RESEARCH ARTICLE

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Key Points:

- Insolation retrievals from the GOES satellite tend to reduce overestimates of downwelling shortwave radiation in WRF meteorological model
- Using satellite retrievals as inputs reduces MEGAN model estimates of isoprene emissions by an average of 20% during an episode over Texas
- Introducing the GOES assimilated clouds can improve model performance for simulated ground-level ozone over Texas

Supporting Information:

- Supporting Information S1

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Incorporating GOES Satellite Photosynthetically Active Radiation (PAR) Retrievals to Improve Biogenic Emission Estimates in Texas

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Abstract This study examines the influence of insolation and cloud retrieval products from the Geostationary Operational Environmental Satellite (GOES) system on biogenic emission estimates and ozone simulations in Texas. Compared to surface pyranometer observations, satellite-retrieved insolation and photosynthetically active radiation (PAR) values tend to systematically correct the overestimation of downwelling shortwave radiation in the Weather Research and Forecasting (WRF) model. The correlation coefficient increases from 0.93 to 0.97, and the normalized mean error decreases from 36% to 21%. The isoprene and monoterpene emissions estimated by the Model of Emissions of Gases and Aerosols from Nature are on average 20% and 5% less, respectively, when PAR from the direct satellite retrieval is used rather than the control WRF run. The reduction in biogenic emission rates using satellite PAR reduced the predicted maximum daily 8 h ozone concentration by up to 5.3 ppbV over the Dallas-Fort Worth (DFW) region on some days. However, episode average ozone response is less sensitive, with a 0.6 ppbV decrease near DFW and 0.3 ppbV increase over East Texas. The systematic overestimation of isoprene concentrations in a WRF control case is partially corrected by using satellite PAR, which observes more clouds than are simulated by WRF. Further, assimilation of GOES-derived cloud fields in WRF improved CAMx model performance for ground-level ozone over Texas. Additionally, it was found that using satellite PAR improved the model's ability to replicate the spatial pattern of satellite-derived formaldehyde columns and aircraft-observed vertical profiles of isoprene.

Plain Language Summary Models have long struggled to accurately estimate emissions of hydrocarbons from vegetation. Those emissions strongly influence concentrations of pollutants such as ozone and particulate matter. Errors in modeling of cloudiness and solar radiation may contribute to errors in estimates of biogenic emissions, which vary with the intensity of sunlight reaching vegetation. This study applies satellite retrievals of sunlight and cloudiness to adjust model estimates of hydrocarbon emissions from vegetation in a modeling episode over Texas. It then tests how those adjustments influence estimates of ozone, particulate matter, and formaldehyde. Pollutant measurements from satellites, aircraft, and ground-based monitors are used to evaluate model results.

1. Introduction

In the United States, the current national emission inventory (2011NElv2) estimate biogenic sources comprise 75%–80% of all volatile organic compound (VOC) emissions. Texas vegetation emits more biogenic VOC (BVOC) than any other state (The United States Environmental Protection Agency, 2015). Biogenic isoprene and monoterpenes, the dominant BVOC species (Fehsenfeld et al., 1992; Sindelarova et al., 2014), play a critical role in tropospheric chemistry and climate change through reactions with hydroxyl and nitrate radicals (Brown et al., 2013; Zhang et al., 2000), and ozone (Carlton & Baker, 2011; Warneke et al., 2004), and serve as important precursors of ozone and secondary organic aerosol (Carlton, Wiedinmyer, & Kroll, 2009; Hoffmann et al., 1997).

Biogenic emissions surpass anthropogenic emissions over the heavily forested eastern half of Texas and comprise nearly half of the total VOC inventory over transition areas between forest and densely populated areas (Song et al., 2008). A source apportionment study suggested that the contribution of BVOC emissions to ozone formation is about 20% higher than anthropogenic VOC over Southeast Texas (Ying & Krishnan, 2010). Therefore, accurate estimation of BVOC emissions is important for modeling to inform state implementation

plans for ozone nonattainment regions in Texas, such as Dallas-Fort Worth (DFW) and Houston-Galveston-Brazoria (HGB) (Allen et al., 2012).

