Dear authors,

thank you for taking all my remarks into account. I'm left with two minor issues, both on page 18.

* line 383: you always considered the year 2006 in your comparisons, and January and July 2006 in particular in Section 3.2. So, why are you comparing OMI version 3.0 with SSMIS for July 2007 here? Or is it a typo?

* lines 390-391: Why this inconsistency in filtering out pixels affected by rain between Fig. 6 and Table 3? Please give a reason for this approach.

Dear reviewer,

Thanks for your review.

For line 383, it is a typo. The year used should be 2006. Thanks for catching it. We have made the correction.

For line 390-391, SSMIS data have lower quality when there is precipitation. Thus, we have filtered out pixels with rain in both Figure 6 and Table 3. However, Figure 6 is dedicated to the comparison under "clear-sky" condition and Table 3 is for investigating the influence of different cloud fractions. We have therefore filtered out SSMIS pixels with cloud liquid water in Figure 6 and kept those pixels in Table 3. A comment about this has been added to the paper near line 391.

Regards,

from all authors

OMI Total Column Water Vapor Version 4 Validation and Applications

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7

8 Abstract

9 Total Column Water Vapor (TCWV) is important for the weather and climate. TCWV is 10 derived from the Ozone Monitoring Instrument (OMI) visible spectra using the Version 4.0 11 retrieval algorithm developed at the Smithsonian Astrophysical Observatory. The algorithm uses 12 a retrieval window between 432.0 and 466.5 nm and includes updates to reference spectra and 13 water vapor profiles. The retrieval window optimization results from the trade-offs among 14 competing factors.

The OMI product is characterized by comparing against commonly used reference datasets -15 16 Global Positioning System (GPS) network data over land and Special Sensor Microwave Imager 17 / Sounder (SSMIS) data over the oceans. We examine how cloud fraction and cloud top pressure 18 affect the comparisons. The results lead us to recommend filtering OMI data with cloud fraction 19 less than f = 0.05 - 0.25 and cloud top pressure > 750 mb (or stricter), in addition to the data 20 quality flag, fitting RMS and TCWV range check. Over land, for f = 0.05, the overall mean of 21 (OMI-GPS) is 0.32 mm with a standard deviation (σ) of 5.2 mm, the smallest bias occurs when 22 TCWV = 10 - 20 mm, and the best regression line corresponds to f = 0.25; Over the oceans, for f 23 = 0.05, the overall mean of (OMI-SSMIS) is 0.4 mm (1.1 mm) with σ = 6.5 mm (6.8 mm) for 24 January (July), the smallest bias occurs when TCWV = 20 - 30 mm, and best regression line 25 corresponds to f = 0.15. For both land and the oceans, the difference between OMI and the 26 reference datasets is relatively large when TCWV is less than 10 mm. The bias for Version 4.0 27 OMI TCWV is much smaller than that for Version 3.0.

As test applications of the Version 4.0 OMI TCWV over a range of spatial and temporal scales, we find prominent signals of the patterns associated with El Niño and La Niña, the high 30 humidity associated with a corn sweat event and the strong moisture band of an atmospheric

31 river (AR). A data assimilation experiment demonstrates that the OMI data can help improve the

32 Weather Research and Forecasting model (WRF)'s skill at simulating the structure and intensity

33 of the AR and the precipitation at the AR landfall.

34 **1 Introduction**

Water vapor is of profound importance for weather and climate. Through condensation, it forms clouds that modify albedo, affect radiation and interact with particulate matter. In addition, latent heat released from water vapor condensation can influence atmospheric energy budget and circulation. Water vapor is the most abundant greenhouse gas, accounting for ~50% of the greenhouse effect (Schmidt et al., 2010). Thus, monitoring the spatial and temporal distributions of water vapor is crucial for understanding water-vapor related processes.

41 Water vapor has been measured using a variety of in situ and remote sensing techniques from 42 the ground, air and space. Satellite data provide global perspective and are indispensable for 43 constraining reanalysis products (Dee et al., 2011; Gelaro et al., 2017). The current satellite 44 water vapor datasets are evaluated through the Global Energy and Water cycle Exchanges 45 (GEWEX) Water Vapor Assessment program (Schröder et al., 2019). These datasets are derived 46 from visible, near infrared (NIR), Infrared (IR), microwave and Global Positioning System 47 (GPS) measurements. Each dataset has its own characteristics and contributes to the 48 understanding of water vapor in its own way. For example, microwave data are useful for both 49 clear-sky and cloudy-sky conditions, but are best suited for non-precipitating ice-free oceans due 50 to the complications associated with land surface emissivity; NIR data are best suited for the 51 land, as the surface albedo is low over the oceans; IR data are available over all surface types, 52 but are strongly influenced by clouds and less sensitive to the planetary boundary layer; visible 53 data are sensitive to the boundary layer over both land and the oceans, but are complicated by 54 uncertainties in clouds and aerosols (Wagner et al., 2013).

Total Column Water Vapor (TCWV, also called Integrated Water Vapor - IWV, or
Precipitable Water Vapor - PWV) can be retrieved from the 7v water vapor vibrational polyad
band (around 442 nm) despite the weak absorption (Wagner et al., 2013). This made it possible
to derive TCWV from instruments measuring in the blue wavelength range. Since water vapor is
a weak absorber here, saturation of spectral lines is not of concern (Noël et al., 1999). Moreover,

the similarity between the land and ocean surface albedo in the blue wavelength range suggests a
roughly uniform sensitivity of the measurement over the globe (Wagner et al., 2013). However,
weaker absorption tends to result in larger relative uncertainties, especially for low TCWV
amount.

64 Using the visible spectra measured by the Ozone Monitoring Instrument (OMI), Wang et al. 65 (2014) retrieved Version 1.0 TCWV from 430 - 480 nm and publically released the data on the Aura Validation Data Center (AVDC, https://avdc.gsfc.nasa.gov). Wang et al. (2016) found that 66 67 the Version 1.0 data generally agree with ground-based GPS data over land but are significantly 68 lower than the microwave observations over the oceans. They found that using a narrower 69 retrieval window (427.7 - 465 nm) in Version 2.1 could improve the data over the oceans 70 without adversely affecting the results over land much. However, the Version 2.1 data were only 71 generated for a few test months and not released to the public. An interim Version 3.0 OMI 72 TCWV product was available at AVDC. Compared with Version 2.1, Version 3.0 uses the 73 reference spectrum for water vapor from the latest HITRAN database (Gordon et al., 2016) and 74 that for liquid water from Mason et al. (2016), as well as the newest cloud product (Veefkind et 75 al., 2016). The Version 3.0 retrieval window (427.0 - 467.0 nm) is adjusted from that for 76 Version 2 within 2 nm on each end based on fitting uncertainty for a randomly selected test orbit. 77 This paper focuses on Version 4.0 OMI TCWV which has replaced Version 3.0 on AVDC. 78 We present the Version 4.0 retrieval algorithm which incorporates a more vigorous systematic 79 optimization for the retrieval window and miscellaneous updates. We characterize the 80 performance of the Version 4.0 dataset by comparing with well-established references, such as 81 the GPS network data and the Special Sensor Microwave Imager / Sounder (SSMIS) 82 observations. We also assess the performance of Version 4.0 against that of Version 3.0. To 83 provide practical guide to users of the new data, we investigate the influence of cloud fraction 84 and cloud top pressure on the comparisons. Based on the results, data filtering criteria are 85 recommended. As an additional check on the Version 4.0 product, we show test applications of 86 the data to a range of spatial and temporal scales, including El Niño / La Niña, a corn sweat 87 event and an atmospheric river (AR) event. For the first time, a data assimilation experiment for 88 the AR event demonstrates that the OMI TCWV data can provide useful constraint for weather 89 prediction.

90 2 Retrieval Algorithm

OMI on board the Aura spacecraft is a UV/Visible imaging spectrometer (Levelt et al.,
2006). It has been making daily global observations at a nominal 13×24 km nadir resolution
from a 1:30 PM equator crossing time polar orbit since October 2004. The UV-Visible channel
of OMI covers 350-500 nm at a spectral resolution of about 0.5 nm.

95 TCWV is derived from the OMI visible spectrum using a commonly used two-step approach. 96 First, the Slant Column Density (SCD, molecules/cm²) is retrieved from a spectral fitting 97 algorithm. Then, the Vertical Column Density (VCD, molecules/cm²) is calculated from the ratio 98 of SCD and Air Mass Factor (AMF) (Palmer et al., 2001). VCD can be converted to TCWV 99 using 10^{23} molecules/cm² = 29.89 mm. The details of the two-step procedure can be found in 100 González Abad et al. (2015). The specifics of Version 4.0 are discussed below.

