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Key Points:

- Water vapor data from the Stratospheric Aerosol and Gas Experiment on the International Space Station are assessed
- Data screening procedures are described for removing anomalous data and data impacted by cloud interference
- With appropriate filtering, the new data agree with other correlative measurements within ~10% in the stratosphere

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Validation of SAGE III/ISS Solar Water Vapor Data With Correlative Satellite and Balloon-Borne Measurements

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Abstract Since June 2017, the Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station (SAGE III/ISS) has been providing vertical profiles of upper tropospheric to stratospheric water vapor (SWV) retrieved from solar occultation transmission measurements. The goal of this study is to evaluate the publicly released SAGE III/ISS beta version 5.1 WV retrieval through intercomparison with independent satellite- and balloon-based measurements, and to present recommendations for SAGE III/ISS data quality screening criteria. Overall, we find that SAGE III/ISS provides high quality water vapor measurements. Low quality profiles are predominately due to retrieval instabilities in the upper stratosphere that cause step-like changes in the profile, and aerosol/cloud-related interferences (below ~20 km). Above 35 km, the retrieved uncertainty and noise in the data rapidly grow with increasing altitude due to relatively low extinction signal from water vapor. Below the tropopause, retrieved uncertainty increases with decreasing altitude due to enhanced molecular scattering and aerosol extinction. After screening low-quality data using the procedures described herein, SAGE III/ISS WV is shown to be in good agreement with independent satellite and balloon-based measurements. From 20 to 40 km, SAGE III/ISS WV v5.1 data exhibit a bias of 0.0 to −0.5 ppmv (~10%) relative to the independent data, depending on the instrument and altitude. Despite its status as a beta version, the level of SAGE III/ISS WV agreement with independent data is similar to previous SAGE instruments, and therefore the data are suitable for scientific studies of SWV.

Plain Language Summary Measurements of water vapor (WV) in the stratosphere are important for understanding climate change. This study presents new measurements of SWV from an instrument aboard the International Space Station, and describes methods for filtering the data to retain only the highest quality profiles for scientific analysis. The new measurements compare well to existing satellite and scientific balloon measurements of SWV, and therefore will be of use for studying year-to-year and longer-term changes in SWV.

1. Introduction

Water vapor plays an important role in determining the radiative balance of Earth's atmosphere, and variations in stratospheric water vapor (SWV) concentrations have been shown to affect radiative forcing (Forster & Shine, 1999; Solomon et al., 2010), ozone concentrations (Dvortsov & Solomon, 2001), and atmospheric circulation (Maycock et al., 2013). These variations in SWV can occur on subseasonal to decadal timescales, so accurate and continuous global measurements of SWV are essential in order to understand SWV variability over the range of relevant timescales. Although no formal satellite-based monitoring program exists for SWV, a number of temporally overlapping satellite instruments have been making measurements of SWV continuously since the launch of the Stratospheric Aerosol and Gas Experiment II (SAGE II) in

1984. This collection of satellite SWV measurements, which is described comprehensively by the second Stratosphere-troposphere Processes And their Role in Climate (SPARC) water vapor assessment (WAVAS-II, Lossow et al., 2019), includes both the SAGE II instrument (1984–2005, Damadeo et al., 2013), as well as the SAGE III instrument that flew aboard the METEOR-3M satellite (SAGE III/M3M, 2002–2005, Thomason et al., 2010).

In June 2017, a new SAGE III instrument aboard the International Space Station (SAGE III/ISS) began regular operation and has been making ∼30 solar occultation measurements per day since that time. From these sunrise and sunset transmittance measurements, vertical profiles of ozone (Wang et al., 2020), nitrogen dioxide, water vapor, and aerosol extinction at multiple wavelengths are retrieved, and have been made publicly available as version 5.1.

2. SAGE III/ISS Solar Water Vapor Data

2.1. Instrument Description and Retrieval

The SAGE III/ISS instrument is essentially the same as the SAGE III/M3M instrument (W. Chu et al., 1997; W. P. Chu & Veiga, 1998), with additional hardware to operate onboard the International Space Station and an improved neutral density filter to eliminate thick plate etalon features in the solar events (Cisewski et al., 2014; Thomason et al., 2010). Like previous SAGE instruments, it uses the technique of solar occultation to produce line-of-sight (LOS) transmission profiles at each wavelength from the top of the atmosphere down to the cloud top (W. P. Chu & Mccormick, 1979). SAGE III/ISS is also capable of making observations using lunar occultation or limb scatter modes, but those measurements do not produce water vapor as a retrieval product and are thus not discussed here. As a CCD spectrometer, observations of absorption by water vapor in the atmosphere are made using 27 different pixel columns on the CCD between 933 and 958 nm, each with a spectral resolution of ∼3 nm. Two additional pixel columns with similar resolution near 920 and 971 nm are also used. Collectively, this spectral range measures in the rho-sigma-tau bands in the water vapor spectrum as well as the Wulf band in the ozone spectrum.

This study discusses the results of the version 5.1 beta release of water vapor. The retrieval algorithm is a nonlinear Levenberg Marquardt, onion-peeling algorithm making use of the Curtis-Godson approximation forward model to turn wavelength-dependent LOS transmission profiles into profiles of water vapor, ozone, and aerosol simultaneously. The retrieval provides profiles of both the retrieved quantities and their uncertainties. The reported uncertainties in the water vapor product are the best estimate of the random measurement uncertainty in the SAGE instrument propagated through the retrieval and do not include any systematic component.

Contributions from Rayleigh/molecular scattering are removed first, but ozone is not simply cleared out as an interfering species despite having an arguably more robust solution (of ozone extinction) from another part of the SAGE III/ISS retrieval algorithm (e.g., see Wang et al., 2020 for a description of the SAGE III/ISS ozone product). This is because doing so would make the water vapor solution dependent upon the relative accuracy of the ozone cross-section database used here (Bogumil et al., 2003) between the primary ozone solution spectral range (∼600 nm) and that used for water vapor (∼945 nm). Similar retrievals in SAGE II using the same cross-section database suggest that the relative difference in ozone cross-sections between the two spectral regimes could be off by about 10% (Damadeo et al., 2013). Instead, the increased spectral resolution of SAGE III/ISS (compared to SAGE II) makes the retrieval sensitive only to the relative shape of the ozone cross-sections in the water vapor channel and not their overall magnitude (Thomason et al., 2010). However, the ozone and aerosol solutions that derive from the water vapor retrieval are not reported as part of the public data product. It is important to point out that in v5.1, unlike other SAGE III/ISS data products, the water vapor retrieval is performed on a 1 km grid and the results are interpolated to a 0.5 km grid. The LOS transmission profiles are also smoothed with a 1-2-1 smoothing on a 1 km grid for use with the water vapor retrieval, giving the final product a 2 km vertical resolution.

The SAGE III/ISS instrument and its operation in solar occultation mode is similar to its predecessors (e.g., SAGE II and SAGE III/M3M), but includes some advances which permit measurement of additional wavelengths. A general description of the solar occultation measurement technique is provided by McCormick