Biogenic emission models typically represent BVOC as a function of land use/land cover classification, temperature, soil moisture, and the amount of photosynthetically active radiation (PAR) reaching the canopy. PAR is the light intensity between the wavelengths 0.4–0.7 μm available for photosynthesis. Models often show PAR to be one of the strongest influences on isoprene emissions, while monoterpenes from some plant species exhibit a weaker dependence on PAR (Guenther et al., 2012).

The Model of Emissions of Gases and Aerosols from Nature (MEGAN) (Guenther et al., 2012) is one of the most sophisticated and widely used models for simulating BVOC. The robustness of this biogenic emission model has been demonstrated through comparisons with direct flux measurements over forested areas (Acton et al., 2016; Eerdekens et al., 2009; Hu et al., 2015; Warneke et al., 2010). One of the key recommendations for using MEGAN for regional biogenic emission estimates is to use localized high-resolution emission factors and land cover data (Guenther et al., 2012; Huang et al., 2014; Misztal et al., 2016). Specific to Texas, some studies reported that MEGAN overestimated isoprene emissions (Song et al., 2008; Ying & Krishnan, 2010; Kota et al., 2015; Wang et al., 2017), though others find reasonable performance (Huang et al., 2015; Yu et al., 2015).

Overprediction of PAR by meteorological models has been suggested as a possible explanation for the overprediction of isoprene by MEGAN (Sakulyanontvittaya et al., 2012). Mesoscale weather models often fail to simulate clouds in the observed locations and times (Pour-Biazar et al., 2011; White et al., 2017). In particular, meteorological models tend to underpredict the presence of thin clouds or clouds that are smaller than the size of a grid cell. Since clouds reduce the availability of PAR, errors in simulated clouds influence emission estimates of BVOCs.

Observations of clouds and radiation fields from satellites such as the Geostationary Operational Environmental Satellite (GOES) provide an opportunity to enhance PAR estimates used by biogenic emissions models. The most widely used satellite PAR retrieval products were developed by the University of Maryland (UMD) (Pinker et al., 2003) in support of the GEWEX (Global Energy and Water Cycle Experiment, www.gewex.com) Continental-Scale International Project and the GEWEX Americas Prediction Project. This product had been used in biogenic emission models to evaluate associated impacts on BVOC (e.g., Carlton & Baker, 2011; Guenther et al., 2012; Song et al., 2008). However, this PAR retrieval product was discontinued in 2010. For this study, a new satellite-based PAR retrieval produced by the University of Alabama in Huntsville (UAH) was used. UAH collaborates with the Infrared Measurements and Water Vapor Studies Group (IR group) at the National Aeronautics and Space Administration (NASA)/Marshall Space Flight Center to generate and archive several GOES-derived products including cloud albedo, surface albedo, and surface insolation for the use in meteorological and air quality models (Haines et al., 2003). Daily GOES retrieval products are available online from 2006 through 2016 (<http://www.nsstc.uah.edu/uahgoes>). Over the years, these products have been evaluated and used in many air quality studies (Haines et al., 2003; McNider et al., 1998; Mackaro et al., 2011; Pour-Biazar et al., 2007). To meet the air quality community needs, UAH developed a new PAR retrieval algorithm and provided satellite-based PAR for this study.

This study applies two new methods for utilizing GOES imagery to improve the radiation fields that influence biogenic emission estimates. The first method assimilates clouds observed by GOES into the Weather Research and Forecasting (WRF) meteorological model. The second method directly estimates PAR from the GOES retrievals. These methods are applied over Texas during the September 2013 Deriving Information on Surface Conditions from COlumn and VERTically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) field campaign (<http://discover-aq.larc.nasa.gov/>) (Crawford et al., 2014). The associated meteorological fields and PAR estimates are then used by MEGAN to estimate emissions of BVOCs. Additionally, a series of Comprehensive Air Quality Model with extensions (CAMx) (Ramboll Environ, 2014) simulations were performed to evaluate the impact of emission and meteorological changes on air quality predictions.

