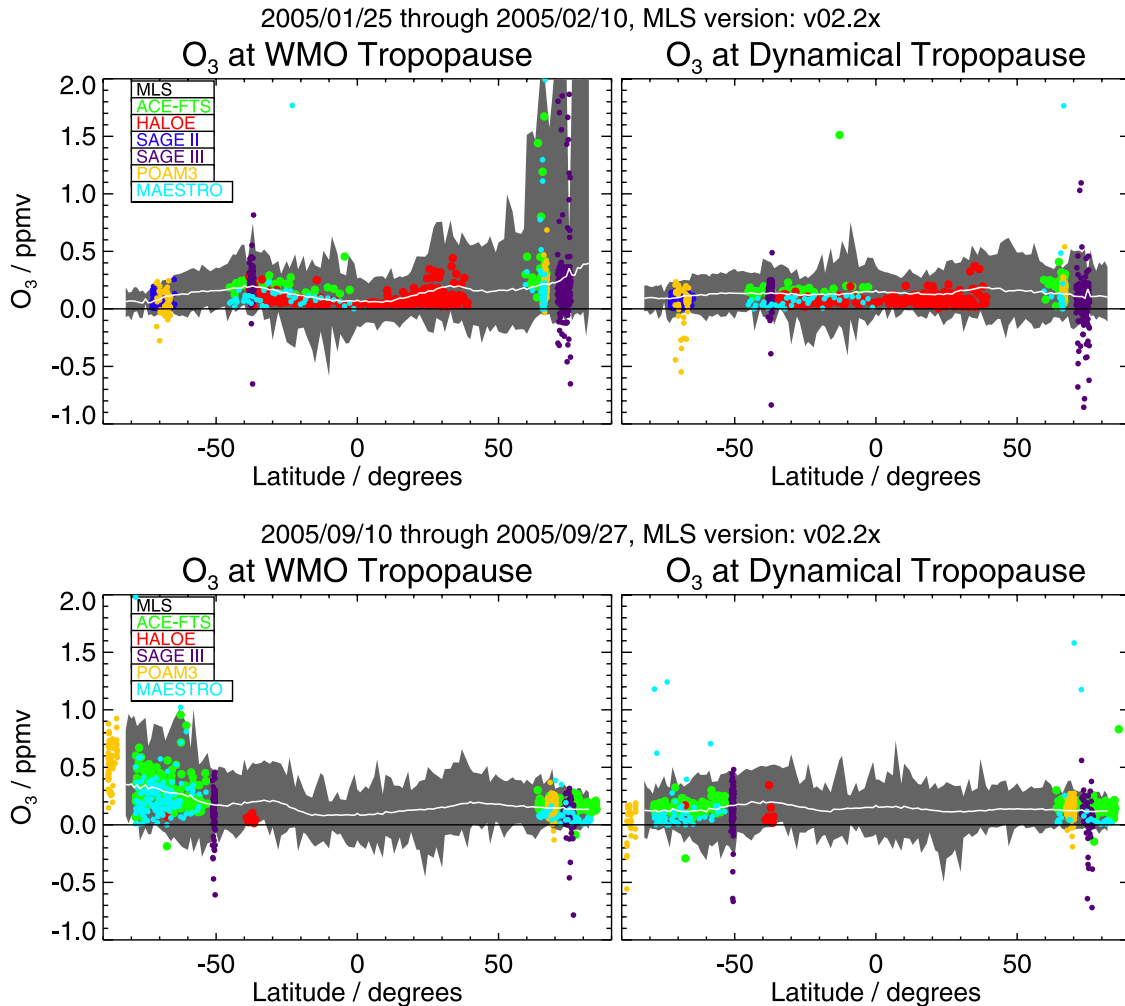


Figure 14. O_3 (ppmv) at the (left) WMO and (right) dynamical tropopause for MLS v2.2 (range shown as grey shading, average white line), ACE-FTS (green), MAESTRO (cyan), HALOE (red), SAGE II (blue), SAGE III (purple) and POAM III (gold) for all measurements during (top) 25 January to 10 February 2005 and (bottom) 10–27 September 2005. Tropopause locations for interpolation of O_3 are from MetO DMPs.

symmetric conditions in the SH winter resulting in more uniform sampling.

[45] Figures 15 and 16 compare v2.2 MLS O_3 with each of the solar occultation instruments during March 2005. First, Figure 15 shows MLS O_3 mapped in EqL/ θ using the GEOS-5 and the MetO DMPs, and the difference between them; this demonstrates that the differences in gridding from using different DMPs are small compared to differences seen below between instruments. ACE-FTS and MAESTRO comparisons in Figure 16 use GEOS-5 DMPs and extend to higher levels; other comparisons use MetO DMPs for MLS as well as the solar occultation instruments.

[46] Figure 16 shows very good agreement between all instruments in the lower stratosphere and around the tropopause; differences are typically less than 0.2 ppmv, and, even at these low O_3 values, less than $\sim 5\%$. An exception is a slight high bias of MLS with respect to HALOE at NH midlatitudes near 20 km, consistent with previously reported biases between HALOE and SAGE II [e.g., Morris

et al., 2002]; Jiang *et al.* [2007] and Froidevaux *et al.* (submitted manuscript, 2007) also show some evidence (albeit inconclusive) of a small high bias in MLS v2.2 O_3 at the lowest retrieval levels. MLS also shows a slight low bias with respect to ACE-FTS at the lowest levels shown near $\pm 40^\circ$ EqL, at the edges of the ACE-FTS coverage.

[47] Good agreement between MLS and the solar occultation instruments in O_3 mapped using DMPs from the tropopause through the lower stratosphere (Figures 13, 14, and 16) is consistent with the dominance of transport processes (or, in the polar winter, chemical processes that are generally well correlated with the vortex) in controlling the O_3 distribution. At higher altitudes, O_3 chemical lifetimes decrease, and the situation becomes more complex.