101 The Version 4.0 spectral fitting parameters are summarized in Table 1. In the nonlinear least square fitting, we consider wavelength shift, under-sampling, closure polynomials (3rd order 102 103 multiplicative and additive), reference spectroscopic spectra of water vapor, interfering 104 molecules (O₃, NO₂, O₄, liquid water, C₂H₂O₂ and IO) and Raman scattering (the Ring effect, 105 vibrational Raman scattering of air and the water Ring effect). In comparison with previous 106 versions, Version 4.0 no longer fits common mode (i.e. the mean of the fitting residual, González 107 Abad et al., 2015). It turns out that the common mode for land is different than that for ocean 108 (Wang et al., 2014). Previous retrievals derive a common mode for each orbit swath using the 109 pixels in the low latitudes which often includes both land and ocean scenes. Thus, the derived 110 common mode depends on the proportion of land versus ocean pixels of the spacecraft orbit and 111 is not universally suitable for all the pixels of the swath. Statistics for Orbit 10423 show that 112 although the mean of SCD differs little between the retrievals with and without common mode in 113 the fitting (0.1 mm), the standard deviation of SCD between them can be significant (1.7 mm). 114 Most of the settings in Table 1 are shared between Version 3.0 and 4.0, except that Version 3.0 115 uses HITRAN 2016 (Gordon et al., 2016) as the water vapor reference spectrum, includes 116 common mode in the fitting, but does not consider vibrational Raman scattering of air (Lampel et 117 al., 2015a). We revert to the HITRAN 2008 water vapor spectrum (Rothman et al., 2009) in 118 Version 4.0 because validation results show that it leads to better agreements with the GPS and 119 SSMIS TCWV data (Section 3). We did not apply the correction of Lampel et al. (2015b) to the

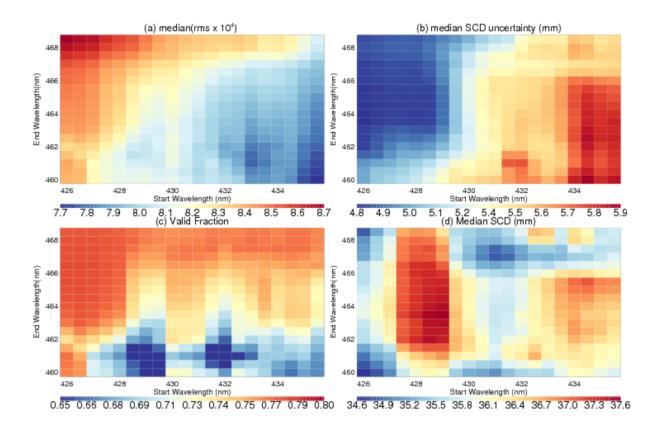
- 120 HITRAN 2008 water vapor spectrum. It is recently found that HITRAN 2016 is adversely
- 121 affected by an issue with line broadening for water vapor in the blue wavelength range and
- 122 improvements are being made for the next HITRAN release (the HITRAN group, personal
- 123 communication).

Wavelength shift	Solar reference spectrum	Dobber et al. (2008)			
Target	H ₂ O	288K, Rothman et al. (2009)			
Interference	O ₃	228K, Brion et al. (1993)			
molecules	NO ₂	220K, Vandaele et al. (1998)			
	O4	293K, Thalman and Volkamer (2013)			
	Liquid water	Mason et al. (2016)			
	C ₂ H ₂ O ₂	296K, Volkamer et al. (2005)			
	ΙΟ	298K, Spietz et al. (2005)			
Raman scattering	Ring effect	Chance and Spurr (1997)			
	Water Ring	Chance and Spurr (1997)			
	Air Vibrational Raman	Lampel et al. (2015a)			
Other	Additive polynomial	3 rd order			
	Multiplicative polynomial	3 rd order			
	Under-sampling	Chance et al. (2005)			

124 **Table 1.** Parameters used in Version 4.0 spectral fitting for OMI total column water vapor.

125

To optimize the retrieval window, we randomly selected OMI Orbit number 10426 (on July 1, 2006) to examine the effect of varying the starting and ending wavelengths around the 7vwater vapor absorption band. The orbit swath contains 60×1644 ground pixels and covers parts of Australia, the Pacific, China and other areas. We systematically adjust the starting wavelength within 426.0-435.0 nm and the ending wavelength within 460.0-468.5 nm, both at 0.5 nm steps.



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Figure 1. Sensitivity of the retrieval to the start and end wavelengths (nm) of the retrieval
window for OMI Orbit number 10426. (a) Median of fitting RMS×10⁴; (b) median of water
vapor SCD fitting uncertainty in mm; (c) valid fraction for retrievals; (d) median SCD in mm.

135 In previous versions, the fitting window is selected based on the fitting uncertainty (Wang et 136 al., 2014, 2016). For Version 4.0, we consider the following four factors. (1) Figure 1a shows that the median of the fitting Root Mean Squared error (RMS) is smaller toward the lower right 137 138 corner of the domain (i.e., longer start wavelength and shorter end wavelength); (2) Figure 1b shows that the medium fitting uncertainty of water vapor SCD decreases toward the upper left 139 140 corner; (3) Figure 1c shows that the fraction of valid retrievals for the orbit generally increases 141 toward the upper part of the domain. Valid retrievals here refer to those that pass the main data 142 quality check (MDQFL = 0) and have positive SCDs. The main data quality check ensures that the fitting has converged, the SCD is $< 5 \times 10^{23}$ molecules/cm² (149.45 mm) and within 2σ of the 143 fitting uncertainty. The SCD threshold here is meant to filter out large outliers. For reference, the 144 largest TCWV of the GPS and SSMIS datasets used in Section 3 is about 75 mm. At low 145 146 latitudes where TCWV is large, more than 90% of the OMI AMFs are between 0.5 and 2.0; (4) 147 The length of the retrieval window increases with the difference between the end and start

wavelengths. The general patterns exhibited by Orbit number 10426 in Figure 1 also hold forOrbit number 10423 which cuts across the Pacific near the dateline.

150 Ideally, we would like to have small fitting RMS to reduce the residual's amplitude and structure, a small fitting uncertainty to reduce error, a large fraction of valid data to increase data 151 152 volume and a long retrieval window to include more information into the fitting. However, these 153 criteria cannot be met simultaneously. As a compromise, we select the wavelength interval 154 between 432.0 nm and 466.5 nm as the retrieval window for Version 4.0. For Orbit number 10426, this leads to a median fitting RMS of 8.1×10^{-4} , a median SCD uncertainty of 5.4 mm, a 155 156 valid fraction of 0.75 and a window length of 34.5 nm (Figure 1). Figure 1d shows that the 157 median SCD for Orbit number 10426 varies between 34.6 mm and 37.6 mm. This 3 mm 158 difference corresponds to an 8% variation and exhibits a complex pattern within the domain. The 159 Version 4.0 retrieval window leads to a median SCD of 35.5 mm for Orbit number 10426 which 160 is near the beginning of the middle third of the SCD range. The ratio between the median SCD 161 uncertainty and the median SCD (i.e., the relative SCD uncertainty) is about 0.15. Note that this 162 value is for the whole orbit which includes a wide range of SCDs. As shown in Supplementary 163 Figure 1, the relative SCD uncertainty is >1.2 for SCD = 0 - 10 mm, drops to about 0.4 for SCD 164 = 10 - 20 mm, and to about 0.1 for SCD > 40 mm.

165 The AMF is calculated by convolving scattering weights with the shape of water vapor 166 vertical profile (González Abad et al., 2015). The scattering weight is interpolated from the same 167 look-up table as that used in Wang et al. (2016). The scene specific information used in the AMF 168 calculation is listed in Table 2. By propagating typical errors for surface albedo (15%), cloud 169 fraction (10%) and cloud top pressure (15%), we find that the AMF error due to scattering 170 weight for a typical orbit (number 10426) is mostly < 3%, though for cloudy pixels, the error can 171 be 15% or more. Version 4.0 uses the 0.5°×0.667° monthly mean MERRA-2 water vapor profile 172 (Gelaro et al., 2017) for the month and year corresponding to the retrieval, while previous 173 versions used the monthly mean of 2007 for all years. To evaluate the error associated with gas 174 profiles, we compare the TCWV calculated using the daily MERRA-2 profile against that 175 calculated using the monthly MERRA-2 profile for July 2006 (for TCWV within the 0-75 mm 176 range). Results show that (TCWV(daily) – TCWV(monthly)) has a mean (median) of 0.3 mm (0 177 mm) with a standard deviation of 5.0 mm. When comparing the TCWV calculated using the 178 daily MERRA-2 profile against that calculated using the daily ERA-Interim profile for July