2. Methodology

2.1. UAH PAR Retrieval Algorithm

Details of the UAH PAR retrieval are documented elsewhere (Pour-Biazar et al., 2015). Here we present a short summary of the technique used to produce the PAR product for this study.

One of the important factors impacting plant photosynthesis, and thus BVOC emission, is light availability. PAR is the part of the visible spectrum (0.4–0.7 μm) that stimulates photosynthesis by activating chlorophyll in plants. In general, about 45% of the incoming sunlight is used for photosynthesis by plants (Larcher, 2003). However, since the blue (0.4–0.5 μm) and red (0.6–0.7 μm) parts of the visible spectrum have a greater influence on photosynthesis, converting total insolation to PAR must account for this wavelength dependency (Salisbury & Ross, 1992). Additionally, previous studies have indicated that diffuse sunlight, i.e., incoming solar radiation scattered by aerosols and clouds, is more effective at increasing plants' photosynthesis than direct light (Cheng et al., 2015; Ge et al., 2011; Gu et al., 2002; Zhang et al., 2010). However, the scattering that is responsible for diffuse light also reduces the total energy reaching the canopy and in many cases results in a net reduction in PAR.

To produce PAR from satellite observations, a functional form of the conversion factor is needed to quantify its ratio to the total broadband surface insolation. The formulation must encapsulate the complexities involved in partitioning the total incident energy into direct and diffuse light. Such parameterization for PAR should also incorporate the dependency on zenith angle and cloud optical depth. Since PAR is a fraction of the total solar insolation, it is necessary to first derive the surface insolation from GOES. The algorithm developed by Diak and Gautier (1983) with improvement by Pour-Biazar et al. (2007) is used for the retrieval of surface insolation. This algorithm uses the GOES Imager visible channel (0.55 – 0.75 μm) data at 1 km resolution to explain the observed upwelling radiant energy for a clear and a cloudy atmosphere. The technique accounts for the effects of Rayleigh scattering (Coulson, 1959), ozone absorption (Lacis & Hansen, 1974), water vapor absorption (Paltridge, 1973), cloud absorption, and cloud reflection.

With the total surface insolation known, the portion of the incoming solar radiation that impacts photosynthesis can be estimated as

$$\text{PAR} = \text{Insolation} \times \text{CF} \quad (1)$$

where CF is the conversion factor and PAR and Insolation have units of W/m^2 . The average CF value is about 0.5 but varies with time and location depending on atmospheric parameters such as water vapor, total overhead ozone, aerosol and cloud optical depth, and zenith angle (Frouin & Pinker, 1995; Pinker & Laszlo, 1992).

A formulation for CF was developed that encapsulated the impact of cloud attenuation (C_{factor}) and zenith angle (Z_{factor}):

$$\begin{aligned} \text{CF} &= \frac{\text{PAR}}{\text{Insolation}} = 0.42 + 0.28 \times C_{\text{factor}} \times Z_{\text{factor}} \\ &= 0.42 + 0.28 \times \left(1 - 1.8^{-\sqrt{0.1 \times \tau}}\right) \times \left(1.1 - 0.1 \times \sqrt{\cos(Z)}\right)^{-\tau} \end{aligned} \quad (2)$$

where τ is the cloud optical depth and Z is the zenith angle in degrees. Optical depth is estimated from the satellite-derived cloud albedo (α_c), based on the parametrizations proposed by Stephens (1978):

$$\tau = \frac{8\alpha_c}{(1 - \alpha_c)^2} \quad (3)$$

The CF formulation was validated against the data provided by Pinker and Laszlo (1992) and Frouin and Pinker (1995), which showed the variation in CF for different optical depths and zenith angles. In equation (2), CF increases with optical depth due to the impact of diffused sunlight and approaches a maximum of 0.7 under thick clouds and low zenith angles. The dependence of CF on zenith angle and cloud optical depth is given in Figure S1 in the supporting information.