[48] In the middle to upper stratosphere (~ 900 – 1600 K) above $\sim 40^\circ$ EqL, Figure 16 shows that MLS is higher than ACE-FTS, POAM III and SAGE III (high-latitude-sampling instruments) and lower than SAGE II and HALOE (low-

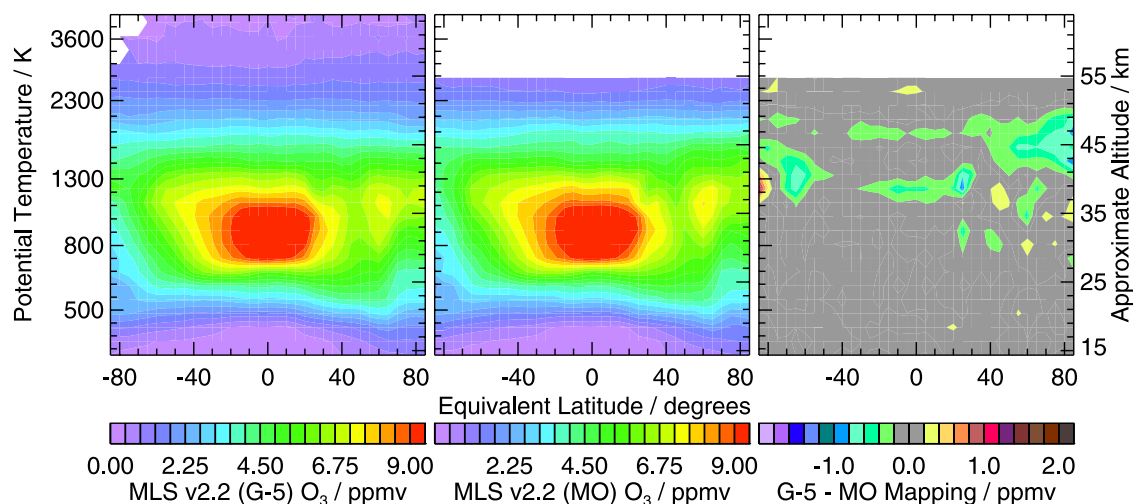


Figure 15. Global EqL/ θ cross sections for 10–16 March 2005 comparing MLS v2.2 O₃ (ppmv) mapped using (left) GEOS-5 and (middle) MetO DMPs and (right) the difference (ppmv). Vertical range is 360 through 4300 K.

latitude-sampling instruments). MLS is higher than MAESTRO (with same sampling as ACE-FTS, with sunset profiles in the NH and sunrise profiles in the SH at this time) from ~ 900 to 1300 K, above which a substantial high bias in sunset MAESTRO profiles with respect to SAGE III and POAM III has been reported [Kar *et al.*, 2007]. This is the region where “low-O₃ pockets” [Manney *et al.*, 1995b; Harvey *et al.*, 2004] are common: High O₃ from low latitudes is drawn into and trapped in the anticyclone for many days. When thus confined at high latitudes, O₃ relaxes chemically toward the lower equilibrium values for these latitudes (whereas air outside the anticyclones is continually being mixed with higher-O₃ air from low latitudes) [Morris *et al.*, 1998; Nair *et al.*, 1998]. The pattern seen in MLS data (Figure 15), with highest values apparently excluded from this EqL band, is characteristic of the morphology seen when a low-O₃ pocket is present [e.g., Manney *et al.*, 1999, 2001]. Low-O₃ pockets were observed continuously from early December 2004 through late March 2005, and were sampled by MLS and all solar occultation instruments examined here (V. L. Harvey *et al.*, Low-ozone pockets observed by EOS-MLS, submitted to *Journal of Geophysical Research*, 2007, hereinafter referred to as Harvey *et al.*, submitted manuscript, 2007). A detailed discussion of effects of sampling on low O₃ in the anticyclones as observed by MLS and the solar occultation instruments, and discussion of potential pitfalls in using EqL coordinates for this type of analysis, is given by Harvey *et al.* (submitted manuscript, 2007). EqL/ θ comparisons like those in Figure 16 constructed using only MLS observations coincident with the solar occultation instruments (not shown) reduce the differences in the middle stratosphere to less than ~ 0.4 ppmv, and in some cases change the sign (e.g., MLS is slightly lower than ACE-FTS in this region), conclusively demonstrating that these differences result from the interplay of sampling, transport and chemistry in this region.

[49] In the upper stratosphere (and lower mesosphere for ACE-FTS, above ~ 1600 K, ~ 45 km), Figure 16 shows MLS O₃ to be low with respect to ACE-FTS and SAGE III; this difference is global and persistent across the time periods

examined. Similar differences were seen by Froidevaux *et al.* [2006] for MLS v1.5 comparisons with ACE-FTS v2.1 data; Walker *et al.* [2005] also noted that ACE-FTS v1.0 O₃ was high with respect to other instruments from about 40 to at least 60 km, and this difference persists in ACE-FTS v2.2 O₃ update data. MAESTRO is also high in this region, consistent with the sunset occultation biases reported by Kar *et al.* [2007]. Froidevaux *et al.* (submitted manuscript, 2007) show a few percent increase in MLS v2.2 over v1.5 in the upper stratosphere, with a continuing low bias (by ~ 5 –10%) with respect to ACE-FTS v2.2 data. The high bias of MLS with respect to ACE-FTS in the lower mesosphere above ~ 3000 K is also persistent across the periods examined, and consistent with the results of Froidevaux *et al.* (submitted manuscript, 2007). Thus, although O₃ chemical lifetimes are short in the upper stratosphere, raising the possibility of sampling issues arising from chemical processes not well correlated with the vortex, the biases seen here are consistent with those reported in traditional coincidence analyses.