- 179 2006, we find that (TCWV(MERRA-2) TCWV(ERA-Interim)) has a mean (median) of -0.1
- 180 mm (0 mm) with a standard deviation of 2.8 mm. Thus, gas profiles can introduce substantial
- 181 scatter to the retrieved TCWV. AMF is highly sensitive to clouds (Wang et al., 2014; Vasilkov et
- al., 2017). Version 4.0 uses the cloud information from Veefkind et al. (2016). The primary
- 183 difference with the Acarreta et al. (2004) cloud product used in Version 1.0 and 2.1 is in the
- 184 cloud top pressure for cloud fraction f < 0.3. In addition to the factors in Table 2, aerosol and
- 185 surface bi-directional reflectance distribution function (BRDF) influence the AMF (Lorente et
- al., 2017; Vasilkov et al., 2017), but have not been considered in the retrieval yet.
- 187 **Table 2.** Parameters used in AMF calculation

Solar Zenith Angle	OMI L1B data
View Zenith Angle	
Relative Azimuth Angle	
Surface Albedo	OMLER (Lambert equivalent reflectance) Kleipool, et al.
	(2008)
Cloud fraction	OMCLDO2 (derived from O ₂ -O ₂) Veefkind et al. (2016)
Cloud top pressure	
Surface pressure	MERRA-2 monthly data $(0.5^{\circ} \times 0.667^{\circ})$, Gelaro et al. (2017)
Water vapor profile	

189 **3 Validation**

- 190 To validate the Version 4.0 OMI TCWV data, we compare them against two commonly used
- 191 reference datasets a GPS network dataset for land and a microwave dataset for the oceans.

192 **3.1 OMI and GPS over land**

193 To assess the Version 4.0 OMI TCWV over land, we compare against the GPS network data

downloaded from NCAR (rda.ucar.edu/datasets/ds721.1). The GPS data are composed of 2-

195 hourly TCWV at International GNSS Service (IGS), SuomiNet and GEONET stations, and have

an estimated error of < 1.5 mm (Wang et al., 2007; Ning et al., 2016). The subset of IGS-

197 SuomiNet data for the whole year of 2006 is used in this paper. The geographical distribution of

198 the stations can be found in Wang et al. (2016). Most of the stations are concentrated in North

199 America and Europe, fewer are scattered on other continents.

200 OMI TCWV data are filtered using the following criteria. The stripes in Level 2 swaths due 201 to systematic instrument error are removed using the SCD scaling procedure described in Wang 202 et al. (2016). The pixels affected by OMI's row anomaly are filtered out

203 (projects.knmi.nl/omi/research/product/rowanomaly-background.php), as well as negative or
204 extremely large (i.e., TCWV > 75 mm) values. For the clear-sky comparison in Figure 3, we

205 require cloud fraction < 5% and cloud top pressure > 750 mb, in addition to MDQFL = 0 and

206 fitting RMS < 0.001. The cloud fraction and cloud top pressure are from the OMCLDO2 cloud

207 product (Veefkind et al., 2016) and are included in the Level 2 OMI product for ease of data

filtering. On a typical day (July 1, 2006), among the OMI data that pass the MDQFL and TCWV
range test, cloud fraction < 0.05 accounts for 35% of the data, cloud top pressure > 750 mb
accounts for 53% of the data and RMS < 0.001 accounts for 72% of the data.

211 To co-locate GPS and OMI data, we select the GPS data observed between 1200 LT and 212 1500LT. This 3-hour local time range covers the OMI overpass time. We average the qualified 213 OMI data within 0.25° longitude $\times 0.25^{\circ}$ latitude of the GPS stations for each day. To minimize 214 the influence of local topography (e.g., mountain peaks, river valleys), if a station's elevation is 215 more than 250 m different than the mean elevation within the corresponding $0.25^{\circ} \times 0.25^{\circ}$ grid 216 square, then it is excluded from the analysis. The $0.25^{\circ} \times 0.25^{\circ}$ topography was downloaded from 217 www.temis.nl/data/topo/dem2grid.html. The comparison between OMI and GPS is made for 218 TCWV within the range of 0-75 mm as the largest TCWV for the GPS data is about 75 mm. 219 The co-locating procedure leads to about 11,000 co-located data points for the entire year of 220 2006.

Figure 2 shows the comparison between the resulting co-located GPS and Version 4 OMI TCWV. The top panel shows the histogram of OMI-GPS (in 0.5 mm bins). The bin from -0.5 to 0.0 mm corresponds to the peak of the distribution. The overall mean (median) of OMI-GPS is 0.32 mm (0.35 mm), with a standard deviation of 5.2 mm. The mean (median) absolute error is 3.9 mm (3.0 mm).

The bottom panel of Figure 2 shows the joint distribution of the co-located GPS and Version 4.0 OMI data. The count for each 0.5 mm bin is normalized by the maximum of all bins. About 34% of the data have TCWV < 10 mm, 72% have TCWV < 20 mm and 90% have TCWV < 30 mm. There is a general linear correlation between GPS and OMI data, with a correlation coefficient of r = 0.87 ($R^2 = 0.76$). The linear regression line (OMI = 2.22 + 0.88 * GPS, where OMI and GPS TCWV are in mm) has a significant positive intercept and a slope that is less than one. This indicates a positive bias of OMI against GPS for small TCWV and a negative bias for

- 233 large TCWV. Indeed, as indicated at the top of the panel, the mean of OMI-GPS for each 10 mm
- 234 GPS TCWV bin decreases from 1.7 mm for TCWV = 0 10 mm to -2.3 mm for TCWV = 40 10
- 50 mm, though the fraction of data for TCWV > 40 mm is < 3%. The corresponding standard
- deviation (σ) increases from 3.5 mm to 7.9 mm. The minimum bias of 0.2 mm occurs for TCWV
- in the 10 20 mm bin. The large positive bias of the 0 10 mm bin (as compared with the
- 238 TCWV of the bin) has significant adverse effect on the regression line. For TCWV > 10 mm, the
- regression line (OMI = $1.51 + 0.91 \times \text{GPS}$) is better.
- 240 In comparison, although Version 3.0 OMI is similarly correlated with GPS (correlation
- 241 coefficient r = 0.86), it has a much larger positive bias of 2.8 mm (with a standard deviation of
- 5.5 mm). The large bias is attributed to the much larger SCD of Version 3.0 (Supplementary
- 243 Figure 2b), as the AMFs of both versions roughly follow the 1:1 line (Supplementary Figure 2a).
- 244 Sensitivity tests show that the larger Version 3.0 SCD is primary due to the water vapor
- reference spectrum. If the water vapor reference spectrum in Version 4.0 is replaced with that of
- Version 3.0 (Test 1), then the median SCD increases by about 4.5 mm for Orbit 10423
- 247 (Supplementary Figure 2c). Modifying the retrieval window for Version 3.0 cannot sufficiently
- reduce the retrieved SCD, therefore cannot make significantly better agreement with the
- 249 reference TCWV data. As Version 4.0 shows better performance, this paper focuses on
- 250 characterizing Version 4.0 to provide useful information to potential users. In subsequent
- discussions, OMI data refer to Version 4.0 unless specified otherwise.

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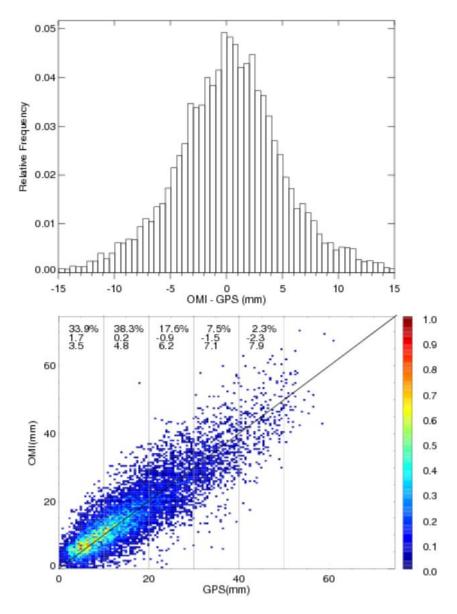


Figure 2. Comparison between co-located GPS and OMI TCWV (mm) for all days in 2006. The
data filtering criteria include cloud fraction < 5%, cloud top pressure > 750 mb, and others
discussed in the text. (Top) Relative frequency of occurrence for OMI-GPS (mm). (Bottom)
Normalized joint distribution of GPS versus OMI TCWV (mm). The three lines of text from top
to bottom indicate the percentage of data points (1st), the mean of OMI-GPS in mm (2nd), and
the standard deviation of OMI-GPS in mm (3rd) for each 10 mm GPS TCWV, respectively. The
1:1 is plotted for reference.