Since the PAR product is computed as a fraction of the satellite-derived insolation, any error in insolation retrieval will carry over to the PAR product. Thus, a thorough examination of insolation product was conducted by comparing it to surface pyranometer measurements. More information can be found in Pour-Biazar et al. (2015).

2.2. WRF-MEGAN-CAMx Simulation Platform

The WRF-MEGAN-CAMx simulation platform was used in this study to quantify the impact of satellite-based PAR and cloud assimilation on biogenic emission estimates and ozone formation. Table 1 outlines the model configurations used here. The modeling domain followed the configuration set by the Texas Commission on

Table 1
Configurations of WRF-MEGAN-CAMx Modeling Platform Used in This Study

		Mesoscale weather model (WRF)	
Version	WRF-ARW v3.6.1	Shortwave radiation	RRTMG ^a
Domain Setting	CONUS (D1), Texas (D2), and E Texas (D3)	Longwave radiation	RRTMG ^a
Vertical resolution	43 Layer with $P_{top} = 50$ hPa	Surface layer scheme	Monin-Obukhov
Land surface model	Unified Noah (four-soil layer)	PBL scheme	YSU ^b scheme
Microphysics	Thompson	Cumulus physics	Kain-Fritsch with moisture-advection trigger
Analysis nudging	T, Q, and Winds in D1 and D2 with nudging coefficients of 3×10^{-4} , 1×10^{-5} , and 3×10^{-4}	Nudging within PBL	Winds only in D1–D3
Version	MEGAN v2.10	Biogenic emission model (MEGAN)	
		Emission factor (EF)	EFvE2011 (Global emission factor database based on ecoregion-averaged PFT) Guenther et al., 2012
Plant functional type (PFT)	PFT16v2011 (spatial resolution: 30 arcsec) Guenther et al. (2012)	Leaf area index of vegetation fraction (LAIV)	2011 LAIV (2008 MODIS ^c 8 day average (MCD15A.005), spatial resolution: 30 arcsec) Guenther et al. (2012)
		Regional chemistry transport model (CAMx)	
Version	CAMx v6.10	Anthro. emission	NEI2011 with TCEQ updates
Domain grids	D1 (36 km), D2 (12 km), and D3 (4 km)	Biogenic emission	MEGAN with WRF PAR
Boundary condition	MOZART-4 ^e	Vertical diffusion	ACM2 ^f
Gas mechanism	CB05 ^g	Deposition scheme	Zhang et al. (2003)
Photolysis	TOMS ^h ozone column data measured by OMI ⁱ	Initial condition	Default concentration profiles with spin-up

^aThe Rapid Radiative Transfer Model for GCMs. ^bYonsei University. ^cModerate Resolution Imaging Spectroradiometer. ^dGeostationary Operational Environmental Satellite. ^eModel for Ozone and Related Chemical Tracers, version 4. ^fAsymmetrical Convective Model version 2. ^gCarbon Bound version 5. ^hTotal Ozone Mapping Spectrometer. ⁱOzone Monitoring Instrument.

Figure 1. Domain coverage of the WRF-MEGAN-CAMx platform used in this study, locations of monitoring sites for model evaluation, and map of the 10 climate divisions in Texas.

Environmental Quality (TCEQ) State Implementation Plan modeling (<https://www.tceq.texas.gov/airquality/airmod/data/domain>). The parent domain (D1) with 36 km horizontal grid spacing covers the whole contiguous United States (CONUS), the nested middle domain (D2) with 12 km horizontal grid spacing covers Texas, and the innermost nested domain (D3) with 4 km horizontal grid spacing focuses on East Texas. The innermost domain contains large biogenic emissions over the heavily forested region north and northeast of Houston. It also includes two ozone nonattainment metropolitan areas: Houston-Galveston-Brazoria and Dallas-Fort Worth (see Figure 1).