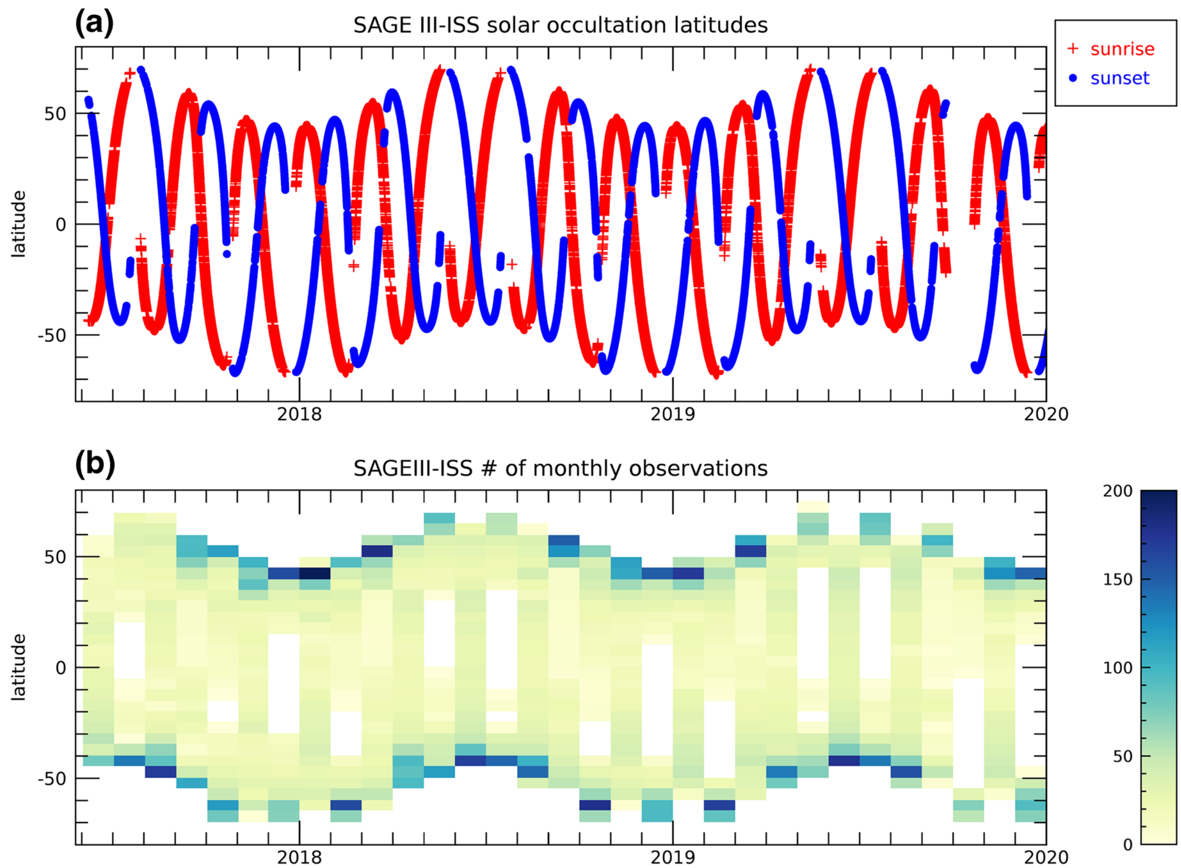

Figure 1. (a) SAGE III/ISS solar occultation latitudes as a function of latitude and time, separated by event type (sunrise and sunset). (b) The number of SAGE III/ISS solar occultation measurements as a function of latitude and time, in monthly 5° latitude bins. Data shown are from the mission start (June 2017) through December 2019. SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station.

et al. (1979), but here we briefly describe how SAGE III/ISS acquires the radiant target and uses a scanning mirror to scan the target image across the instrument field-of-view aperture. A measurement is considered to occur at the point along the line of sight from the instrument to the target that comes closest to the Earth's surface (i.e., the subtangent point). The altitude of that point above the Earth's surface is commonly referred to as the tangent altitude.

The use of a scanning mirror provides multiple samples at each tangent altitude that are combined to construct transmission profiles from the Earth's surface (or cloud top) to an altitude of 100 km. Above this altitude, irradiance measurements are acquired between 100 and 250 km to characterize the instrument's performance across its wavelength range. This information is used to calibrate the instrument for each solar occultation event. By using this procedure, SAGE III data are relatively unaffected by changes in the instrument characteristics over the lifetime of the mission.

2.2. SAGE III/ISS Solar Sampling Characteristics

The ISS is inclined in a 52° orbit, and as such, sunrise and sunset latitudes oscillate from their extreme latitude in one hemisphere to their extreme in the other hemisphere approximately every 30 days (Figure 1a). This pattern results in expanded sampling coverage compared to SAGE III/M3M. The latitudinal sampling envelope varies seasonally, in phase with the subsolar latitude, such that the sampling is shifted northward during boreal summer and southward during boreal winter. As with other mid- and high-inclination orbit solar occultation instruments, the sampling is denser at higher latitudes and sparser in the tropics, with on average 2–3 months per year of no tropical data at near-equatorial latitudes (Figure 1b).

Table 1
Frost Point Hygrometer Soundings Used in This Study (June 17, 2017 to December 31, 2019)

Station	Instrument	Latitude	Longitude	# Soundings	# SAGE coincidences
Lindenberg (GER)	CFH	52.2	14.1	64	4
Boulder (USA)	FPH	40	−105.2	38	13
Hilo, HI (USA)	FPH	19.7	−155.1	28	2
San Jose (CRI)	CFH	10	−84.1	29	4
Lauder (NZL)	FPH	−45	169.7	28	7
TOTAL				187	30

3. Correlative Data and Methods

3.1. Aura MLS

The Aura Microwave Limb Sounder (MLS) instrument began taking data in August 2004 from aboard the NASA Earth Observing System Aura satellite (Waters et al., 2006). MLS measures thermally emitted microwave radiation from Earth's limb, and retrieves water vapor using the 190 GHz channel (Lambert et al., 2007; Read et al., 2007). MLS achieves nearly global coverage (82°S–82°N), sampling ∼3,500 profiles per day with a vertical resolution of 2.5–3.5 km for SWV (100 hPa–1 hPa). Here, we use version 4.2 data, which are provided at 12 levels per decade (∼1.25 km) for pressures greater than 1 hPa. Over this range, the estimated accuracy (precision) for water vapor ranges from 4% to 19% (4%–15%, Livesey et al., 2020), based on both retrieval characterization and validation with independent measurements (Hurst et al., 2014; Lambert et al., 2007; Read et al., 2007; Vomel, Barnes, et al., 2007; Vömel, David, & Smith, 2007). The MLS data are broadly in agreement with correlative satellite data sets at this level, as addressed by the recent second SPARC data initiative and water vapor assessment (WAVAS-II) activities (Hegglin et al., 2013; Khosrawi et al., 2018; Lossow et al., 2019). MLS data are screened according to the recommendations in the Aura MLS version 4.2 data quality document (Livesey et al., 2020).

3.2. ACE-FTS

The Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) is a solar occultation limb sounder launched in 2003 aboard the SCISAT satellite. ACE-FTS measures mid-infrared radiances (750–4,400 cm^{-1}) with a vertical field of view of ∼3–4 km to retrieve numerous trace gases on a 1 km altitude grid. Measuring since February 2004, ACE-FTS observes up to 30 solar occultation events per day, with sampling focused on high latitudes due to its high inclination orbit (74°). In this study, we use both ACE-FTS v3.6 data, which is a minor update to the validated v3.5 data (Boone, 2013; Sheese et al., 2017), and the recently released v4.1 data (Boone et al., 2020). The newest version of ACE-FTS is included here to assess any potential differences between it and the well validated earlier version of the data. Validation efforts for ACE-FTS v3.5 data have demonstrated that the water vapor product has good stability and mean bias within 10% (17–70 km) in comparison to the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) and Aura MLS measurements (Sheese et al., 2017). The assessment of ACE-FTS data in WAVAS-II also corroborates these results (Khosrawi et al., 2018; Lossow et al., 2019).

3.3. Frost Point Hygrometer Measurements

The balloon-borne frost point water vapor measurements used here consist of NOAA Frost Point Hygrometer (FPH, Hurst et al., 2011) and Cryogenic Frostpoint Hygrometer (CFH, Vomel, Barnes, et al., 2007; Vömel, David, & Smith, 2007) soundings at five sites (see Table 1) during both routine monthly soundings and specially chosen times to correspond to ISS overpasses. The CFH and NOAA FPH use the same basic principle to measure frost point temperatures at high vertical resolution (∼5 m), but there are subtle differences in the way they operate. Each uses a different optical system and control parameters to regulate a thin layer