[50] The preceding discussion of O₃ indicates overall very good agreement between MLS and all of the solar occultation instruments studied when viewed with respect to EqL, but highlights sampling issues that are important in interpretation of sparse measurements. Mapping in EqL is very valuable in scientific studies with SO data, allowing examination of the full range of conditions sampled and averaging of air from similar air masses; the above results show it to be a valuable tool for O₃ from the tropopause through the lower stratosphere. At higher levels, chemical processes that are not well correlated with the vortex can complicate the interpretation of EqL-mapped O₃.

4.3. Other Fields

4.3.1. HNO₃

[51] HNO₃ in the middle and lower stratosphere is often well correlated with the vortex, but situations do occur for which the sparse sampling of solar occultation instruments can lead to apparent disagreements with MLS. In the middle stratosphere (Figure 17), qualitative time evolution appears generally consistent between MLS and ACE-FTS, with

lower overall MLS values in agreement with the results of *Santee et al.* [2007]. The low MLS HNO_3 regions inside the vortex and along the vortex edge in January and February provide an illustrative example of differences related to the sparse ACE-FTS sampling. Maps of MLS 850 K HNO_3

during this period (Figure 18) show the evolution of a partial band of low HNO_3 just inside the vortex edge. ACE-FTS observation locations are overlaid, and show that ACE-FTS typically measured near the edge of this low HNO_3 region where values were slightly higher; this pattern, and the 3 d time half-width used for the ACE-FTS gridding, result in a faint and smeared echo of the feature in the ACE-FTS data.

[52] In the lower stratosphere, HNO_3 is critical in both the activation and the deactivation of chlorine, and thus indirectly regulates O_3 destruction [Solomon, 1999; Santee et al., 2004, and references therein]. The time evolution of MLS v2.2 and ACE-FTS HNO_3 as a function of EqL in the lower stratosphere (not shown) agrees quite well, but ACE-FTS misses some of the lowest values in the vortex indicative of sequestration in PSCs. EqL/ θ comparisons of MLS v2.2 and ACE-FTS HNO_3 in January 2005 (Figure 19), during a period of strong PSC activity [Jin et al., 2006a], show good qualitative agreement, including the position and morphology of the primary HNO_3 peak and a secondary peak in the polar winter upper stratosphere (~ 900 – 1300 K) that is a common feature of the HNO_3 distribution [e.g., Orsolini et al., 2005a]. Quantitative agreement is fairly good in the levels surrounding the peak (~ 550 to 900 K), with MLS typically up to 1.0 ppbv (~ 5 – 20%) lower, consistent with the results of Santee et al. [2007]. Somewhat larger differences are seen in the mid to low EqL lower stratosphere, below ~ 500 K, and above ~ 900 K, with MLS biased low. ACE-FTS does not capture the region of lowest HNO_3 in the NH lower stratospheric vortex indicative of sequestration in PSCs, an effect of the sparse sampling of ACE missing the region of strongest PSC activity, which is not aligned with PV contours and is limited in spatial extent.

4.3.2. HCl

[53] As a primary chlorine reservoir species, HCl also plays an important role in polar processing in the lower stratosphere [e.g., Solomon, 1999]. EqL/time evolution of MLS v2.2 and ACE-FTS HCl in the lower stratosphere during the 2004–2005 NH winter (not shown) indicates very good quantitative agreement in the evolution of the region of low HCl associated with chlorine activation, and in other features of the time evolution. Figure 20 shows EqL/ θ comparisons of MLS v2.2, ACE-FTS, and HALOE HCl in January 2005. Agreement between ACE-FTS and MLS is very good, typically better than 5%, everywhere above ~ 550 K, consistent with Froidevaux et al. [2007]. In the low-HCl region in the NH vortex, ACE-FTS is higher than MLS by up to ~ 0.4 ppmv, resulting from ACE-FTS sampling not covering the location of minimum values in the vortex core sampled by MLS. HALOE HCl is ~ 5 – 25% lower than MLS through most of the range, consistent with Froidevaux