The WRF model with Advanced Research WRF (ARW) core v3.6.1 (www.wrf-model.org) is a mesoscale weather model used to simulate local- and synoptic-scale meteorological conditions during the period of interest (Skamarock et al., 2008). For this study, the model's initial and lateral boundary conditions were derived from the 12 km (grid 218) North American Mesoscale 6-hourly analysis (http://nomads.ncdc.noaa.gov/data.php#hires_weather_datasets). Important physical parameterizations used in this study include the following: the Rapid Radiative Transfer Model for General Circulation Models (GCMs) (RRTMG) scheme (Iacono et al., 2000) for shortwave and longwave radiations, Yonsei University (YSU) planetary boundary layer (PBL) scheme (Hong et al., 2006), Unified Noah 4 soil layer land surface model (Tewar et al., 2004), Thompson microphysics scheme (Thompson et al., 2008), and Kain-Fritsch cumulus parameterization scheme (Kain, 2004) with Ma and Tan (2009) trigger function. Analysis nudging of temperature (T), moisture (Q), and wind speed (U and V) was used in the WRF simulations with the nudging coefficient given in Table 1.

In addition to the base WRF simulation, a second simulation was conducted, which assimilated GOES-derived cloud fields to improve the placement of clouds in space and time within WRF. Based on GOES-derived cloud albedo and cloud top temperature, the assimilation technique determines the necessary vertical motion required to either dynamically create clouds by introducing positive vertical motion where the model underpredicts clouds, or dissipate clouds by introducing a negative vertical motion in locations where the model overpredicts clouds. In order to create the necessary vertical motion within the model, the horizontal wind field is adjusted using a one-dimensional variational technique based on O'Brien (1970). The adjusted horizontal wind field is then nudged into the model through Four Dimensional Data Assimilation by replacing the original analysis wind field. Further details on the assimilation technique can be found in White et al. (2017).

MEGAN version 2.1 (Guenther et al., 2012) was used to estimate the biogenic emissions under different PAR. MEGAN has the capability to use either the generic PAR, which is directly scaled from the WRF incoming solar radiation (with the scaling factor 0.5), or the satellite-retrieved PAR. Two sets of land use characterization as well as BVOC emission factor database were used in this study. One (version 2011) is the default inputs provided with MEGAN v2.1 (<https://bai.ess.uci.edu/megan/versions>) with leaf area index of vegetation

fraction (LAIv) from the 2008 8 day averaged Moderate Resolution Imaging Spectroradiometer (MODIS) MCD15A2 product (2011 LAIv) and 16 Community Land Model plant functional type (PFT) classification over North America with the horizontal resolution 30 arcsec (PFT16v2011). The global emission factors for 10 BVOC compound class are based on ecoregion-averaged PFT (EFvE2011). The other one (version 2015) is the update version based on a recent local study for TCEQ (Yu et al., 2015) with PFT derived from 30 m resolution 2012 Land Fire Existing Vegetation Type (EVT) data along with Forest Inventory and Analysis data (<http://www.fia.fs.fed.us>) for tree species composition (PFT16v2015). The LAIv data used in the update version are from 2013 8 day averaged MODIS MCD15A2 product (2013 LAIv). The updated emission factors (EFvA2015) are based on higher resolution land cover data, and isoprene emission factor is constrained with aircraft flux measurements (Yu et al., 2017).

CAMx version 6.10 was used to quantify the impact of different PAR/insolation inputs to ozone formation through 3-D photochemical transport modeling. Anthropogenic emissions for the simulation domains were provided by TCEQ based on the National Emission Inventory (NEI) version 2011 with local updates over the Texas region (ftp://amdaftp.tceq.texas.gov/pub/TX/camx/basecase/bc12_12jun.reg3a.2012_wrf361_p2a_i2_a/input/ei/Components/). Point sources were calculated inline in CAMx using the environmental conditions to estimate buoyancy rise and plume dispersion. Gas phase chemistry was simulated with the Carbon Bond mechanism version 2005 (CB05) (Yarwood et al., 2005). The photolysis rates were calculated off-line from the day-specific ozone column data observed by the Ozone Monitoring Instrument (OMI). The initial and boundary conditions for CAMx were provided by Model for Ozone and Related Chemical Tracers version 4 (MOZART-4) (Emmons et al., 2010).