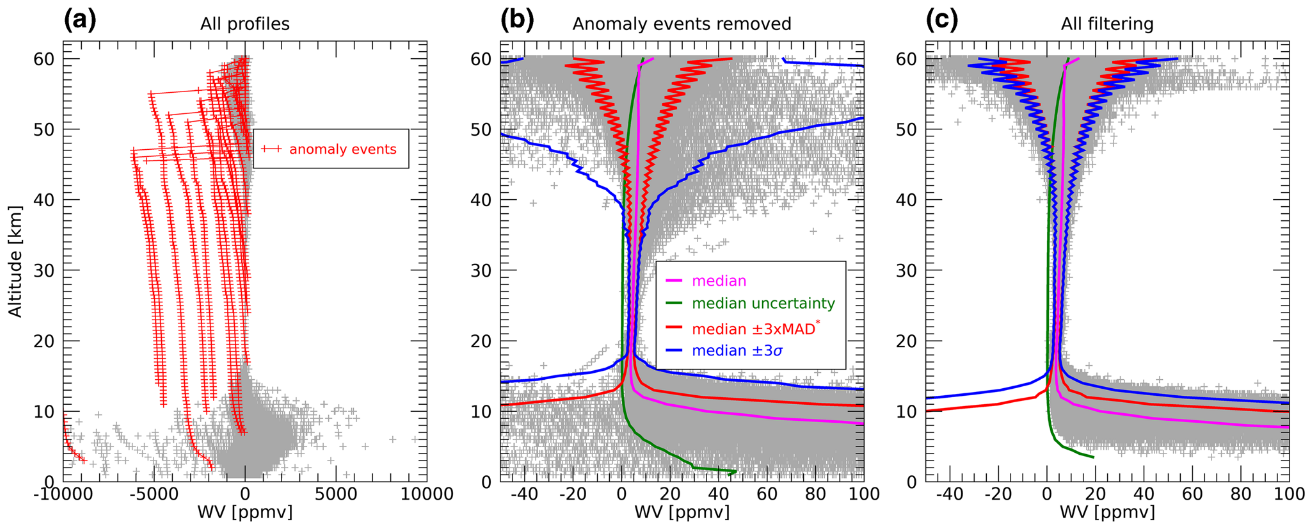

Figure 2. (a) All retrieved water vapor values collected by SAGE III/ISS through the end of 2019 (gray +). Anomalous water vapor profiles are shown in red (see Table 2), and have been removed in the middle and right panels. (b) SAGE III/ISS WV values on an enlarged scale, along with the median values (magenta), median uncertainties (green), and two diagnostics of the dispersion of the data: the median ± 3-standard deviation lines (blue) and corresponding median ± 3 times the scaled median absolute deviations (MAD* = 1.48 x MAD, red). (c) SAGE III/ISS WV values after removal of anomalous profiles (Section 4.1), keel-over profiles (Section 4.2), and aerosol/cloud contaminated data (Section 4.3). SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station; WV, water vapor.

of ice on a temperature-controlled mirror, and there are also differences in the way unwanted stray light (i.e., sunlight) is filtered. Several dual flights of the two hygrometers since 2005 have demonstrated their agreement is well within the stated measurement uncertainties (<10%), especially in the stratosphere (Hall et al., 2016; Vomel, Barnes, et al., 2007; Vömel, David, & Smith, 2007). Laboratory measurements between 2and 600 ppmv show biases relative to a reference instrument of 1% for the NOAA FPH (Hall et al., 2016).

3.4. Coincident Profiles

For identifying coincident measurements from correlative data sources, it is necessary to define coincidence criteria since measurements are generally not made at the exact time and geographical location. Here, we use criteria very similar to that used by Wang et al. (2020) to identify matched pairs of ozone profiles from SAGE III/ISS and correlative satellite data sets. For matching other data sets with SAGE III/ISS, we consider profiles to be matched with SAGE III/ISS if they fall within ±1 day, ±2° latitude, and ±1,113 km in longitude (i.e., equivalent to ±10° longitude at the equator). For the case of multiple correlative profiles meeting this match criteria, the profile with the closest spatial distance is chosen.

These criteria lead to 16% of frost point (FP) profiles obtained at the five sites between the start of SAGE III/ISS data and the end of 2019 being matched with SAGE. Of the matched FP-SAGE measurements, the median separation is 500 km and the root-mean-square time difference is 13 h. It is worth noting that while the matching criteria used here are generally sufficient to obtain a good comparison in the overworld stratosphere, large geophysical variability in the upper troposphere and a small sample size mean the matched profile comparisons are highly uncertain in that region.

4. SAGE III/ISS Data Quality Screening Criteria

4.1. Known Anomalies and Outliers in Version 5.1

As of the end of 2019, SAGE III/ISS has collected 21,879 solar occultation profiles of water vapor, all of which are shown in Figure 2. An analysis of these reveals a number of anomalous profiles that can be broken into two categories: failed retrievals and "keel-over" profiles. Both of these anomalies have a similar

Table 2
Anomalous Water Vapor Events in SAGE III/ISS Version 5.1 (June 17, 2017 to December 31, 2019)

Event number	Date	Time	Latitude	Longitude	Reason
1128120	May 11, 2018	12:51:54	−39.97	60.35	anomaly
1495410	January 2, 2019	16:59:41	43.92	−139.92	anomaly
1587720	March 3, 2019	3:01:49	−54.70	−122.50	anomaly
1587920	March 3, 2019	6:07:17	−54.45	−169.04	anomaly
1589520	March 4, 2019	6:50:56	−52.29	178.72	anomaly
1592220	March 6, 2019	0:34:43	−48.09	−89.27	anomaly
1596720	March 8, 2019	22:08:09	−39.07	−55.50	anomaly
1630910	March 3, 2019	22:05:22	−43.44	123.49	anomaly
1632310	March 31, 2019	19:44:11	−45.70	159.39	anomaly
1683520	May 3, 2019	18:50:00	−46.95	−30.86	anomaly
1739820	June 9, 2019	0:20:16	33.84	−78.85	anomaly
1756710	June 19, 2019	22:29:33	−1.39	113.57	anomaly
1762620	June 23, 2019	17:13:27	−32.26	−3.68	anomaly
1766110	June 25, 2019	22:25:57	28.04	100.89	anomaly
719620	August 21, 2017	20:23:56	−6.69	−36.65	eclipse

cause. The amount of extinction from water vapor in the spectral region surrounding 945 nm is very small in the upper stratosphere and mesosphere and the SAGE III/ISS water vapor retrieval uses a nonlinear onion peeling technique, meaning it starts at the top of the profile and iteratively works its way down while using the previous solutions for the next iteration. With a weak signal and a nonlinear solution, instabilities can arise that result in mixing ratios that tend to oscillate back and forth between very large positive and very large negative through the onion peeling process. This oscillatory behavior, a byproduct of error propagation (Clarmann et al., 1991), is a common outcome of any onion peeling retrieval in a weak signal regime and results in a noisy solution at the top of the profile that relaxes with decreasing altitude. Occasionally the solution arrives at a negative value that is so large it cannot properly recover, resulting in the anomalous profiles shown in red in Figure 2a. Similarly, the solution sometimes arrives at a very large positive value high in the profile and then slowly relaxes toward a more realistic value as the retrieval moves to lower altitudes, resulting in the "keel-over" profiles, so named because the mixing ratio appears to keel over toward very large values in the upper part of the profile.

In version 5.1, the data are screened for failed retrievals or obviously unphysical results by the SAGE team prior to their release as part of a Quality Assurance (QA) step that was also done during the SAGE III/M3M mission. The large, unphysical, negative anomalies are intentionally removed during the QA step, but this is still a manual process and, as evident by Figure 2a, sometimes an error is made and failed retrievals slip through for release to the public. A list of these missed anomalies identified for manual removal is shown in Table 2. Also included in this list of bad events is one profile affected by solar eclipse conditions (i.e., with bit flag 6 set, see NASA, 2018).

While the large, unphysical, negative anomalies were intentionally, though incompletely, removed during the QA process, the keel-over profiles were intentionally left in the data set. These profiles were included so that they could be evaluated by data users to determine if the data in the lower part of the profiles were usable. Keel-over events are easily identifiable by large statistical outliers in the upper stratosphere in Figure 2b and are responsible for the divergence above ∼35 km between the standard deviation (blue line in Figure 2b) and the scaled median absolute deviation (red line in Figure 2b), which is an outlier resistant measure of the dispersion in data (Leys et al., 2013). For a normal distribution, the MAD is directly related to the standard deviation by a scale factor of 1.48, so in Figure 2 we plot the scaled MAD (i.e., MAD* = 1.48*MAD) for comparison with the standard deviation. For a normal distribution with outliers, the standard deviations are larger than the scaled MADs and is a poor measure of the dispersion in the data. The fact that the two diagnostics are in good agreement in the lower-to-middle stratosphere suggests that the data below the keel of keel-over events may still be of good quality. A method of diagnosing these events and filtering out the keel-over portion is discussed in Section 4.2, and the impact of removal of these data is show in Figure 2c.