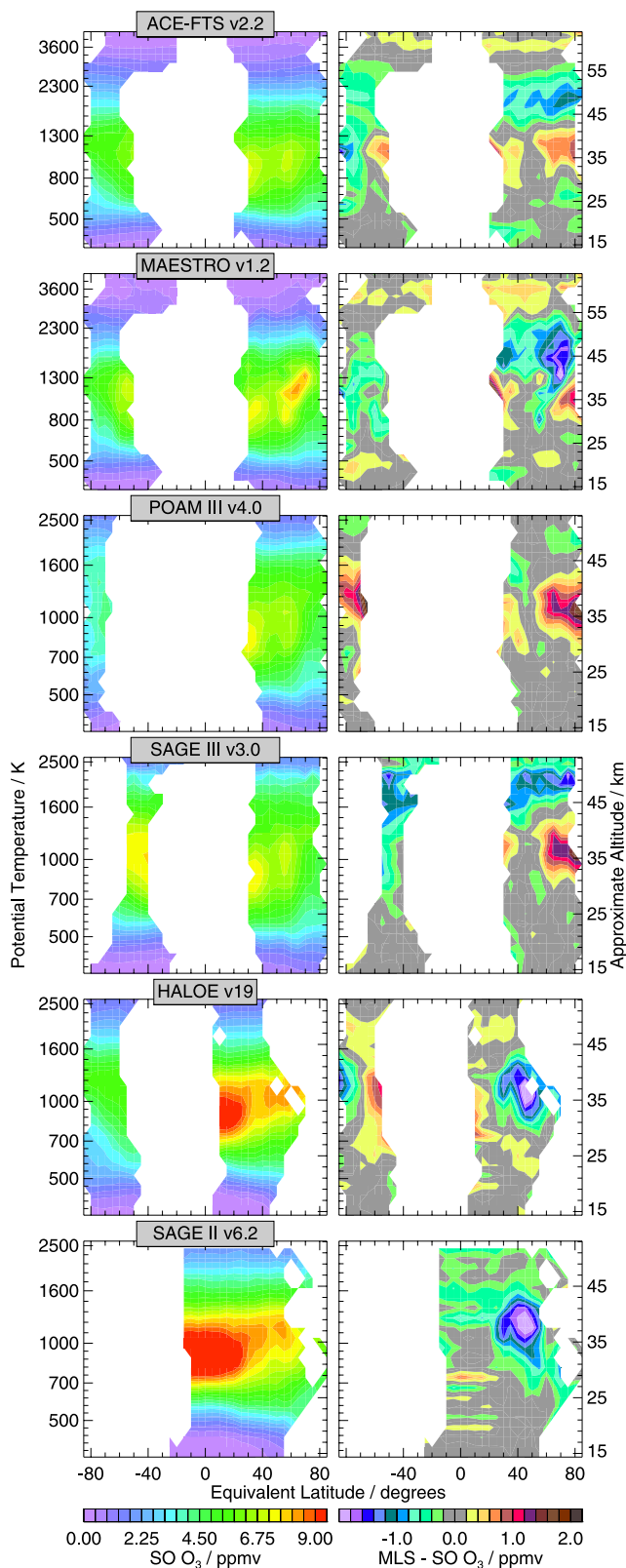


Figure 16. Global EqL/ θ cross sections for 10–16 March 2005 comparing MLS v2.2 O_3 with (top to bottom) ACE-FTS, MAESTRO, POAM III, SAGE III, HALOE, and SAGE II. (left) Solar occultation instruments' O_3 and (right) the MLS-solar occultation instrument O_3 difference (ppmv). For comparisons with ACE-FTS and MAESTRO, GEOS-5 DMPs are used for EqL/ θ mapping; others comparisons use MetO DMPs. MLS/ACE comparisons are shown from 360 through 4430 K; others are 360 through 2500 K (the top limit of the MetO DMPs).

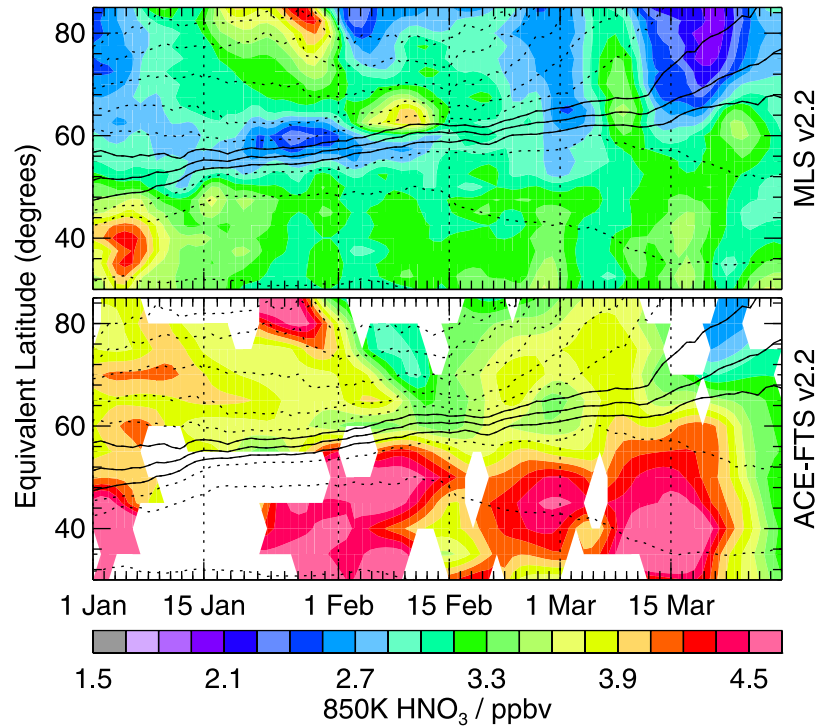


Figure 17. As in Figure 13 but for (top) MLS v2.2 and (bottom) ACE-FTS HNO_3 (ppbv) at 850 K, using GEOS-4 DMPs.

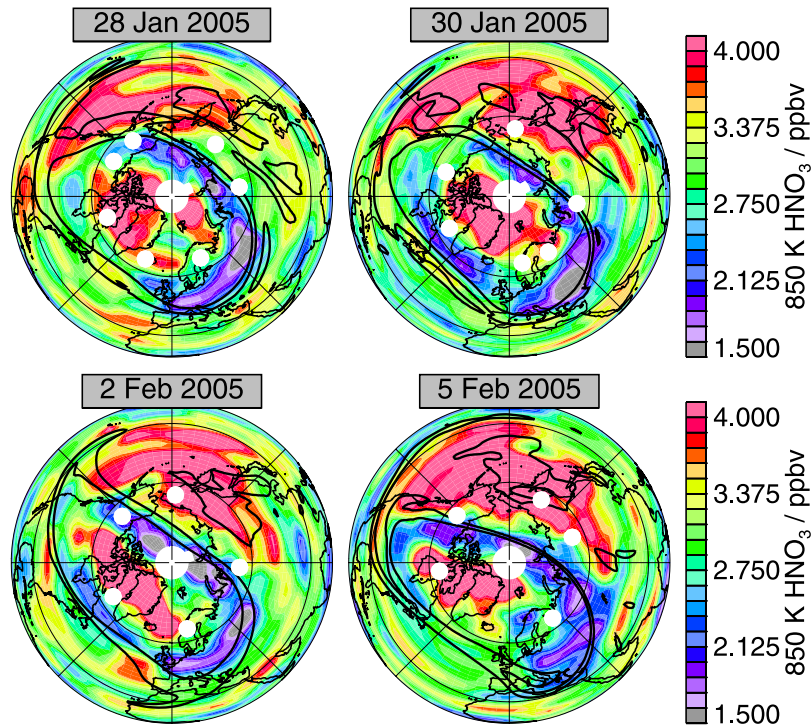


Figure 18. Maps of MLS v2.2 HNO_3 (ppbv) at 850 K for 28 and 30 January and 2 and 5 February 2005, with ACE-FTS observation locations (white dots) overlaid. PV contours in the vortex edge region are overlaid in black. Projection is orthographic, with 0° longitude at the bottom; latitude range is from 0 to 90°N . White space above $\sim 82^\circ\text{N}$ is region not sampled by MLS.