2.3. Simulation Case and Model Evaluation Arrangement

The time period chosen for this study was September 2013, which coincides with the Houston-based NASA's DISCOVER-AQ field campaign (Crawford et al., 2014). In situ trace gas measurements from P-3B flights during this campaign provide a unique opportunity to evaluate model performance for ozone and BVOCs.

MEGAN and CAMx were applied over the three modeling domains during September 2013 using three sets of meteorological fields. The first case "WRF_base" used the standard configuration of WRF (see Table 1). The second case applied WRF with cloud assimilation of GOES data as described in section 2.2 ("WRF_assim"). The third case used the PAR fields computed from the GOES satellite retrieval but kept the other meteorological fields from the WRF_base case ("GOES_UAH"). These three simulations allow us to quantify how MEGAN estimates of BVOC are impacted by assimilation of satellite-observed clouds into WRF and by direct use of satellite PAR retrievals.

Seven available sites for direct continuous measurements of PAR in the Surface Radiation Budget Network (SURFRAD) (<http://www.esrl.noaa.gov/gmd/grad/surfrad/>) as well as 47 local broadband radiation sites from the Texas Air Monitoring Information System (TAMIS, <http://www17.tceq.texas.gov/tamis/index.cfm>) were chosen to evaluate the PAR/insolation retrieval products. In order to evaluate CAMx model performance, 38 Continuous Ambient Monitoring Stations (CAMS) for ground-level ozone observations and 18 CAMS sites for ground-level isoprene concentrations were extracted from TCEQ's Geographical Texas Air Monitoring interface database Web page (<https://gisweb.tceq.texas.gov/geotam3/>, see Figure 1 for the locations of those evaluation sites).

Daily satellite-based observations of the formaldehyde (HCHO) from OMI and the 0.25° Global Ozone Monitoring Experiment-2 (GOME-2) Level 3 data were used to verify the model performance of isoprene vertical column concentrations (<http://h2co.aeronomie.be/>). The in situ P-3B flight measurements made during the 2013 DISCOVER-AQ field campaign (<https://www-air.larc.nasa.gov/cgi-bin/ArcView/discover-aq.tx-2013>) were also utilized to evaluate the CAMx model performance above the surface with different MEGAN estimates.

Routine statistical metrics such as observation mean (OBS), simulation mean (SIM), Pearson correlation coefficient (R), root-mean-square error (RMSE), mean bias (MB), normalized mean bias (NMB), and normalized mean error (NME) were used for model evaluation. In order to evaluate how well the cloud assimilation in WRF improved the simulation of clouds, a contingency-based metric is used called the cloud agreement index (AI). AI is defined as the fraction of grid cells that are in agreement with GOES satellite observations of whether clouds are present (White et al., 2017):

$$AI = \frac{A + D}{A + B + C + D} \quad (4)$$

where A is the number of cells where both model and GOES indicate clouds, B is the number of cells where GOES indicates clouds while the model is clear (under-prediction), C is the number of cells where GOES is clear while the model is cloudy (overprediction), and D is the number of cells where both the model and GOES are clear.

3. Results and Discussion

3.1. Evaluation of PAR/Insolation Products

Measurements from the SURFRAD network were used to evaluate three PAR products: the control WRF simulation, the WRF simulation with cloud assimilation, and the GOES satellite retrieval. In order to compare the PAR products to the SURFRAD observations, the closest satellite pixel or WRF model grid cell containing the pyranometer location was used. Additionally, since the GOES data occurring 45 min past the hour was used, it was interpolated to the end of each hour to match the observations and WRF output.