Apart from the known anomalies discussed above, there are other statistical outliers in the upper troposphere (below ∼15 km), again evidenced by the divergence between the standard deviations and the scaled MADs. While some of this is attributable to increasing geophysical variability with decreasing altitude in this region, negative values of water vapor are not expected in the troposphere. Instead, these outliers are likely to occur due to contamination of the transmission profiles by clouds. Solar occultation retrievals assume spherical homogeneity of the atmosphere (i.e., a concentration of a species is constant for a given altitude). While this assumption generally breaks down further in the troposphere, it is particularly incorrect in the presence of clouds. This causes the data obtained when viewing a cloud to corrupt the data obtained below it during the inversion process, producing statistical outliers that are both positive and negative. As such, simply removing negative values would be insufficient which is why it

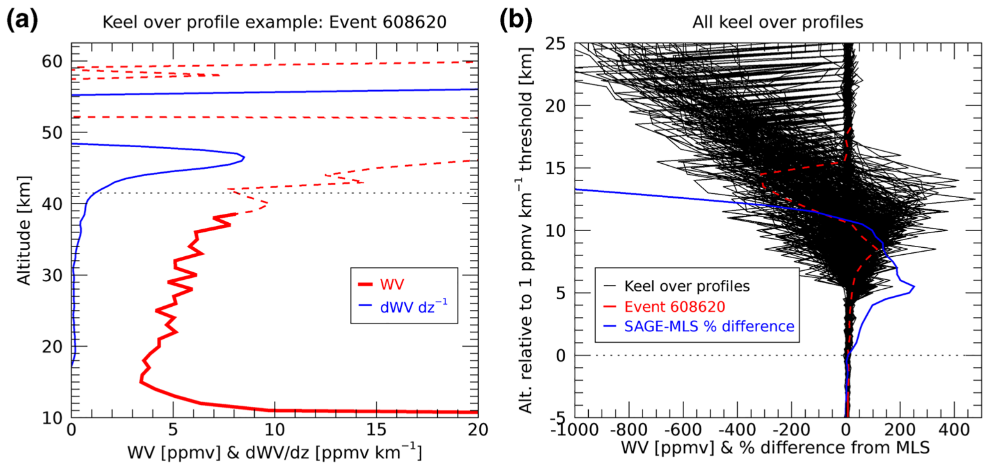

Figure 3. (a) An example keel-over profile from event #608620 taken on 2017-06-11 at 11:10:14 UTC (46.3° N, 128.9° (e). The thick red line is retained, and the dashed line is removed using the keel-over filtering described in Section 4.2. (b) A plot of all 573 keel-over profiles identified in the SAGE III/ISS data through 2019 (black lines). Also highlighted in red is the event from (a), as well as the mean percent differences from MLS for the keel-over profiles (blue). In both plots, the horizontal dotted line indicates the level at which the vertical derivative of water vapor reaches 1 ppmv km^{-1}. MLS, Aura Microwave Limb Sounder; SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station.

has always been recommended to ignore data below the top of a cloud obtained from occultation instruments. A technique for filtering this data is discussed in Section 4.3.

While negative values are not expected in the troposphere, where water vapor values are typically large, they can be present as a result of noise in the weak signal regime (i.e., in the upper stratosphere). This is clearly shown by the increasing reported uncertainties (green line in Figure 2b) and increasing spread of the scaled MADs (red line in Figure 2b) in the upper stratosphere that encompasses negative values. The oscillatory pattern in the MADs is a result of the retrieval being performed on a 1 km grid and interpolated to the 0.5 km grid, thus making the outer envelope of the MADs indicative of the spread in the retrieved data while the inner envelope is a result of the interpolation that acts like a form of smoothing in the presence of oscillatory noise patterns from onion peeling. It is generally recommended to not attempt to filter out negative values (or values with large uncertainties) in the presence of noise (such as in the upper stratosphere), as doing so has the potential to bias spatially averaged data (e.g., zonal means) high.

After applying the filtering described in the next two sections, the SAGE III/ISS data set is much more well behaved, as illustrated in Figure 2c. For example, both the 3σ and MAD* estimates are in agreement in the upper stratosphere, indicating successful removal of the outlier values in this region. Also, outliers in the upper troposphere (both negative values and large positive outliers) are removed.

4.2. Filtering Keel-Over Profiles

As mentioned in Section 4.1, keel-over profiles in the SAGE III/ISS WV data manifest as a systematic increase in WV value upwards along the profile, as illustrated in the example shown in Figure 3. In these profiles, there is a strong vertical gradient in water vapor that leads to a large positive peak in the profiles, often followed by an oscillation and large negative peak above that (see example in Figure 3a).

The general strategy for identifying keel-over profiles is to find the presence of a large positive vertical gradient in water vapor (dWV/dz), and then remove the part of the profile above the point where this occurs. Because of noise in the profiles, particularly in the mid and upper stratosphere where keel-overs occur, we smooth the profiles before computing the vertical derivatives. Through experimenting with different averaging and vertical derivative thresholds, we found that a 5 km boxcar average and derivative of 1 ppmv km^{-1} adequately identifies keel-over profiles without creating too many false positives. To be

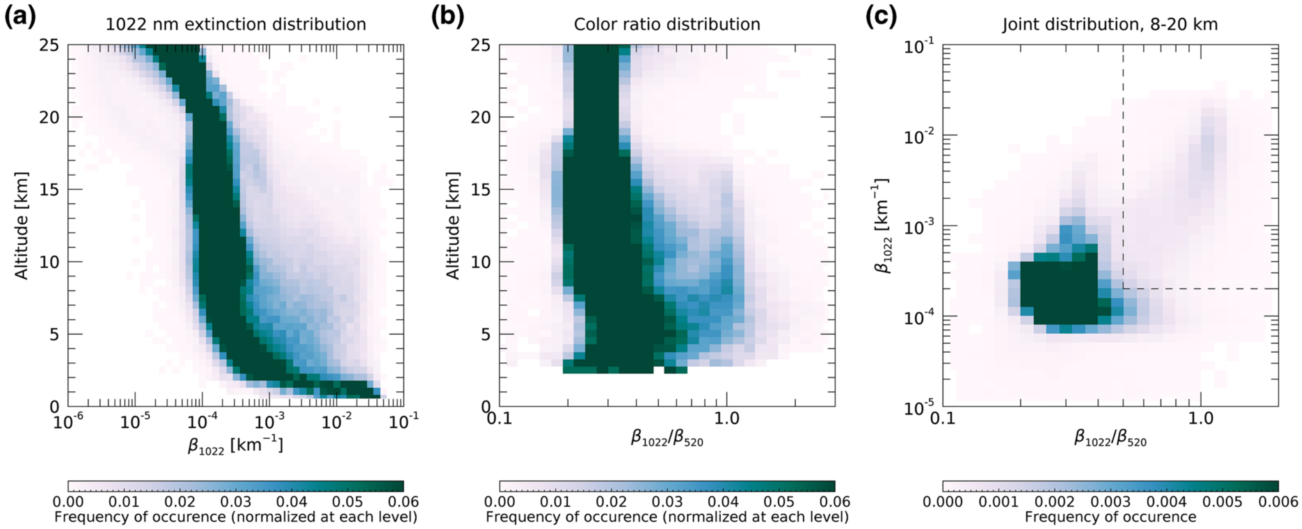

Figure 4. (a) The frequency of occurrence histogram of extinction and (b) color ratio in SAGE III/ISS data, normalized at each vertical level. (c) The joint distribution of 1,020 nm extinction and color ratio, normalized over all data between 8 and 20 km. The dashed line illustrates the threshold chosen for screening SAGE III/ISS WV data based on extinction and color ratio, as described in the text. SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station; WV, water vapor.

conservative in the filtering, we remove the portion of the profile above the level 2.5 km below the point at which the smoothed derivative is 1 ppmv km^{-1} (see dashed red lines in Figure 3 showing the removed portion of the profile).

In this filtering, we are assuming that the bottom part of the keel-over profile is of reasonable quality, which is a reasonable assumption since the retrieval iterates from the top of atmosphere downwards and the retrieval instability occurs in the tops of these profiles. However, to test this we compared the 573 keel-over profiles to their closest matched MLS profiles to verify that the SAGE III/ISS data problems occur above the 1 ppmv km^{-1} point. Indeed, the mean percent differences from MLS (blue line, Figure 3b) only appears to show extreme deviations near and above the 1 ppmv km^{-1} level, not in the lower part of the profile. In the 5 km below the keel over point, the median percent difference of SAGE III/ISS from MLS is 6%.

4.3. Filtering of Data Affected by Clouds

In general, SAGE III/ISS water vapor data become unusable in the presence of clouds. This is both within the cloud, where the LOS optical depth becomes so large that the water vapor signal is comparatively too weak to retrieve, and below the cloud, where the assumption of atmospheric spherical homogeneity corrupts data during the inversion process. For previous SAGE data, these points were identified through the use of the visible (525 nm) and/or near-infrared (1,020 nm) aerosol extinction values, and techniques could be simpler (e.g., Kent et al., 1993) or more complicated (e.g., Thomason & Vernier, 2013). Recommendations for ozone have traditionally relied on the extinction "color ratio" (β_{1022}/β_{520}); values of color ratio ~0.2–0.4 are typical for stratospheric aerosols, and values greater than ~0.5 are indicative of large (>1 μm) cloud particles. For this study, we do not attempt to create a robust analysis to differentiate between aerosol and cloud; instead we implement a set of filtering criteria that aggressively attempts to filter out cloud-like influences that would detrimentally impact retrieved water vapor.