262 OMI TCWV retrieval is highly sensitive to clouds (Wang et al., 2014). In Figure 3, we 263 examine the effect of OMI cloud fraction threshold (f) on the comparison while keeping other 264 data filtering criteria the same as those for Figure 2 (i.e., cloud fraction < f, cloud top pressure < 265 750 mb, MDQFL = 0, fitting RMS < 0.001 and 0 < TCWV < 75 mm). From f = 0.05 to f = 0.55, 266 the number of co-located data pairs (N) more than triples, the mean of OMI-GPS increases from 267 0.32 mm to 1.66 mm, the standard deviation of OMI-GPS increases from 5.2 mm to 6.1 mm. The 268 linear correlation coefficient (r) increases from r = 0.87 at f = 0.05 to $r \sim 0.90$ at f = 0.15, then 269 levels off for larger cloud fraction thresholds. It should be noted that the error in cloud top 270 pressure decreases with cloud fraction in the OMCLDO2 product (Veefkind et al., 2016). As a 271 result, f = 0.05 corresponds to the largest uncertainty in cloud top pressure, and the error will 272 propagate into OMI TCWV through AMF, leading to smaller correlation coefficient than those 273 for larger f values.

274 In addition, as shown by the GPS versus OMI joint distributions for different cloud fraction 275 thresholds in Figure 4, the $f \ge 0.15$ cases have larger effective dynamical ranges which tend to 276 favor better correlations. For example, there is a larger fraction of data pairs with TCWV > 30277 mm for f = 0.15 than for f = 0.05. The regression line for f = 0.15 (OMI = 1.26 + 0.96 * GPS) 278 shows an apparent improvement over that for f = 0.05 (OMI = 2.22 + 0.88*GPS). The best 279 regression line is arguably that for f = 0.25 (OMI = 1.16 + 0.99*GPS) or f = 0.35 (OMI = 1.19 + 0.99*GPS) 280 1.00*GPS), though the mean bias and scatter are larger than those for f < 0.25 (Figure 4). 281 In brief, f = 0.05 leads to the lowest overall bias and scatter of the co-located data; f = 0.15282 doubles the number of co-located data pairs and leads to the largest improvement in the 283 correlation coefficient; f = 0.25 (or 0.35) leads to the best linear regression line; the bias and 284 standard deviation increase with cloud fraction threshold. Hence, cloud fraction thresholds in the

range of f = 0.05 - 0.25 seems reasonable for filtering OMI TCWV, depending on applications.

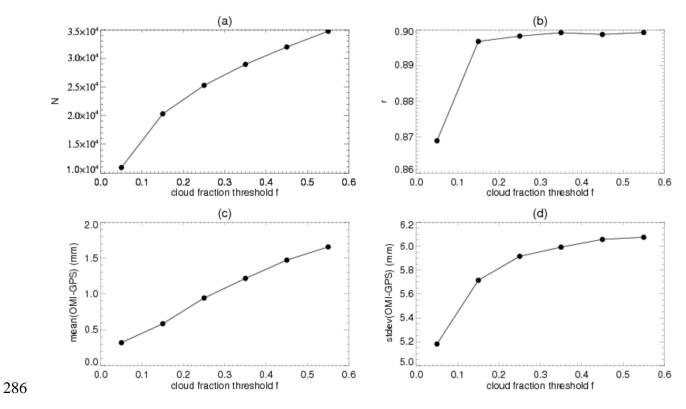


Figure 3. Dependence of various parameters on the cloud fraction threshold (f) used for filtering
OMI data. Other filtering criteria remain the same as those for Figure 2. The parameters are (a)
number of co-located OMI and GPS data pairs; (b) linear correlation coefficient between OMI
and GPS TCWV; (c) mean of OMI-GPS in mm; (d) standard deviation of OMI-GPS in mm.
Results are derived from the co-located Version 4.0 OMI and GPS data for the whole year of
2006.

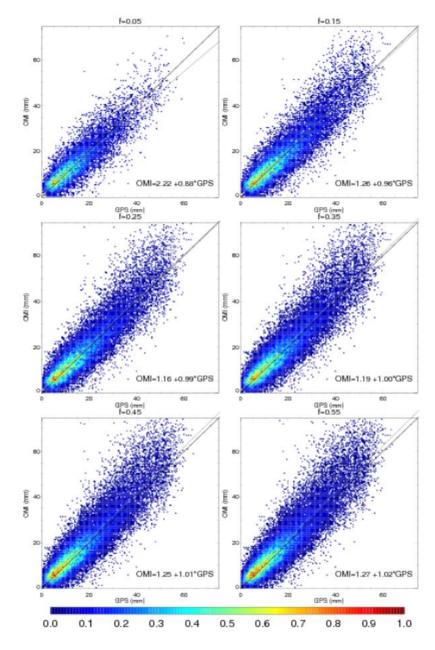


Figure 4. Normalized joint distributions of GPS versus Version 4.0 OMI TCWV for different cloud fraction thresholds. Results are derived from the co-located data pairs for 2006. The OMI data filtering criteria are the same as those for Figure 3. In each panel, the 1:1 line is plotted in black, the linear regression line is plotted in gray and indicated by the formula in the lower right corner.

To further characterize the effect of cloud fraction threshold on the comparison between GPS
and OMI, in Figure 5, we examine the mean and standard deviation (σ) of OMI-GPS for each 10
mm GPS TCWV bin. The results are derived from the same sets of co-located GPS and OMI

302 data as those used in Figure 3 and Figure 4. The filled symbols are for the cases where the

303 number of GPS and OMI data pairs within the corresponding TCWV bin is > 1% of the total

number of data pairs, and the open symbols are for < 1%. As the filled symbols represent better

305 statistics, we will focus on them below.

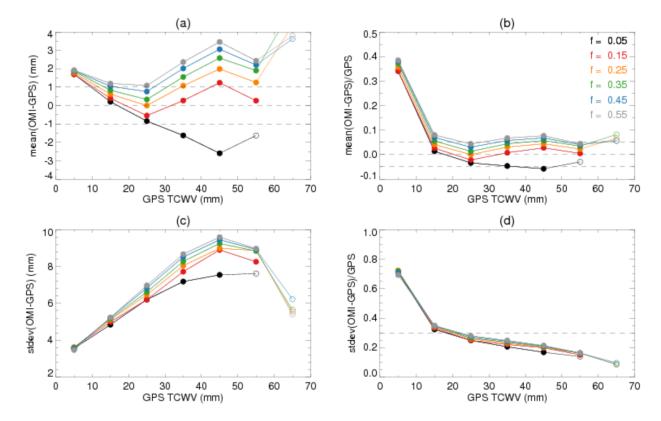


Figure 5. Parameters for each 10 mm TCWV bin. Curves with different colors are for different cloud fraction thresholds f as indicated in Panel (b). The OMI filtering criteria remain the same as those for Figure 3 and 4. Symbols are filled if the fraction of data pairs within the TCWV interval is > 1% of all the available data pairs and are open otherwise. The parameters are (a) mean of OMI-GPS in mm, (b) relative bias defined as mean(OMI-GPS)/GPS, (c) standard deviation (σ) of OMI-GPS in mm, and (d) relative scatter defined as σ /GPS. Results are for all days in 2006. Dashed lines are meant to facilitate visualization.

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Figure 5(a) shows that the means of OMI-GPS vary between ± 4 mm following "V"-shaped curves whose minima occur in the TCWV = 20 – 30 mm bin except for f = 0.05. The curves shift upward with increasing cloud fraction thresholds, suggesting that OMI cloudy-sky TCWV is generally larger than OMI clear-sky TCWV. Other things being equal, cloud formation indicates 319 water vapor saturation and therefore a larger amount of TCWV than that under clear-sky 320 condition. The smallest absolute bias for 10 < TCWV < 20 mm occurs at f = 0.05, that for 20 < 10321 TCWV < 30 mm occurs at f = 0.25, and that for 30 < TCWV < 40 mm occurs at f = 0.15. The f =322 0.15 and f = 0.25 curves show the best overall performance according to Figure 5(a) as they are 323 within 1 mm of zero for 10<TCWV<40 mm, while other curves come within 1 mm of zero in 324 narrower TCWV ranges. Figure 5(b) shows the relative bias which is defined as the mean of 325 (OMI-GPS)/GPS. The relative biases decrease sharply from ~40% to ~5% as GPS TCWV 326 increases from the TCWV = 0 - 10 mm bin to the TCWV = 10 - 20 mm bin, and generally stay 327 less than $\sim 5 - 10$ % for larger TCWV values. Figure 5(c) shows that σ increases from ~3.5 mm for TCWV = 0 - 10 mm to \sim 9.5 mm for TCWV = 40 - 50 mm (the percentage of data with 328 329 TCWV > 50 mm is very small). In most cases, larger cloud fraction thresholds correspond to 330 larger σ values. This is consistent with the larger dynamical range (due to a larger fraction of 331 data with high TCWV) for larger cloud fraction threshold (Figure 4). In fact, the relative scatter, 332 defined as the mean of σ /TCWV, shows little difference among the f values (Figure 5d). The 333 relative scatter decreases with TCWV, with the sharpest decrease from ~ 0.7 to ~ 0.3 between 334 TCWV = 0 - 10 mm and TCWV = 10 - 20 mm (Figure 5d). The relative scatter continues to 335 decrease for larger TCWV and the overall scatter is about 20%.