First, the UAH PAR retrieval product was evaluated at SURFRAD sites in August 2006 in order to compare the performance to the discounted UMD PAR product as well as corresponding WRF simulation results (Table 2 and Figure S2). Both satellite retrieval products statistically outperformed WRF, with correlation value $R \geq 0.96$ and mean bias value $NMB \leq \pm 12\%$, compared with $R = 0.94$ and $NMB = 13\text{--}23\%$ for WRF simulation cases. Satellite retrieval products achieved much better linear regression (closer to 1:1 ratio line with smaller intercept value) at all seven evaluation sites. Due to its smaller footprint (4 km resolution) than its counterpart (0.5°), the UAH PAR product exhibits less scatter than the UMD product though still tended to slightly overestimate PAR (Figure S2).

Table 2 presents evaluation statistics for different PAR and insolation products against SURFRAD and TCEQ monitors during September 2013. Consistent with evaluation results in 2006, the PAR retrieval products outperformed WRF predictions in terms of combined higher correlation coefficients ($R = 0.95$ versus 0.93) and smaller simulation errors ($NME = 24\%$ versus 32–33%). In evaluations of total insolation, using satellite data substantially reduced the positive bias from the WRF control run, reducing the NMB from 17% to 8% for the cloud-assimilated WRF run and 5% for the UAH retrieval. While cloud assimilation was able to reduce the positive bias in WRF, the UAH retrieval strongly outperformed both WRF runs in terms of error and correlation (Table 2).

Figure 2 provides the spatial distribution of insolation performance in terms of correlation and normalized mean bias for the three cases. Considering individual sites, the WRF_base case exhibits the lowest correlation ($R \sim 0.85$) near the coastal sites, especially near Houston. It performs better at inland sites near the Dallas region ($R \sim 0.92$). The WRF_assim case slightly improves model correlation at most of the sites. The GOES_UAH case achieved stronger correlation with the observational data, with the R values at inland sites approaching 1 and at the coastal sites mostly around 0.95. In terms of NMB, all three products performed better around Dallas and other inland sites than near Houston, and the satellite-based cases outperformed the base WRF simulation. The persistent relatively poor performance at the single site even with the satellite insolation product may relate to a malfunction in the radiative transfer retrieval algorithm (Haines et al., 2003).

3.2. Performance of Cloud Assimilation in WRF

The cloud AI metric (equation (4)) is used to evaluate the agreement between clouds simulated by WRF and observed by the GOES satellite. The AI metric was calculated for each hour in the time range 15–23 UTC to ensure maximum daylight coverage across the domains whenever GOES imager observations are available.

Figure 3 shows the average hourly AI without (black) and with (green) GOES cloud assimilation in WRF across the three modeling domains for the month of September 2013. Overall, the assimilation technique led to better cloud agreement, improving the hourly average AI from 0.65–0.71 to 0.71–0.77. Comparing the AI improvements at different grid resolutions, the improvement in the finer resolution domain (i.e., D3) was less significant than in the coarser resolution domains (D2–D1). The maximum hourly average percentage change in AI for D3 is 8.3%, while the corresponding values for D2 and D1 are 10.5% and 13.8%, respectively. This can likely be attributed to two factors. The first is that the advection of the clouds between 4 km grid cells in the

Table 2

Summary of Statistics for PAR and Insolation Retrievals and Simulations Evaluated at SURFRAD and Texas Ground Pyranometer Observation Network During August 2006 and September 2013

Parameter	Case	OBS ^a (W/m ²)	SIM ^b (W/m ²)	R ^c	RMSE ^c (W/m ²)	MB ^d (W/m ²)	NMB ^e	NME ^f
PAR	WRF_base(2006)	107	131	0.94	65	23	23%	35%
	WRF_assim(2006)	107	121	0.94	60	13	13%	33%
	GOES_UAH(2006)	107	93	0.97	39	−14	−12%	21%
	GOES_UMD(2006)	107	118	0.96	43	10	10%	21%
Insolation	WRF_base(2013)	114	143	0.93	67	28	21%	33%
	WRF_assim(2013)	114	129	0.93	59	15	15%	32%
	GOES_UAH(2013)	114	123	0.95	44	9	9%	24%
	WRF_base(2013)	259	303	0.91	132	54	17%	27%
	WRF_assim(2013)	259	277	0.91	133	17	8%	28%
	GOES_UAH(2013)	259	269	0.96	117	10	5%	26%