For SAGE III/ISS data, we consider both color ratio and extinction for filtering bad WV data in the troposphere, since the combination more clearly isolates the cloud-affected portion of the data. This separation is illustrated in Figure 4, which shows the distributions of 1,022 nm extinction and color ratio as a function of altitude, and their joint distribution for data below 20 km. Filtering solely based on extinction is not straightforward, because at a given altitude the distribution is unimodal with a long tail (see

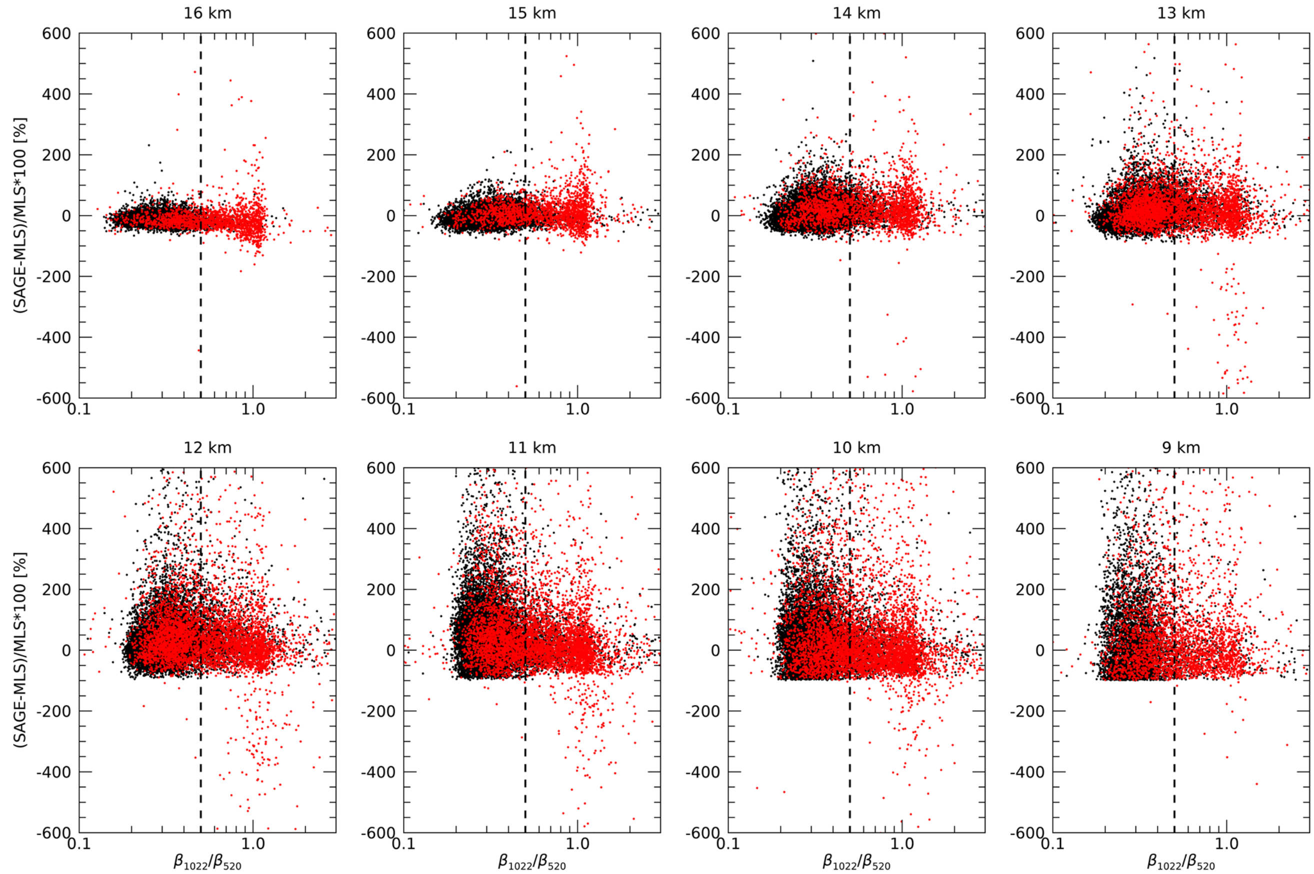

Figure 5. Percent difference of SAGE III/ISS from MLS at select levels in the upper troposphere as a function of color ratio. Black dots show all data, and red dots show data removed by the extinction and color ratio filtering described in the text. The vertical dashed line shows the color ratio threshold (0.5). Note that points with color ratio values less than 0.5 are removed in some cases. These cases occur because the color ratio and 1,022 nm extinction thresholds are exceeded at a higher altitude in the profile and the bottom part of the profile is discarded. MLS, Aura Microwave Limb Sounder; SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station; WV, water vapor.

Figure 4a); this makes identification of a threshold extinction value difficult. However, for color ratio (Figure 4b), the distribution is bi-modal, with one mode around 0.3 and another mode near 1.0. Similarly, for the joint distribution of 1,022 nm extinction and color ratio, there is a separate mode containing large values of both extinction and color ratio that is likely due to clouds (upper right, Figure 4c).

Next, we test how removing the presumed cloud-affected data affects the large number of negative SAGE III/ISS WV values in the troposphere and the comparison with MLS in this region. To filter out the affected data, for each profile we discard WV values below the point 1 km above the highest level at which both the color ratio is greater than 0.5 and the 1,022 nm extinction is greater than 2×10^{-4} km^{-1}. These thresholds are illustrated as dashed lines in the joint distribution in Figure 4c. Discarding data 1 km above the level of this exceedance is done because of the smoothing applied to the measured transmission profile during the water vapor retrieval. In addition to the extinction/color ratio filtering, we also discard WV values below the point 1 km above the highest level at which an invalid/fill value occurs in extinction from either the 520 or 1,022 nm channel, for levels at and below 19 km. These fill values typically occur when the LOS optical depth becomes large enough to cause the retrieval to terminate in a channel, and are typically indicative of clouds along the line of sight. It is perhaps obvious but worth noting that this additional filtering is necessary because it is not possible to apply the aforementioned color ratio and extinction filtering when one or both of the channels contains a fill value.

Overall, the cloud filtering removes 35% of the SAGE III/ISS WV data below 19 km, including almost all of the negative WV values in this region (e.g., Figure 1). Figure 5 illustrates the impact of this filtering on

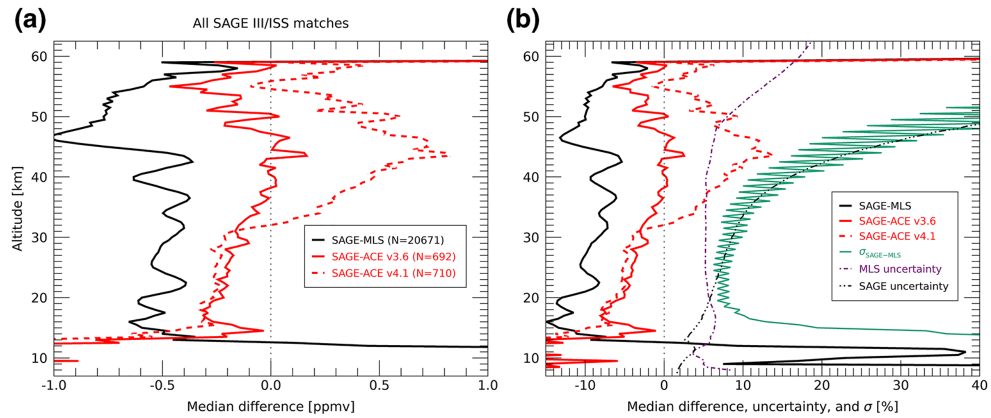

Figure 6. (a) The median absolute difference between matched pairs of SAGE III/ISS and Aura MLS (black) or ACE-FTS (red). (b) The median percent difference between SAGE III/ISS and these other satellites (defined as [SAGE-other]/other*100, black and red lines), the standard deviation of these differences (green line), and the median uncertainties for SAGE III/ISS (black) and Aura MLS (purple). MLS, Aura Microwave Limb Sounder; SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station.

comparison of SAGE WV data with matched MLS profiles. As can be seen in this figure, the largest differences occur at higher values of color ratio, and these outliers are successfully removed by the filtering (red points in Figure 5). It is worth noting that these filtering criteria are inherently conservative in that they are likely removing some valid SAGE III/ISS WV values, as evidenced by the large number of data points that are removed yet in reasonable agreement with MLS. While the overall agreement with MLS is improved by this aggressive filtering, we do not further evaluate the accuracy of the tropospheric SAGE III/ISS WV data due to large uncertainties in the MLS data and high intrinsic variability of WV in this region. Furthermore, SAGE III/ISS WV profiles often "turn over" and decrease with decreasing altitude for a few kilometers below their maximum value at the bottom of the retrieved profile, without any other obvious indications of a problematic retrieval. We do not attempt to remove these artifacts, although it is possible that these artifacts could be robustly removed following a more extensive analysis. Although validation of SAGE III/ISS WV data in the troposphere is beyond the scope of this study, previous results from SAGE II suggest that the tropospheric WV data should be scientifically useful (Chiou et al., 1997; Liao & Rind, 1997).