In short, Version 4.0 OMI agrees with GPS within 1 mm for 10 < TCWV < 40 mm when f = 0.15 and f = 0.25 are used; when f = 0.05 is used, the bias and scatter are the smallest for 10 < TCWV < 20 mm; but, for TCWV < 10 mm, OMI TCWV is too high and has large relative scatter. The latter is expected from the low signal-to-noise ratio when TCWV < 10 mm in the OMI retrieval.

341 **3.2 OMI and SSMIS over ocean**

To evaluate Version 4.0 OMI TCWV over the oceans, we compare against the microwave TCWV data from SSMIS on board the Defense Meteorological Satellite Program (DMSP)'s F16 satellite. The SSMIS data are derived by Remote Sensing Systems (RSS) using their Version 7 algorithm (www.remss.com) and have a retrieval accuracy of better than 1 mm (Wentz, 1997; Mears et al., 2015). For clear-sky comparison, we use the daily 0.25°×0.25° SSMIS data for January and July 2006 and filter out the pixels affected by rain and cloud liquid water. Diedrich et al. (2016) found that the diurnal cycle in TCWV is generally within 1% to 5% of the daily mean, with a minimum between 0600 LT and 1000 LT and a maximum between 1600 LT and
2000 LT. To reduce the influence of diurnal cycle, we average the SSMIS data for the ascending
and descending orbits of F16 (~2000 LT and 0800 LT in 2006).

We generate daily $0.25^{\circ} \times 0.25^{\circ}$ Level 3 OMI TCWV from the de-striped Level 2 OMI swaths, with the requirement that MDQFL = 0, fitting RMS < 0.001, 0<TCWV<75 mm, cloud fraction < 0.05, and cloud top pressure > 750 mb. There are typically 15 Level 2 swaths per day. The gridding program uses a tessellation method that weighs the contribution of a Level 2 data point by its area within the Level 3 grid square and its spectrum fitting uncertainty (Wang et al., 2014, 2016). The filtered daily Level 3 SSMIS and OMI data are compared for each month. We find 548,223 and 847,678 co-located data pairs for January and July 2006, respectively.

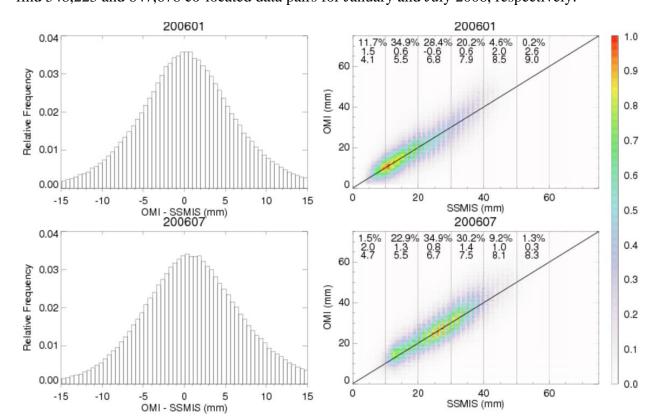


Figure 6. Comparisons between Version 4.0 OMI and SSMIS over the oceans for (top) January
2006 and (bottom) July 2006. Panels in the left column show the relative occurrence frequency
of OMI-SSMIS (mm). Panels in the right column show the normalized joint distribution of
SSMIS versus OMI TCWV (mm).

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365 The left column of Figure 6 shows the distribution of OMI-SSMIS for January and July 366 2006. For July, the mean of OMI-SSMIS is 1.1 mm with a standard deviation of 6.8 mm, the 367 mean absolute error |OMI-SSMIS| is 5.2 mm; for January, the mean error, standard deviation and 368 mean absolute error are 0.4 mm, 6.5 mm and 5.0 mm, respectively. This suggests a slightly better 369 agreement for January than for July. In comparison with the (OMI-GPS) over land (Section 3.1), 370 OMI-SSMIS over the oceans has somewhat larger bias and standard deviation. However, as 371 TCWV over the oceans are generally larger than that over land (compare Figure 6 with Figure 372 2), the relative bias and scatter are actually similar.

373 The right column of Figure 6 shows the normalized joint distribution of SSMIS versus OMI 374 for January and July 2006. The correlation coefficients are r = 0.84 and 0.82 for January and 375 July, respectively. For January, OMI-SSMIS remains within 0.6 mm of zero for TCWV in the 10 376 -40 mm range, but is 1.5 mm for TCWV in the 0-10 mm range (only a small fraction of data 377 pairs have TCWV > 40 mm); for July, OMI-GPS is 0.8 mm for the TCWV = 20 - 30 mm bin, 378 and varies between 0.8 and 1.4 mm for TCWV in the 10-50 mm range (only a small fraction of 379 data pairs have TCWV < 10 mm or > 50 mm). For TCWV bins that have > 5% of the data pairs, 380 the standard deviation of OMI-SSMIS vary between 4.1 and 8.1 mm. Overall, Version 4.0 OMI 381 data compare reasonably well with SSMIS data for TCWV in the 10-40 mm range, with the 382 smallest bias occurring in the TCWV = 20 - 30 mm bin.

The agreement between Version 4.0 OMI with SSMIS is better than that between Version 3.0 OMI and SSMIS. For July 2006, using the same data filtering criteria as before, we find that Version 3.0 OMI – SSMIS has a mean of 3.2 mm with a standard deviation of 7.8 mm. The bias is much larger than that for Version 4.0 OMI – SSMIS. Again, this is because of the much larger SCD of Version 3.0 OMI TCWV due to the water vapor reference spectrum (Supplementary Figure 1).

Table 3 shows the effect of cloud fraction threshold (f) on the comparison between SSMIS and Version 4.0 OMI TCWV. The comparisons are performed using daily filtered Level 3 data for July 2006. For SSMIS, we only filter out pixels affected by rain. To investigate the influence of clouds, cloud liquid water is not used to filter the SSMIS data here. This is less restrictive than the criteria used for Figure 6 as the SSMIS pixels with cloud liquid water are filtered out in Figure 6 for the "clear-sky" comparison there. For OMI, we require MDQFL = 0, RMS < 0.001,

- 0 < TCWV < 75 mm, cloud top pressure > 750 mb and cloud fraction < f. Results show that OMI
- is higher than SSMIS by 0.02 3.07 mm for f = 0.05 0.45. The difference between the f = 0.05
- 397 case of Table 3 and the f = 0.05 case of Figure 6 is due to the relaxed SSMIS filtering criteria.
- 398 The closest agreement in terms of the mean and standard deviation of OMI-SSMIS occurs when
- f = 0.05. The number of SSMIS and OMI data pairs more than doubles between f = 0.05 and f = 0.05.
- 400 0.15. The linear correlation coefficient varies between 0.82 and 0.85 within the range of f values
- 401 considered. The best linear regression line (OMI = 0.70 + 1.02 * SSMIS) occurs when f = 0.15.
- 402 Therefore, for OMI over the oceans, we recommend using cloud fraction threshold f = 0.05 0.05
- 403 0.15, in combination with the other usual data filtering criteria, though users are advised to make
- 404 their own decisions based on their tolerance and applications.