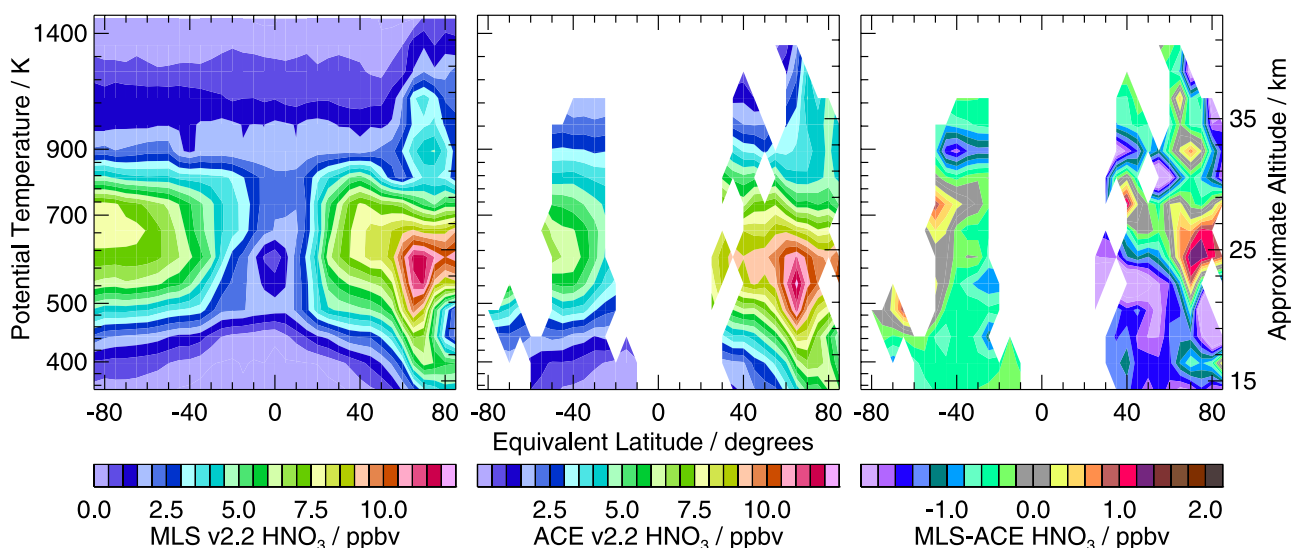


Figure 19. As in Figure 9 but for MLS v2.2 and ACE-FTS HNO_3 (ppbv) for 25–31 January 2005, using GEOS-5 DMPs. Vertical range is 400–1600 K.

et al. [2007]. Because the depletion of the reservoir HCl by activation of Cl is largely well correlated with the vortex, sampling effects on HCl comparisons are minimal.

4.3.3. Temperature

[54] The use of vortex centered (i.e., EqL) coordinates is not an obvious choice for temperature from a scientific point of view, since temperature is not, in general, expected to be closely spatially correlated with the vortex [e.g., Manney *et al.*, 1996a, 2003b; Mann *et al.*, 2002]. However, we are often interested in temperatures within the vortex, and the comparison between MLS and solar occultation instruments can help us understand how the sparse sampling of the solar occultation instruments may affect studies of processes depending on temperature. Also, the EqL coordinate still provides a method of comparing solar occultation measurements with other data sets over a broader range of conditions than can easily be done with individual coincidences or zonal means.

[55] Figure 21 compares EqL/ θ -mapped MLS and ACE-FTS temperatures in September 2005, during the SH late winter. MLS appears lower than ACE-FTS almost everywhere, by a much larger amount than the small bias noted by Schwartz *et al.* (submitted manuscript, 2007). During this period, there was strong wave activity throughout the stratosphere, with the vortex distorted and shifted off the pole, and a dipole pattern of low/high temperatures across the vortex edge on the side with the anticyclone (Figure 22). ACE-FTS measurements were in the outer part of the vortex, so tended to miss the coldest region and sample near the warmest region on most days during the period (Figure 22), resulting in the apparent low bias of MLS with respect to ACE-FTS. This shows how strong a factor sampling is in comparisons of temperature, and demonstrates the care that must be taken in interpreting temperatures in vortex-centered coordinates.

5. Summary and Outlook

[56] Derived meteorological products (DMPs) have been calculated and made available for Aura MLS and the solar

occultation instruments ACE-FTS, MAESTRO, HALOE, POAM II and III, and SAGE II and III. The DMPs are fields calculated from gridded meteorological analyses that are interpolated to the observation locations of the satellite instruments. The DMP fields include θ , horizontal winds, PV, horizontal PV gradients, EqL, geopotential height, vortex edge criteria, and tropopause locations; DMP files for some instruments include additional potentially useful quantities such as temperature gradients and line-of-sight PV and temperature gradients. The DMPs have been calculated from the Met Office stratosphere-troposphere assimilation data set for all instruments; in addition, DMPs from GEOS-4 and GEOS-5 are available for ACE-FTS and MLS, and from NCEP/CPC data for SAGE II. DMPs are not limited to the Aura mission, but have been calculated for the entire mission for each instrument. DMPs are provided (see Appendix A) with the hope that other researchers will find them useful both for validation and in science studies combining multiple data sets.