Finally, while the filtering described in this section removes almost all negative WV values from the SAGE III/ISS data, a few values (∼10 for the data set considered here) remain below 19 km. We therefore recommend that users also manually remove data below the point 1 km above the occurrence of any negative WV value occurring below 19 km.

5. Comparisons Between SAGE III/ISS and Correlative Data Sets

5.1. Satellite Data: Basic Comparisons

In this section, we present comparisons of SAGE III/ISS WV data with correlative satellite data from Aura MLS and ACE-FTS. These comparisons are done after the quality control screening from Section 4 has been applied to the SAGE III/ISS data.

Of the 21,879 solar occultation profiles collected by SAGE III/ISS by the end of 2019, over 20,000 of these profiles have a matched MLS profile meeting the coincidence criteria described in Section 3.3. As illustrated in Figure 6 and shown in Table 3, SAGE III/ISS water vapor values are consistently drier than MLS in the lower to mid stratosphere, where the SAGE III/ISS uncertainty is smallest (see black dash-dot line in Figure 6b). In the median, SAGE III/ISS water vapor values are 0.5 ppmv (10%) drier than MLS over the 15–35 km altitude range. Above ∼35 km, the SAGE III/ISS uncertainties increase with increasing altitude (black dash-dot line in Figure 6b), with the same being true for MLS above ∼48 km (purple dash-dot line

Table 3
Summary of SAGE III/ISS Uncertainty and Differences From Correlative Measurements

Altitude [km]	SAGE III/ISS median uncertainty	SAGE III/ISS—MLS v 4.2 median difference		SAGE III/ISS—ACE v3.6 median difference		SAGE III/ISS—frost point median difference	
	%	%	ppmv	%	ppmv	%	ppmv
8	1.7	210	8.5	−34	−27	−14	−45
10	2.8	23	2.2	−22	−3.9	−40	−4.1
12	3.8	9.2	0.45	−28	−1.9	−14	−0.86
14	3.3	−11	−0.5	−5.7	−0.23	−18	−1.2
16	4.5	−15	−0.66	−7	−0.27	−10	−0.47
18	5.2	−12	−0.54	−7.7	−0.31	−6.5	−0.29
20	5.8	−13	−0.59	−5.1	−0.22	−10	−0.42
22	6.3	−8.4	−0.4	−4.3	−0.2	−8.6	−0.39
24	6.9	−9.7	−0.49	−4.2	−0.2	−4.8	−0.23
26	7.4	−10	−0.55	−3.7	−0.19		
28	7.9	−9.6	−0.51	−4.1	−0.21		
30	8.6	−8.3	−0.46	−2.8	−0.15		
32	9.2	−7.2	−0.4	−2.7	−0.15		
34	10	−8.3	−0.5	−0.98	−0.056		
36	11	−6.4	−0.39	−0.44	−0.026		
38	13	−7.5	−0.48	−0.31	−0.017		
40	16	−9.3	−0.63	0.24	0.016		
42	20	−6.1	−0.42	−0.77	−0.052		
44	24	−6.9	−0.48	2.3	0.15		
46	30	−13	−0.99	0.63	0.04		
48	37	−11	−0.88	−1.3	−0.092		
50	46	−10	−0.77	0.53	0.039		
52	57	−10	−0.77	−2.2	−0.15		
54	69	−9.6	−0.73	−4.3	−0.33		
56	80	−7.3	−0.55	−3.9	−0.27		
58	88	−2.1	−0.15	−0.16	−0.013		
60	69	70	5.3	74	5.3		

Abbreviation: SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station.

in Figure 6b). As a result, the median difference between SAGE III/ISS and MLS changes with altitude above ∼45 km.

In comparison with ACE-FTS, SAGE III/ISS data are consistently drier below 30 km. In the 20–30 km range, SAGE III/ISS is 0.1–0.3 ppmv drier than both versions of ACE-FTS. Below ∼15 km, SAGE III/ISS becomes significantly drier than ACE-FTS, but wetter than MLS. However, there are many caveats in these comparisons, including increased geophysical variability in this region, larger vertical gradients in water vapor which can exacerbate differences due to differing spatial resolution among the instruments, and the known "turn over" in SAGE III/ISS WV values discussed in Section 4.3. Above 30 km, the behavior of the two versions of ACE-FTS is quite different. Version 4.1 transitions to having a positive bias with increasing altitude, whereas v3.6 is more consistent with altitude. The behavior of v4.1 has not been fully explored at this time, so for the remainder of the study we use the more extensively validated v3.6.

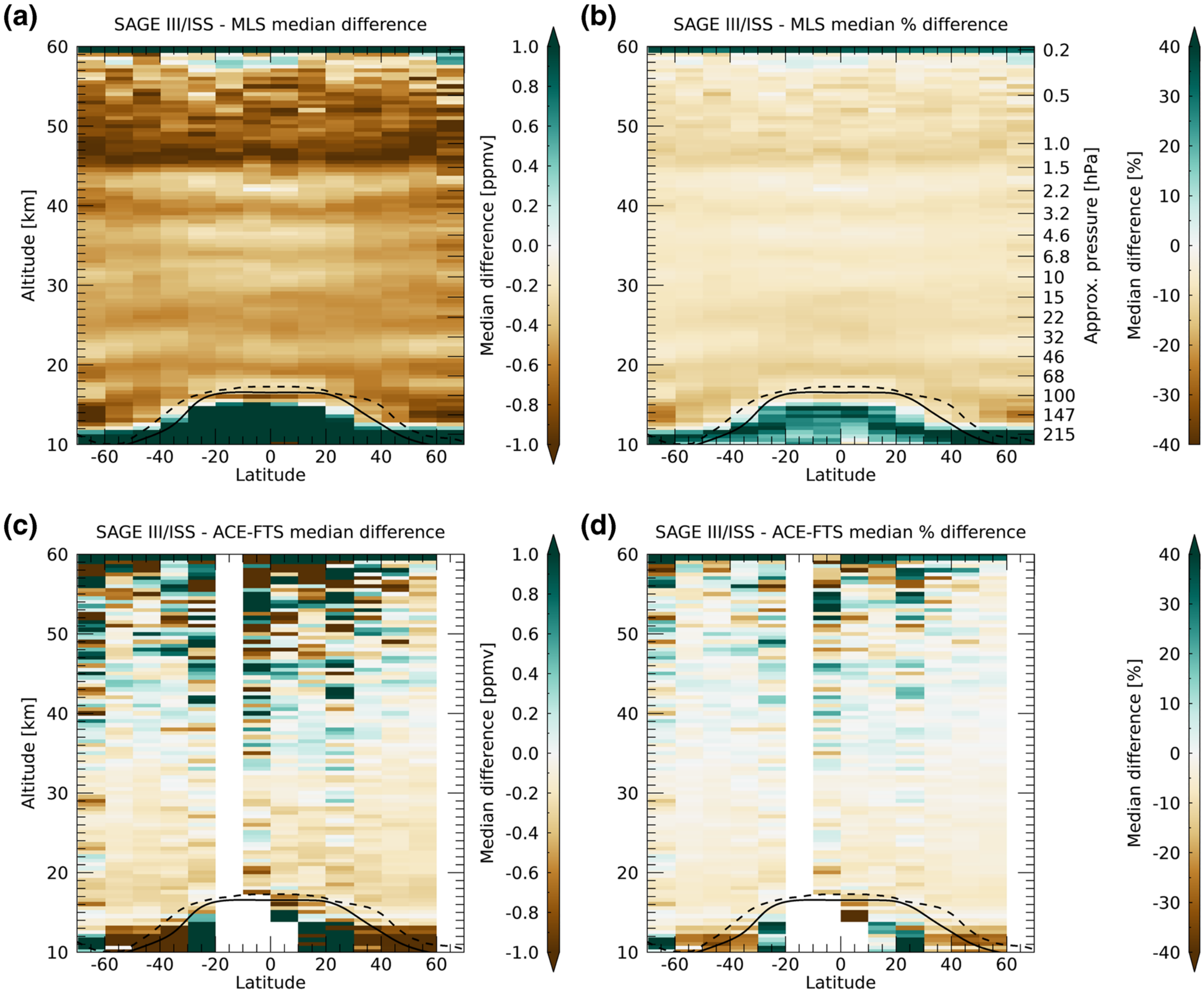

Figure 7. (a) The median difference of SAGE III/ISS minus Aura MLS and (b) median percent difference as a function of altitude and latitude. The approximate locations of the MLS pressure grid are shown on the righthand y axis in panels a and (b) The corresponding plots for ACE-FTS v3.6 are shown in the bottom row (panels c and d, respectively). The mean (solid) and maximum (dashed) thermal tropopause height over the SAGE III/ISS time period (2017-06 through 2019-12) from the MERRA-2 reanalysis is shown in all panels. MERRA-2, Modern-Era Retrospective analysis for Research and Applications, Version 2; MLS, Aura Microwave Limb Sounder; SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station.