405 **Table 3.** Effect of cloud fraction threshold on the comparison between SSMIS and Version 4.0

406 OMI TCWV for July 2006. f: OMI cloud fraction threshold; N: number of qualifying data pairs;

407 P: Percentage of qualifying data pairs with respect to the total number of qualifying SSMIS data

408 points; Mean: mean of OMI-SSMIS in mm; σ: standard deviation of OMI-SSMIS in mm; MAE:

- 409 Mean absolute error |OMI-SSMIS| in mm; r: correlation coefficient between SSMIS and OMI;
- 410 R^2 : coefficient of determination for linear regression OMI = b + k * SSMIS, where OMI and
- 411 SSMIS are in mm; b: Intercept of linear regression; k: slope of linear regression.

f	Ν	P (%)	Mean	σ	MAE	r	\mathbb{R}^2	b	k
0.05	1,048,879	7.4	0.02	7.11	5.39	0.82	0.67	1.43	0.95
0.15	2,837,032	20.0	1.38	7.82	5.84	0.84	0.71	0.70	1.02
0.25	3,932,468	27.8	2.20	8.09	6.09	0.84	0.71	1.11	1.04
0.35	4,819,185	34.0	2.73	8.22	6.24	0.85	0.72	1.45	1.05
0.45	5,537,003	39.1	3.07	8.26	6.32	0.85	0.72	1.62	1.06

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Lowering the value for cloud top pressure threshold also leads to larger bias and scatter. For example, when cloud fraction threshold f = 0.05 and cloud top pressure > 500 mb are used, the mean and standard deviation of OMI-SSMIS become 0.80 mm and 7.9 mm, both are larger than those for f = 0.05 in Table 3, though the linear regression line improves to OMI = 0.63 + 1.01 *RSS due to an increase in the dynamical range of TCWV. It should be noted that the OMCLDO2 cloud product shows good agreement with ground-based observations for clouds at altitudes lower than 2.5 km where single cloud layers dominate, but shows significant bias and large

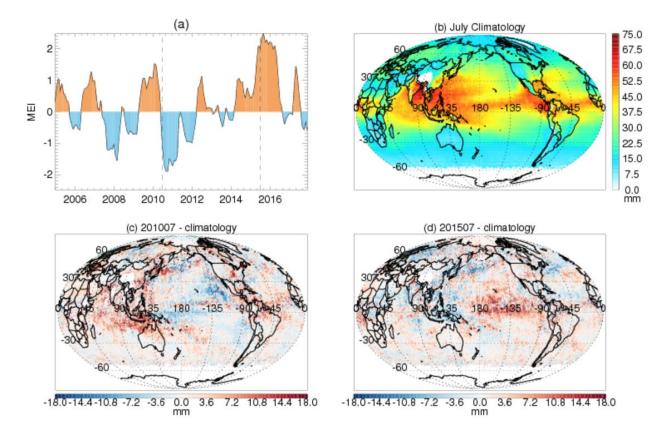
- 420 scatter for clouds at altitudes higher than 2.5 km where multi-layer clouds dominate (Veefkind et
- 421 al., 2016). Thus, OMI TCWV data corresponding to low cloud top pressure (high altitude)
- 422 should be used with caution. Relaxing the filtering criteria for both cloud fraction and cloud top
- 423 pressure will lead to larger bias and scatter, therefore, it is not recommended. As an example, for
- 424 cloud fraction < 0.15 and cloud top pressure > 300 mb, the mean (standard deviation) of OMI-
- 425 SSMIS becomes 2.8 mm (9.0 mm) for July 2006.

426 4 Applications

427 **4.1 El Niño / La Niña**

- 428 In Figure 7, we examine the signals associated with El Niño and La Niña in Version 4.0 OMI
- 429 TCWV. Panel (a) shows the Multivariate ENSO Index (MEI) from NOAA (Wolter and Timlin,
- 430 1998) (https://www.esrl.noaa.gov/psd/enso/mei/). Positive (negative) values correspond to El
- 431 Niño (La Niña) conditions. We examine the anomalies in TCWV for July 2010 (MEI = -1.103,
- 432 La Niña) and July 2015 (MEI = 1.981, El Niño) in the bottom row. Although these events are
- 433 strong within the OMI record (from 2005 to the present), they are mild in comparison with the
- 434 extrema. Between 1950 and 2018, the maximum MEI is 3.008 (in March 1983) and the
- 435 minimum MEI is -2.247 (in June 1955).

436



437

Figure 7. Top row: (a) Multivariate ENSO Index. Dashed vertical lines indicate July 2010 and
July 2015; (b) TCWV (mm) climatology for July derived from Version 4.0 OMI data. Bottom
row: TCWV anomaly (mm) with respect to the climatology for (c) July 2010 and (d) July 2015.

442 To examine the changes in OMI TCWV under different conditions, we first generate the 443 monthly Level 3 $(0.5^{\circ} \times 0.5^{\circ})$ OMI TCWV using the Level 2 data for July 2005 and July 2015 444 using the method described in Section 3.2 (with a cloud fraction threshold of f = 0.15 and a cloud 445 top pressure threshold of 750 mb). Then, using the same data filtering criteria, we derive the 446 climatology for July using all the Level 2 July data between 2005 and 2015 (Figure 7b). Finally, 447 we plot the deviations from the climatology (mm) for July 2010 and July 2015 in Figure 7(c) and 448 7(d), respectively.

The TCWV anomalies exhibit large-scale patterns. The pattern for July 2015 largely opposes that for July 2010. Particularly, in July 2015 under El Niño conditions, TCWV are higher in the equatorial central and eastern Pacific and lower in the Indonesia region; while in July 2010 under La Niña conditions, TCWV are lower in the tropical eastern Pacific and equatorial western Pacific and higher in Indonesia and the Indian Ocean. The overall patterns largely conform to the
results derived from the Hamburg Ocean Atmosphere Parameters and Fluxes from Satellite Data
(HOAPS) data (Shi et al., 2018).

456 **4.2 Corn Sweat**

457 "Corn sweat" refers to a hot and humid condition associated with heat waves which results in 458 large evapotranspiration rate in the Midwestern United States where cropland is often the 459 dominant land usage type. Besides evaporation, transpiration by plants, such as corn, draws 460 water from the soil to the atmosphere, enhancing the humidity and increasing the heat index. A 461 corn sweat event from July 18 to July 24 in 2016 made news in the US. This event is examined 462 in Figure 8 using the Version 4.0 OMI TCWV.

463 Figure 8 (a) and 8(b) show the Level 3 $(0.25^{\circ} \times 0.25^{\circ})$ OMI TCWV for July 18 - July 24

464 (7-day) and June 1 – August 31 (JJA) in 2016, respectively. The 7-day period corresponds to the 465 corn sweat event. The $0.25^{\circ} \times 0.25^{\circ}$ Level 3 data are derived using the same filtering criteria as 466 those used for Figure 7. Figure 8(c) indicates the anomaly associated with the corn sweat event 467 relative to the JJA mean. High TCWV is observed for the 7-day period from the Gulf coast to the 468 Midwestern US. Besides the Gulf region, the largest TCWV enhancements (of up to 18+ mm) 469 occur in parts of Iowa (IA), Missouri (MO), Illinois (IL) and Indiana (IN). Elevated TCWV is 470 also observed by several GPS stations in the general area during the same time period, though 471 coincident OMI data are not found at the stations (Supplementary Figure 3). At a few GPS stations, high TCWV persisted a couple more days after July 24 which is most likely related to a 472 473 change in the weather. As shown by the surface pressure observations at the GPS stations, the 474 Midwest is under the control of a high-pressure system during the corn sweat period and a low-475 pressure system afterwards (Supplementary Figure 4).

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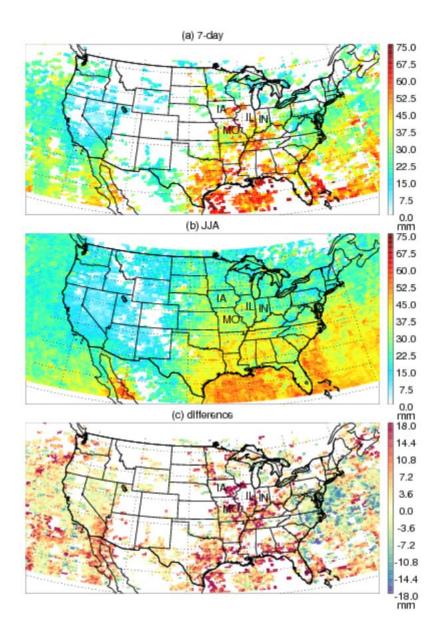


Figure 8. Level 3 (0.25°×0.25°) OMI TCWV (mm) generated using the Level 2 data during (a)
July 18 - July 24, 2016 and (b) June 1 - August 31, 2016. (c) The difference of (a) - (b) in mm.

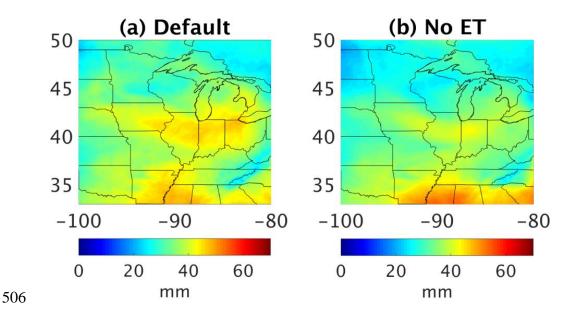
480 The abbreviations for the states most affected by the event are indicated in the map.