[57] Examples comparing MLS and solar occultation data were used to illustrate sampling issues. Situations in which sampling effects can be important include (1) comparison of fine-scale transport features (e.g., filaments and intrusions into the vortex) as represented in high-resolution gridded meteorological analyses and in MLS data; (2) studies using “vortex averages” of long-lived tracers to estimate descent, where the movement of solar occultation sampling from vortex edge to vortex center over time can result in erroneous estimates of descent; (3) studies of O_3 in the middle stratosphere in low- O_3 pockets, where the combination of chemical and dynamical processes results in O_3 distributions that are not closely aligned with the vortex; (4) localized features (such as PSC-induced depressions in gas phase HNO_3) that are captured by MLS but not by sparse solar occultation sampling; and (5) comparisons during polar winter when the temperature field is typically not well correlated with the vortex, such that sparse solar occultation sampling misses extreme values. Solar occultation data are extremely valuable for understanding the

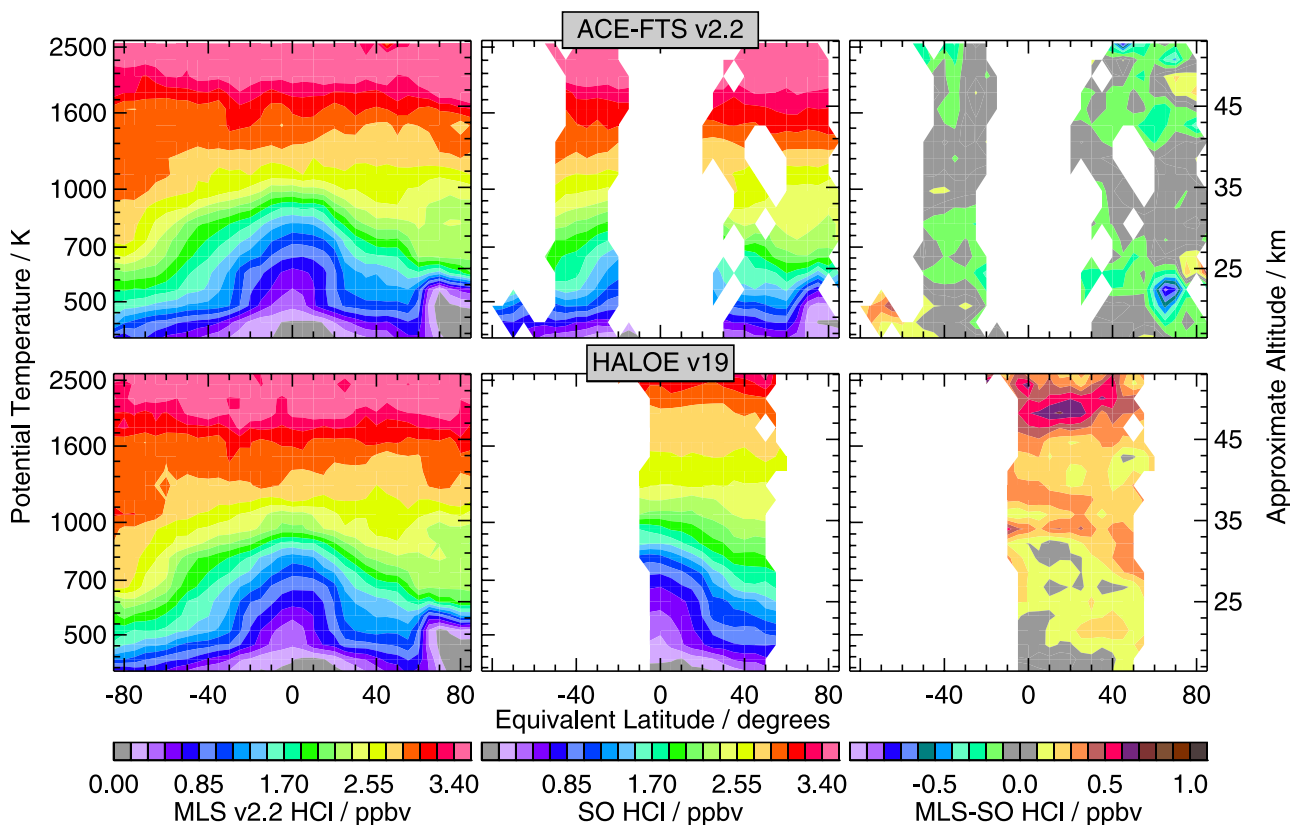


Figure 20. As in Figure 9 but for MLS v2.2, ACE-FTS, and HALOE HCl (ppbv) for 25–31 January 2005. ACE-FTS comparison uses GEOS-5 DMPs, HALOE comparison uses MetO DMPs. Vertical range is 400–2500 K.

atmosphere and monitoring its long-term changes, because of their high vertical resolution and precision, the availability of long, calibrated data sets (e.g., SAGE II, HALOE, POAM), and the potential for detecting many species (e.g., ACE-FTS). Even greater value is realized in studies combining solar occultation with other data, such as those from UARS MLS [e.g., Manney *et al.*, 1999, 2000; Randel *et al.*, 1999] and Aura MLS [Braathen *et al.*, 2006; Singleton *et al.*, 2007; M. L. Santee *et al.*, A study of stratospheric chlorine partitioning based on new satellite measurements and modeling, submitted to *Journal of Geophysical Research*, 2007]. The spatial sparsity of the solar occultation data makes understanding sampling effects critical; sampling limitations have been studied here using DMPs to help guide interpretation of the solar occultation data and combination of them with other data sets.