Interestingly, the standard deviation of the percent difference between SAGE and MLS, which is a combination of the precision of each instrument and the geophysical variability between their coincident locations, tracks quite closely with the SAGE uncertainty above ~25 km. This suggests that random atmospheric variability between the SAGE/MLS measurement pairs is not a major contributor to the observed differences at these levels, and that the reported SAGE III/ISS uncertainties are reasonable. In contrast, below 18 km the standard deviation of the SAGE/MLS difference grows rapidly with decreasing altitude, due to increased atmospheric variability in the upper troposphere lower stratosphere (UTLS) region.

Another important consideration in how SAGE III/ISS compares to other data sets is whether or not there are noticeable geographic variations in the comparison. Figure 7 shows the comparison between SAGE III/ISS and MLS as a function of both height and latitude, along with the thermal tropopause computed from the Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) reanalysis (Gelaro et al., 2017). This figure indicates that the SAGE III/ISS dry bias (relative to MLS) is consistent with latitude throughout most of the overworld stratosphere above ~15 km. There are several

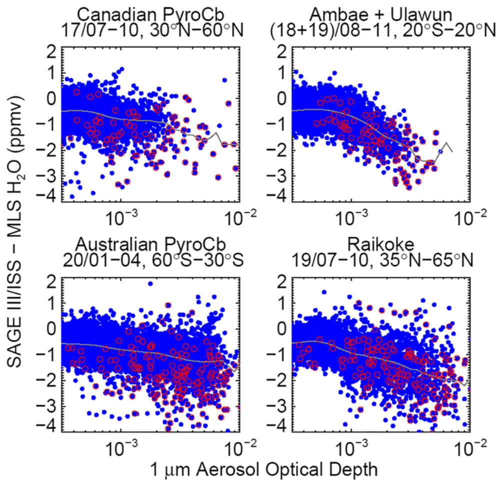

Figure 8. Difference between SAGE III/ISS and MLS WV as a function of SAGE 1 μm aerosol optical depth (AOD) for different stratospheric aerosol injection events. Events, dates, and latitude ranges are labeled for each plot. The Ambae and Ulawun eruptions were combined because of their similar behavior. Points include all data between 14 and 24 km and actively exclude data both below the hygropause and below the peak 1 μm aerosol extinction in each profile to illustrate the impact of elevated aerosol loading on trace amounts of water vapor. Red circles are placed around values where the uncertainty in SAGE water vapor data is ≥100%. The gray line is a running median of the data. MLS, Aura Microwave Limb Sounder; SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station.

geographical regions with less consistency that are worth pointing out. First, in the high latitude lower stratosphere, there are regions where SAGE III/ISS is significantly drier than MLS (i.e., ∼12–15 km and poleward of ∼50° in each hemisphere). This region may be influenced by aerosol contamination from volcanoes and fires, as will be discussed in the next section. These pockets of strong dry bias are also likely related to the relatively weak water vapor signal measured by MLS in these regions at the 147 and 121 hPa levels (Davis et al., 2016). Similarly, the transition to positive biases in the UTLS region is consistent with the known Aura MLS dry bias in this region (Davis et al., 2016; Vomel, Barnes, et al., 2007; Vömel, David, & Smith, 2007). At latitudes poleward of ∼45° in each hemisphere, this transition occurs above the tropopause, as can be seen in the green banding in Figure 7 above the tropopause (dashed and solid lines) in each hemisphere. It is worth stressing that the transition to positive bias in the UTLS is also large in percent difference (Figure 7b), and is not merely the result of moving into a region where the water vapor values are larger (i.e., where a 1 ppmv bias would be relatively small). Finally, it is worth noting that above 45 km the loss of precision in MLS but especially SAGE III/ISS (see, e.g., Figure 6b) leads to increased noise in the comparison shown in Figure 7.

The comparison with ACE-FTS v3.6 in Figure 7 reinforces the behavior apparent in Figure 6. Through most of the stratosphere SAGE III/ISS is dry-biased relative to ACE-FTS, with a decrease in this bias at higher altitudes. Interestingly, there is a suggestion of a latitude-dependence of this bias, with SAGE III/ISS showing relatively wetter values at low latitudes and drier values at high latitudes, in comparison to ACE-FTS. However, it should be stressed that given the predominant high latitude sampling from ACE-FTS, the number of matched profiles in the tropics (N = 74, 30°S–30°N) for these comparisons is significantly lower than at high latitudes (N = 658 for |lat| > 30°).

5.2. Satellite Comparisons: Sensitivity to Aerosol

In the lower stratosphere, near or above the hygropause, water vapor is not the primary contributor to the overall extinction in the spectral region surrounding 945 nm. Instead, it can vary considerably with aerosol loading levels and ranges from ∼10% at "background" conditions down to ∼1% after a major volcanic eruption (Thomason et al., 2004). Studies of previous SAGE instruments looked at the sensitivity of the water vapor product and noticed biases with other measurement systems, recommending filtering criteria based on overall aerosol loading levels. As an example, for SAGE II water vapor data, Taha et al. (2004) recommended removing data in profiles below the highest altitude at which β_{1022} (1,022 nm extinction) was greater than 2×10^{-4} km^{-1}. Herein we investigate the sensitivity of SAGE III/ISS water vapor to aerosol loading in the lower stratosphere using coincident Aura MLS data surrounding five stratospheric aerosol injections since the start of the SAGE III/ISS mission.

Over its first three years, SAGE III/ISS has observed several small volcanic eruptions (i.e., Ambae in 2018 and Ulawun and Raikoke in 2019) and the two largest pyrocumulonimbus (PyroCb) clouds ever recorded (i.e., Canadian wildfires in 2017 [Yu et al., 2019] and Australian bushfires in 2019/2020 [Kablick et al., 2020]). Unlike during SAGE III/M3M, which observed a relatively clean stratosphere that did not appear to impact water vapor (Thomason et al., 2010), these events present an opportunity to assess the impact that moderately elevated aerosol loading has on the retrieved water vapor. Figure 8 looks at the difference between SAGE III/ISS and MLS water vapor between 14 and 24 km as a function of integrated aerosol optical depth near 1 μm in the months after three volcanic eruptions (Ambae, Ulawun, and Raikoke) and the two major PyroCbs. These data show a systematic negative bias in the SAGE III/ISS data that worsens with increasing aerosol loading. At these altitudes and elevated loading levels, the contribution of aerosol to the overall

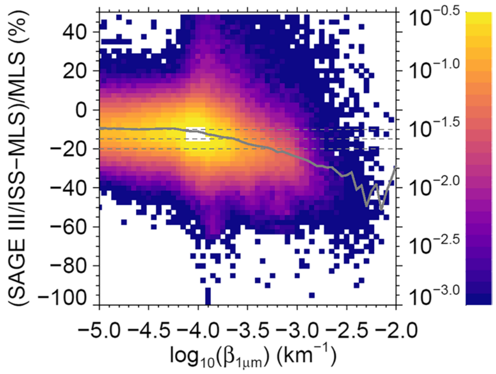

Figure 9. 2D histogram of the percent differences between SAGE III/ISS and MLS as a function of 1 μm aerosol extinction. The data is for all altitudes between 14 and 30 km and for all coincident events between June 2017 and May 2020 and the color scale shows the fractional percentage of data points in each bin. The gray line is a running median of the data showing how the overall negative bias increases with increasing aerosol loading. MLS, Aura Microwave Limb Sounder; SAGE III/ISS, Stratospheric Aerosol and Gas Experiment III instrument on the International Space Station.

extinction near the peak of water vapor absorption in the SAGE channel can be 50 times larger than that of water vapor itself.