481

To assess the significance of evapotranspiration for the Midwestern US during the corn sweat
event, we carried out a sensitivity study using the Weather Research and Forecasting (WRF)
model v3.9.1 (Skamarock et al., 2008). The model was run on a 36-km parent domain and a 12km nested domain, covering the relevant areas of the US. The physics parameterizations

486 included the WRF Single-Moment (WSM) 6-Class Microphysics (Hong and Lim, 2006), the 487 Kain-Fritsch (KF) subgrid cumulus parameterization (Kain, 2004), the Yonsei University (YSU) 488 planetary boundary layer scheme (Hong et al., 2006), the Noah Land-Surface Model (Ek et al., 489 2003; Chen and Dudhia, 2001), and the Rapid Radiative Transfer Model (RRTM). Horizontal 490 turbulent diffusion was based on the standard Smagorinsky first-order closure. The initial and 491 lateral boundary conditions were from the 3-hourly NCEP North American Regional Reanalysis 492 (NARR) at 32-km resolution. To reduce the uncertainty associated with lateral boundary 493 condition for the nested domain, we nudged the model in the parent domain toward the 494 reanalysis, but left the nested domain running freely.

495 To diagnose the contribution of evapotranspiration, the model was run from July 19th to July 22nd of 2016 with and without evapotranspiration (calculated in the Noah Land-Surface model). 496 497 The results for July 21st are shown in Figure 9. TCWV is generally lower in the interior of the 498 domain for the run without evapotranspiration (No ET). The higher TCWV in the No ET run 499 near the southern boundary reflects non-linear water vapor transport from the Gulf region. 500 Turning off evapotranspiration not only directly affects the water vapor flux from the surface but 501 also indirectly influences other meteorological variables, such as winds. Thus, there is a 502 difference in the water vapor flux across the domain boundary. The difference between the 503 default and No ET runs in Figure 9 suggests that evapotranspiration contributes about 15 - 25%504 of the TCWV in the Midwestern US during the corn sweat event. A detailed study incorporating 505 TCWV data with the WRF model will be carried out in future work.



507 Figure 9. WRF simulations of TCWV (mm) for Midwestern US on 07/21/2016 for the run (a)
508 with and (b) without evapotranspiration.

509

510 **4.3 Atmospheric River (AR)**

511 4.3.1 An Intense AR in OMI data

ARs are narrow elongated bands with high TCWV in the atmosphere. With flow rates similar to those of large rivers, ARs are highly important in the global hydrological cycle (Zhu and Newell, 1998). Land-falling ARs can lead to heavy orographic precipitation that affects areas such as the west coast of North America and Europe (Gimeno et al., 2014; Neiman et al., 2008b).

The extreme AR of November $6^{th} - 7^{th}$, 2006 brought devastating flood to the Pacific 516 517 Northwest - the region in western North America bounded by the Pacific to the west and the 518 Cascade mountain range to the east. This AR is described in detail in Neiman et al., 2008a. The 519 signature of this AR is captured in the Version 4.0 OMI TCWV data. The left column of Figure 10 shows the Level 3 OMI TCWV and its anomaly on November 6th, 2006. The Level 3 data are 520 521 generated following the same procedure as that used for Figure 8. Although many pixels are 522 missing because of the cloud filtering (cloud top pressure > 750 mb, cloud fraction < 0.15) and 523 other criteria, the leading edge of the AR is noticeable as an elongated band of high TCWV (15+ 524 mm above the climatology) extending from Hawaii to Northern California (indicated by arrows 525 in Figure 7(b) and 7(c)). The position of the AR in OMI TCWV agrees well with that in Special 526 Sensor Microwave/Imager (SSM/I) microwave observation (Neiman et al., 2008a).

527 The right column of Figure 10 shows the Level 3 OMI ozone mixing ratio interpolated to 200 528 mb and its anomaly. The OMI ozone data are retrieved using the SAO ozone profile algorithm 529 (Liu et al., 2010; Huang et al., 2017, 2018). The climatology is derived by averaging all monthly 530 Level 3 data for November from 2004 to 2017. The global distribution of ozone at 200 mb shows 531 low mixing ratio in the low latitudes and high mixing ratio in the high latitudes, opposite to the 532 global distribution of TCWV. The anomaly shows a curvilinear band of high ozone that is 533 parallel to the AR in the left column, but is located further to the west. This feature indicates 534 intrusion of ozone rich stratospheric air along the polar front, and is associated with the same 535 extra-tropical cyclone as the AR is.

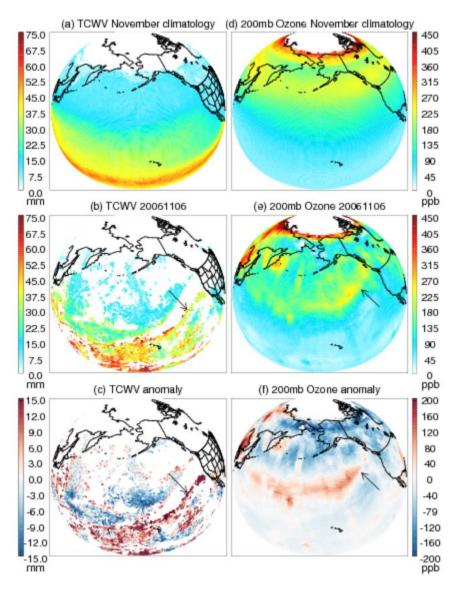


Figure 10. The Level 3 (top row) climatology, (middle row) data on November 6th, 2006 and (bottom row) anomaly on November 6th, 2006 with respect to the climatology for (left column) Version 4.0 OMI TCWV (mm, $0.5^{\circ} \times 0.5^{\circ}$) and (right column) OMI ozone mixing ratio (ppb, $1^{\circ} \times 1^{\circ}$) interpolated to 200 mb.

536

542 **4.3.2 OMI TCWV Assimilation for the AR**

543 To evaluate the potential of OMI water vapor data to improve numerical weather forecasts,

544 we conducted a data assimilation experiment from November 2nd to November 8th of 2006 using

545 WRF v3.9.1 and Version 4.0 OMI TCWV. The model was configured with a 27-km (290×270

546 surface grid points with 51 vertical levels), a 9-km (586×586×51 points) and a 3-km

547 (541×526×51) nested domains in a Lambert projection over the relevant portion of the Pacific

and North America (Figure 11 top left). The domains are designed for the November 6 AR event

549 and its associated precipitation at landfall. The model has the same physics parameterizations as

those used in Section 4.2 except that a more sophisticated double-moment microphysics scheme

is used for quantifying precipitation. The initial and boundary conditions for the 27-km domain

552 were from the $1^{\circ} \times 1^{\circ}$ NCEP FNL reanalysis. One-way nesting is used for the inner domains. To

- evaluate the model's skill at simulating the AR and the contribution of OMI TCWV to the
- quality of the simulation, we did not nudge the run towards the reanalysis, nor assimilate the

observed sea surface temperature within the computational domains.

556 The OMI TCWV is assimilated into the model using analytical optimal estimation (Rodgers, 557 2000). This method minimizes the cost function $J(\mathbf{x}) = (\mathbf{y} - H\mathbf{x})^T \mathbf{E}^{-1} (\mathbf{y} - H\mathbf{x}) +$

558 $(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b)$, where x is the true TCWV, x^b is the a priori TCWV (from the model), y

is the observed TCWV, *H* represents the model Jacobian, **B** and **E** are the error covariance

560 matrices of the a priori and observation. **B** is estimated using the 12-hour and 24-hour forecasts

using the National Meteorological Center method (Parrish and Derber, 1992). E is based on the
fitting uncertainties of OMI data.

The a posteriori analysis $(\hat{\mathbf{x}})$ can be obtained from $\hat{\mathbf{x}} = \mathbf{x}^b + \mathbf{K}(\mathbf{y} - H\mathbf{x})$, where $\mathbf{K} =$ $\mathbf{B}H^T(H\mathbf{B}H^T + W^{-1}\mathbf{E})^{-1}$ is the Kalman gain, $W = \frac{(R^2 - r^2)}{(R^2 + r^2)}$ is the Cressman function to weigh the observations based on their Euclidian distance *r* to the model grids, and *R* is the influence radius of the observations. We simply assume *R* to be 1°, 0.5° and 0.25° for the 27-km, 9-km and 3-km domain to get a quick look at the results in this paper and leave a more vigorous quantification of Data for the observation of the observation observation of the observation of the observation observation

R to future work. The a posteriori TCWV is solved hourly when OMI data are available and isused to initialize the next simulation window.

570 During the assimilation, we adjust the OMI data using the AMF calculated with the modeled 571 water vapor profile $(OMI_{satellite}^{adjusted} = \frac{OMI_{satellite} \times AMF_{satellite}}{AMF_{model}})$ and the scattering weights provided 572 with the Level 2 OMI data. This can reduce the observational error associated with using the 573 monthly mean water vapor profile in the operational OMI product. The standard deviation of the 574 difference between $AMF_{satellite}$ and AMF_{model} is about 20%.