[58] Several of the examples shown here indicate good agreement in time evolution and spatial structure of MLS and solar occultation observations when mapped using DMPs, complementing traditional validation studies shown in other papers in this special section. For these types of studies, using DMPs to combine MLS and solar occultation data sets in a consistent framework is a powerful analysis tool. Two such areas are transport studies based on long-lived tracers, and polar processing in the winter lower stratosphere.

[59] Comparisons of MLS and ACE-FTS long-lived trace gas measurements show the following:

[60] 1. ACE-FTS and MLS v2.2 CO and H₂O provide a similar picture of the descent of mesospheric air into the stratospheric vortex, both in magnitude and timing.

[61] 2. MLS v2.2 N₂O and H₂O show excellent agreement with ACE-FTS data in EqL/time evolution in the middle and lower stratosphere

[62] 3. MLS v2.2 and ACE-FTS CO show excellent agreement in EqL/time evolution in the middle and upper stratosphere.

[63] 4. MLS v2.2 N₂O shows a persistent low bias with respect to ACE-FTS in the polar lower stratosphere. Elsewhere, differences are typically within ~5 ppbv, with localized differences up to ~15 ppbv.

[64] 5. MLS v2.2 and ACE-FTS H₂O agree very well throughout the stratosphere, typically to within 5%. HALOE H₂O shows a persistent low bias with respect to MLS of ~5–10%, consistent with previous studies.

[65] 6. MLS v2.2 and ACE-FTS CO compare very well qualitatively, and overall quantitatively; however, MLS CO data are noisy and still characterized by some vertical oscillations in the stratosphere that compromise detailed quantitative agreement.

[66] The effects of sampling differences on these comparisons are minimal, except for the “vortex averages” described above. Using EqL mapping of long-lived tracers thus facilitates combining solar occultation and MLS data sets for transport studies.

[67] Good agreement is also seen in most analyses of species involved in lower stratospheric polar processing:

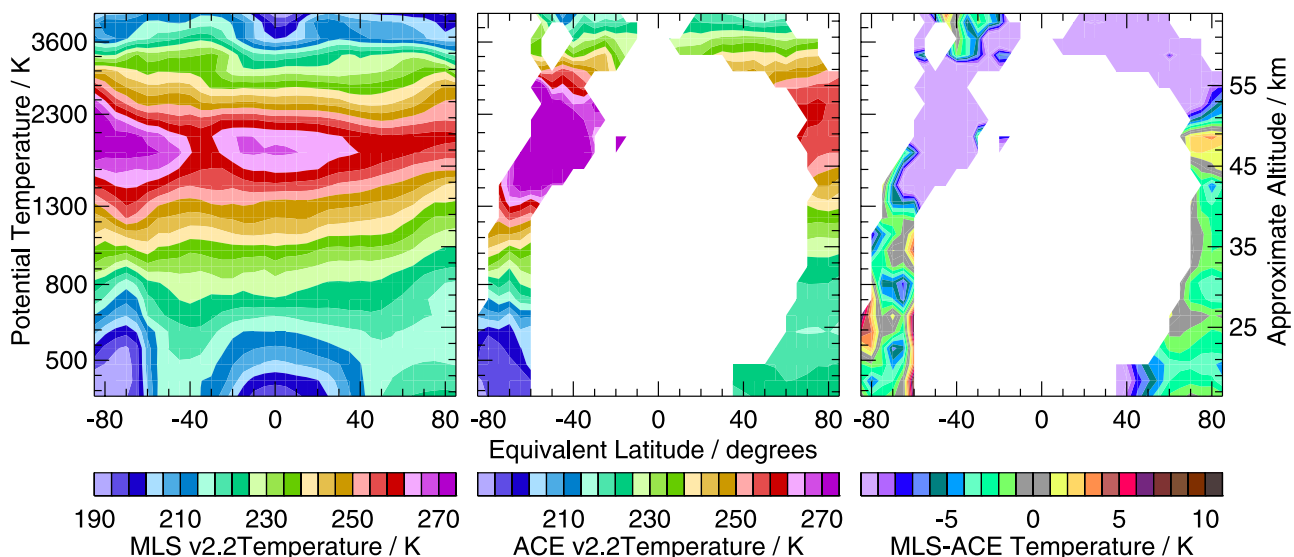


Figure 21. As in Figure 9 but for 17–24 September 2005 MLS v2.2 and ACE-FTS temperatures, using GEOS-5 DMPs. Vertical range is 360 to 4300 K.

[68] 1. Time evolution and values of O₃ in the lower stratospheric vortex agree well between MLS v2.2 and ACE-FTS, MAESTRO, POAM III, and SAGE III (the solar occultation instruments with good coverage of the vortex), and all instruments show a similar amount of decrease related to chemical O₃ loss.

[69] 2. O₃ agrees to within 5% from tropopause level through the lower stratosphere, with larger differences only at higher levels where chemical processes that are not well correlated with the vortex become important.

[70] 3. MLS v2.2 and ACE-FTS HNO₃ agree very well qualitatively, but MLS shows a low bias with respect to ACE-FTS; agreement in morphology and time evolution in the lower stratosphere is good, except when ACE-FTS sampling misses regions of PSCs.

[71] 4. MLS v2.2 and ACE-FTS HCl agree well throughout the stratosphere; HALOE HCl is ~5–25% lower than

MLS and ACE-FTS. Morphology and time evolution of MLS and ACE-FTS HCl in and around the lower stratospheric vortex agree well.

[72] The good agreement and limited impact of sampling issues imply that vortex-centered analyses are useful for detailed polar-processing studies.