Furthermore, it appears that the systematic change in the bias is more pronounced with smaller particles (e.g., volcanic events) than with larger particles (e.g., the fires). This may be because the SAGE retrieval attempts to solve for water vapor, ozone, and aerosol all at once. Sulfate aerosol (from volcanic eruptions) exhibits a larger dependency of extinction with wavelength than smoke aerosol. This enhanced slope can potentially alias into the other terms of the retrieval such as the wings of the ozone cross-sections in the spectral region used by SAGE or into the overall slope of absorption from water vapor. The SAGE team is currently investigating this effect in an effort to correct it in a future version.

While a negative bias of SAGE III/ISS water vapor with increased aerosol loading exists, there is no distinct transition at which this occurs. The effect is gradual, making any clear method of filtering the data difficult. Additionally, filtering the data in the same way as is done for clouds (i.e., removing all data at altitudes below some criteria) should not be necessary, as the contribution of water vapor to the overall signal increases significantly below the hygropause even with elevated aerosol loading, and any negative bias in SWV would have a negligible impact on the retrieval of tropospheric water vapor. That having been said, we investigate the overall change in bias with aerosol loading. Figure 9 shows both a 2D histogram of all of the differences between coincident SAGE III/ISS and MLS events as a function of 1 μm aerosol extinction and a running median of these data. It appears that at low aerosol loading levels ($\leq 10^{-4}$ km^{-1}), there is a roughly 10% offset between the two instruments, consistent with the results shown in the previous section. A−5% aerosol-induced bias (15% total offset) occurs around 2.5×10^{-4} km^{-1} and a −10% bias occurs around 5.0×10^{-4} km^{-1} (20% total offset). It is worth noting that although the reported SAGE III/ISS uncertainties cannot themselves be used as a definitive filtering criterion, the relative uncertainties also tend to increase with increased aerosol loading (not shown), with uncertainties increasing rapidly once the 1 μm aerosol extinction exceeds 10^{-3} km^{-1}. That means the uncertainties can be used for other analyses (e.g., computing weighted vs. unweighted means) to help mitigate the impact of the sensitivity of SAGE III/ISS water vapor to aerosol loading levels.

5.3. Frost Point Hygrometer Soundings

Balloon-borne frost point hygrometer data offer the opportunity to compare SAGE III/ISS water vapor data to independent measurements that have been extensively used for comparisons to other satellite data sets, including both Aura MLS and previous SAGE instruments (e.g., Davis et al., 2016; Read et al., 2007; Vomel, Barnes, et al., 2007; Vömel, David, & Smith, 2007). Since frost point measurements are made at much higher vertical resolution than SAGE, we apply a vertical smoothing to the frost point data. The smoothing used here consists of a triangular averaging window with 2 km full width at half maximum. Although the vertical resolution of each satellite instrument is slightly different, they are all in the 2–3 km range in terms of vertical resolution.

In line with previous validation and intercomparison studies, Figure 10 shows that in the median the satellite data agree with the frost point measurements to within 0.5 ppmv in the stratosphere. The relative dry bias in SAGE III/ISS seen earlier in the comparisons to MLS and ACE-FTS is further borne out in this comparison. SAGE III/ISS is 0.1–0.3 ppmv drier than the frost points in the stratosphere (see also Table 3), with ACE-FTS v3.6 agreeing very closely with the frost points and MLS 0.1–0.2 ppmv wetter, as shown by Hurst et al. (2016).

In the upper troposphere, most satellite instruments are dry-biased relative to the frost points, but the usual caveats regarding comparisons in this region apply. In addition to questionable data quality and large

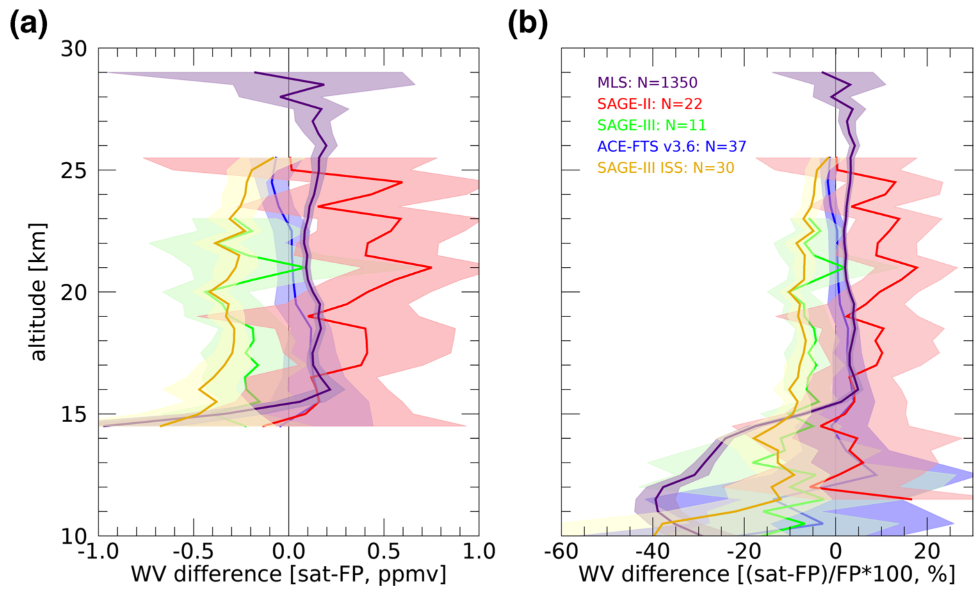

Figure 10. (a) The median differences and (b) median percent differences between various satellites and coincident frost point (FP) measurements. The shading on each instrument shows ±2 standard error estimates. In (a) the axis range is restricted and data are shown for levels at which the mean WV is less than 10 ppmv in order to highlight differences in the stratosphere.

WV gradients, the large geophysical variability coupled with relaxed matching criteria used here (see Section 3.3) could be particularly problematic for the reliability of comparisons in this region.

6. Summary

SAGE III/ISS continues the heritage of satellite SWV vertical profile measurements spanning back to the 1980s, and this data set is one of only a handful of satellite limb sensors currently in operation. This study has assessed the first publicly released beta version 5.1 in comparison to existing balloon and satellite water vapor measurement, in order to provide guidance and recommendations. Based on this analysis, we have devised a set of suggested criteria for data users in order to filter out outliers and data impacted by interference from clouds. Our recommendations are as follows:

1. Remove profiles that are obvious anomalies (events in Table 1)
2. Remove data in "keel over" profiles above the point 2.5 km below the level at which the (5 km) smoothed vertical derivative is 1 ppmv km^{-1}
3. Remove data below the point 1 km above the level at which either criteria occur
   a) Color ratio (β_{1022}/β_{520}) > 0.5 & $\beta_{1022} > 2 \times 10^{-4}$ km^{-1}
   b) Fill value for either β_{1022} or β_{520} below 19 km
   c) Negative WV value below 19 km

Additionally, users of SAGE III/ISS WV data should be aware that there may be an extinction-dependent dry bias in the data that occurs in the presence of clouds or high stratospheric aerosol loading. The source of this bias is likely algorithmic and this issue may be fixed in future versions of the data product. Also, SAGE III/ISS WV data quality in the troposphere is not fully evaluated here and should be treated with caution prior to additional analysis to establish its reliability. Among other potential issues, the profiles have a tendency to "turn over" and decrease with decreasing altitude for a few kilometers below their maximum water vapor value at the bottom of the retrieved profile, without any other obvious indications of a problematic retrieval.

After applying the quality control screening described herein, we find that SAGE III/ISS WV is in good agreement with independent satellite and balloon-based measurements. From 20 to 40 km, SAGE III/ISS WV v5.1 exhibit a bias of 0.0 to −0.5 ppmv (∼10%) relative to ACE-FTS v3.6 and MLS 4.2 data, depending on the instrument and altitude. In comparison to frost point data from 15 to 25 km, SAGE III/ISS has a mean dry bias of 0.3 ppmv. In comparison to the other satellite instruments and the frost point balloon measurements, the SAGE III/ISS WV dry bias is very stable with altitude. It is likely that future versions of the data product with updated line parameters will improve agreement further. Despite its status as a beta version, the level of SAGE III/ISS WV agreement with independent data is similar to previous SAGE instruments, and therefore the data are suitable for extending SWV data records and in scientific studies of SWV.

Data Availability Statement

SAGE III/ISS v5.1 data are publicly available through the NASA Atmospheric Sciences Data Center (https://asdc.larc.nasa.gov/project/SAGE%20III-ISS). The Atmospheric Chemistry Experiment is a Canadian-led mission mainly supported by the Canadian Space Agency. Finally, the authors wish to thank three anonymous reviewers for their insightful comments that helped improve the manuscript.

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