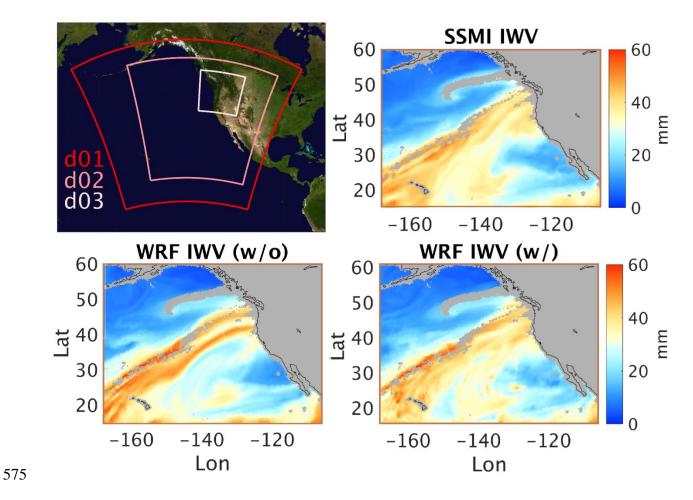
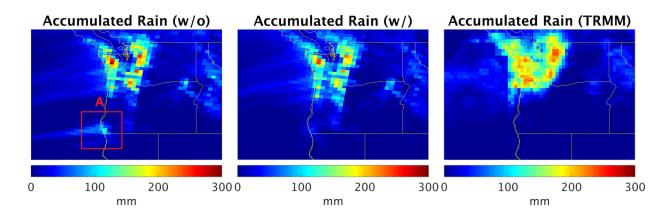


Figure 11. Top left: WRF model domain configuration for the November 2006 AR event. Top
right: TCWV observed by SSM/I on November 6th, 2006. Bottom row: TCWV simulated by
WRF on the same day (left) without and (right) with OMI TCWV data assimilation. Gray color
indicates area with no SSM/I data.

Figure 11 shows the zoomed-in views of the AR on November 6th, 2006. The TCWV independently observed by SSM/I is shown in the upper right panel. The lower left and lower right panels show the model results without and with OMI TCWV assimilation. The model without assimilation shows an AR that is split into two parallel filaments making landfall at separate locations on the west coast of North America, where the TCWV is too high compared to the SSM/I observation, especially for the southern filament. As discussed later, this has a significant impact on precipitation (Figure 12). After assimilating OMI TCWV, the modeled 588 TCWV agrees much better with the SSM/I observation. The spurious southern filament 589 disappeared, the overall shape and amplitude of the AR are significantly improved.

590 The location and intensity of precipitation over land are crucial for local flood control and 591 water resource management, and are closely related to the shape and strength of AR at landfall. 592 The 24-hour accumulated precipitation on November 6 in the 3-km domain is examined in 593 Figure 12. The model output is coarsened to $0.25^{\circ} \times 0.25^{\circ}$ to match the resolution of the Tropical 594 Rainfall Measuring Mission (TRMM) observation product. The model without OMI data 595 assimilation produces spurious rainfall over the Oregon - California border (box A) as a result of 596 the erroneously strong southern filament of the simulated AR (Figure 11, lower left panel). This 597 artifact was removed after OMI data assimilation, showing better agreement with the 598 corresponding TRMM rainfall observation. The difference in rainfall between the assimilation 599 and observation in the Oregon / Washington area is probably related to both the model error and 600 the data error, as well as the data density and distribution. A detailed error attribution for 601 precipitation is beyond the scope of this paper.



602

Figure 12. The simulated rainfall accumulated from 0000 UTC to 2300 UTC (in mm) on
November 6, 2006 for the model (left) without and (middle) with OMI TCWV assimilation. The
rightmost panel show the accumulated rainfall observed by TRMM for the same time period.
Note that the 3-km model result is coarsened to match the resolution of the TRMM product.
Box A highlights the erroneously simulated precipitation in the run without OMI TCWV data
assimilation.

609

610 **5 Summary and Conclusion**

611 The Version 4.0 retrieval algorithm for OMI Total Column Water Vapor (TCWV) is presented 612 in this paper. The algorithm follows the usual two-step approach where Slant Column Density 613 (SCD) is derived from spectral fitting and Vertical Column Density (VCD) is obtained through 614 the ratio of SCD and Air Mass Factor (AMF). In Version 4.0, the spectral fitting no longer 615 considers common mode. The retrieval window (432.0 - 466.5 nm) results from a systematic 616 optimization that reflects trade-offs among several factors, including small fitting RMS, small 617 fitting uncertainty, large fraction of successful retrieval and long retrieval window length. The 618 AMF calculation uses the latest OMI O₂-O₂ cloud product (Veefkind et al., 2016) and monthly 619 variable vertical profiles from the MERRA-2 reanalysis (Gelaro et al., 2017).

620 The Version 4.0 OMI TCWV product is compared against the GPS network data over land 621 and the SSMIS microwave observations over the oceans for 2006. Version 4.0 OMI TCWV has 622 much smaller bias than Version 3.0 and has replaced previous versions on the Aura Validation 623 Data Center website. Version 4.0 OMI TCWV is characterized under different cloud conditions. 624 Under "clear-sky" condition (cloud fraction < 5% and cloud top pressure > 750 mb), the overall 625 mean of OMI-GPS over land is 0.32 mm with a standard deviation of 5.2 mm, and the smallest 626 bias occurs when TCWV is between 10 mm and 20 mm; the overall mean of OMI-SSMIS over 627 the oceans is 0.4 - 1.1 mm with a standard deviation of 6.5 - 6.8 mm, and the smallest bias 628 occurs for TCWV between 20 mm and 30 mm. The correlation coefficient between OMI TCWV 629 and the reference datasets realizes the largest gain when the cloud fraction threshold is increased 630 from 5% to 15%. The regression line appears the best when f = 0.25 is used over land and when f 631 = 0.15 is used over the oceans. But, larger cloud fraction leads to larger bias and scatter. Thus, 632 for most applications, we recommend to consider only OMI data with cloud fraction < 5% to 633 25% and cloud top pressure > 750 mb, in addition to main data quality flag = 0, no row anomaly, 634 fitting RMS < 0.001 and 0<TCWV<75 mm. Relaxing the cloud top pressure threshold has a 635 similar effect as relaxing the cloud fraction threshold. TCWV corresponding to low cloud top 636 pressure (high altitude) should be used with caution due to the degraded accuracy for these 637 clouds in the OMCLDO2 product.

As example applications of the Version 4.0 OMI TCWV data across a variety of temporal and spatial scales, this paper examines the climate pattern associated with El Niño / La Niña, the enhanced humidity during a week-long corn sweat event in the Midwest US, and the linear band of high TCWV associated with an intense atmospheric river which made landfall on the west 642 coast of North America. Strong signals are found in OMI TCWV for all three examples. A data
643 assimilation experiment shows that the OMI TCWV data can help improve WRF's skill of
644 simulating the shape and intensity of the AR, as well as the accumulated rainfall near the coast.

Further improvement of the product can proceed from both spectral fitting and AMF
calculation, such as, water vapor reference spectrum, instrument slit-function and solar irradiance
for spectral fitting, aerosol correction and surface bi-directional reflectance for AMF calculation.

648

649 Data availability

650 The GPS network data are downloaded from NCAR (rda.ucar.edu/datasets/ds721.1). The SSMIS

data used in this paper are downloaded from the Remote Sensing Systems

652 (http://www.remss.com/support/data-shortcut/). The Multivariate ENSO Indices are downloaded

653 from NOAA (https://www.esrl.noaa.gov/psd/enso/mei/table.html). OMI TCWV and ozone

profile data are released through the Aura Validation Data Center (https://avdc.gsfc.nasa.gov/).

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656 Author contribution

657 Huiqun Wang optimized the OMI TCWV retrieval window, performed the data validation 658 and tested most of the data application described in this paper. Amir Souri performed the WRF 659 simulations and data assimilation experiment presented in this paper. Gonzalo González Abad 660 improved and maintained the SAO retrieval code and implemented OMI TCWV data production 661 for the Aura Validation Data Center. Xiong Liu developed the OMI ozone profile retrieval and 662 provided the relevant data used in the AR application. Kelly Chance is the PI of the NASA grant, 663 and is responsible for the overall direction and execution of the project. Huigun Wang prepared 664 and revised the manuscript with contributions from all co-authors. All authors contributed to 665 technical and scientific discussions during this project.

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667 **Competing interests**

668 The authors declare that they have no conflict of interest.

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