[73] Further work to add to and improve DMPs is planned, including calculating DMPs for all solar occultation data sets from GEOS-4 (and, when the reanalysis is completed, GEOS-5) data, and calculating DMPs for SAGE I and possibly for other data sets, such as UARS MLS and UARS Cryogenic Limb Array Etalon Spectrometer. We hope to continue operational production of the DMPs for MLS and ACE-FTS for the duration of those missions. A procedure is available for users to request DMPs calculated at locations that they define (see Appendix A); this system is being used to produce DMPs for ACE-FTS validation

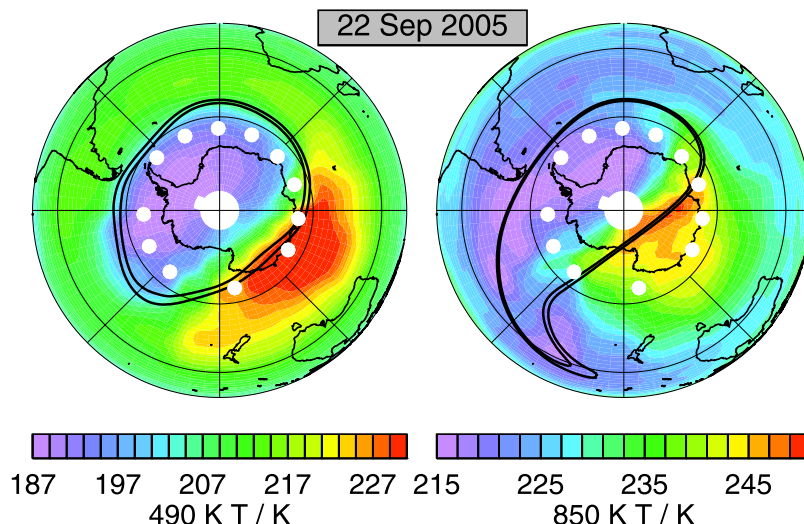


Figure 22. Maps of MLS v2.2 Temperature (colors, K) on 22 September 2005 at (left) 490 K and (right) 850 K. Overlaid contours are 1.4 and $1.8 \times 10^{-4} \text{ s}^{-1}$ sPV. White dots show ACE observation locations.

Table A1. Availability of Solar Occultation Instrument DMPs via FTP

Mission/Instrument	Location ^a	Types	Time Range
ACE	distributed by ACE team	MetO, GEOS{4,5}	Jan 2004 to present
SAGE II ^b	sage2/dmp/v5.0	NCEP/CPC	Oct 1984 to Aug 2005
SAGE II ^b	sage2/dmp/v5.0	MetO	Oct 1991 to Aug 2005
SAGE III ^b	sage3/v03.00/dmp/g3asmb/v1.1/<y>/<d> ^c	MetO	May 2002 to Dec 2005
POAM II ^b	poam2/v6.00/dmp/v1.0	MetO	Oct 1993 to Nov 1996
POAM III ^b	poam3/v4.00/dmp/v1.0	MetO	Apr 1998 to Dec 2005
HALOE	haloe/v19/dmp/v1.1/<y>	MetO	Oct 1991 to Nov 2005

^aRelative to pub/outgoing/manney after logging in via FTP.

^bExample software for reading SAGE II and III and POAM II and III DMPs can be found at https://www.openchannelsoftware.com/projects/Example_IDL_Readers_for_DMPs.

^c<y> = 4-digit year, <d> = 3-digit day-of-year.

campaigns [e.g., Walker et al., 2005; Kerzenmacher et al., 2005] conducted in Eureka in 2004 through 2007 and planned for 2008. Manney et al. [2007] used Eureka DMP products along with ACE-FTS, MLS, Sounding of the Atmosphere through Broadband Emission Radiometry, and ground-based data to provide a meteorological context for the 2004, 2005 and 2006 campaigns, and they, and ACE DMPs, are being used in other ACE validation studies. We are using the DMPs in several studies combining solar occultation data sets and MLS data, and hope that they will be useful to other researchers in similar efforts.

Appendix A: DMP Access, File Format, and Usage

[74] Table A1 shows the locations for solar occultation DMP access via anonymous ftp from mls.jpl.nasa.gov; these can also be accessed from the MLS Web page (<http://mls.jpl.nasa.gov>) under <http://mls.jpl.nasa.gov/research/meteorology.php>. The ACE-FTS DMPs are provided to the ACE-FTS Science Team and distributed by them. For information on these products, please contact ACE-FTS Mission Scientist Peter Bernath (info@acebox.uwaterloo.ca).

[75] DMPs can also be obtained by request at user-defined (UD) times/locations; see <http://mls.jpl.nasa.gov/docs/genericDMPdescription.txt> for information on how to make such a request and the format for the input files.

[76] Aura MLS DMPs are publicly available at <http://mls.jpl.nasa.gov/dmp>. Users must first request access and agree not to redistribute the MLS DMP files. This access request is not intended as a restriction, but rather as a means to gauge community uses for these products and to provide users with updates and information on changes or problems. MLS DMPs can be downloaded for v1.5 and v2.2, GEOS-4 or 5 and MetO, for the full Aura mission.

[77] The formats of the DMP files are designed to follow as closely as possible the formats of the data sets they are provided for. Information on the file formats and links to sample read software are provided on the ftp or web sites along with the DMPs.

[78] **Acknowledgments.** We thank the JPL MLS Science Team, especially Robert P. Thurstans, Ryan Fuller, Brian J. Mills, Paul A. Wagner, and Xuan Sabouchi, for their continuing support and assistance; Sharon Burton and Nina Iyer for assistance with SAGE II data; Randy Moore and David Risley for assistance with SAGE III data; and three anonymous reviewers for their helpful comments. Past and present members of the Met Office Assimilation Applications Group (formerly Middle Atmosphere Group) have been responsible for developing the MetO-SST data set and for maintaining the daily operational flow of these data; MetO data are

provided by the British Atmospheric Data Centre. Research at the Jet Propulsion Laboratory, California Institute of Technology, is done under contract with NASA. Funding for the ACE mission was provided primarily by the Canadian Space Agency and the Natural Sciences and Engineering Research Council of Canada.

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