^aMean observation. ^bMean simulation. ^cCorrelation coefficient. ^dRoot-mean-square error. ^eMean bias. ^fNormalized mean bias. ^gNormalized mean error.

model is more likely to occur within an hour, which is the time scale of satellite observations used here. Thus, a cloud created in the correct place might move to a surrounding grid more quickly than what observations can explain. The second is that the assimilation technique can correct cloudiness in one location but at the same time change cloudiness in neighboring locations (White et al., 2017).

The cloud assimilation scheme improved the AI both when the base WRF simulation performed poorly and even during hours when it already had high AI (e.g., AI > 0.9). An example of the improvement in AI is shown for 16 September 2013, at 19 UTC in Figure S3. For this hour, it can be seen that the WRF_base simulation underpredicted clouds across a large portion of Texas but the WRF_assim simulation was able to correct a sizable portion of this area, improving the AI by greater than 10%. White et al. (2017) showed that GOES-based cloud assimilation in WRF from GOES observations also improves or maintains the model performance for surface temperature, water vapor mixing ratios, and wind speed. Figure S4 compares daily model bias for

Figure 2. Photosynthetically active radiation observed by TCEQ sites and simulated by the (left) WRF base case, (middle) WRF with assimilated clouds, and direct estimates from (right) UAH GOES retrievals.

Figure 3. Comparison of average hourly cloud agreement index (AI) without and with GOES cloud assimilation in WRF across different model resolution domains for September 2013.

the three parameters across the two WRF simulation cases. Assimilating satellite-observed clouds into WRF slightly reduces its overestimation of surface temperature and underestimation of wind speed.

3.3. Biogenic Emission Estimates Using Different PAR

MEGAN emission estimates were computed for September 2013 for isoprene and monoterpenes, the VOCs most strongly emitted by vegetation in Texas (Song et al., 2008; Ying & Krishnan, 2010). Default and update land use characterization as well as BVOC emission factor database in combination with three different PAR inputs were used in MEGAN as inputs (see Table 1). For isoprene, the spatial patterns across different PAR inputs cases were quite similar. Emission hot spots over Texas were mainly concentrated over the Edwards Plateau and East Texas, where broadleaf deciduous and evergreen trees are the dominant plant functional types (Figure S5 for the PFT distribution and Figure S6 for the emission spatial pattern). In terms of the magnitude of isoprene emissions, the GOES_UAH case is the lowest with the maximum emission rate appearing in East Texas at $2.1 \text{ mg m}^{-2} \text{ h}^{-1}$. The overall magnitudes of monoterpene emissions are much smaller, with rates ranging from 0 to $0.6 \text{ mg m}^{-2} \text{ h}^{-1}$. Using different land cover (PFT v2011 and 2011 LAIv versus PFT v2015 and 2013 LAIv) as well as BVOC emission factor database (EFvE2011 versus EFvA2015) in MEGAN yielded different spatial pattern for isoprene and monoterpene emission estimates, with more than 60% lower in less vegetation coverage areas such as Trans-Pecos and High Plains and 16–24% higher in East Texas for the update version (Figure S6). Also, there exists larger emission rate contrast along U.S.-Mexico border due to the abrupt shift in isoprene and α -pinene emission factor map (Figure S5) for version EFvA2015 (Yu et al., 2015).

In order to characterize the BVOC emission patterns from different MEGAN simulations over the heterogeneous plant functional types of Texas, the daily average emission rates over the 10 climate divisions in Texas (see Figure 1) during September 2013 were calculated separately (Figure 4). The climate classification is based on historical climate analyses (1895–2013) for the monitored drought, temperature, precipitation, and heating/cooling degree day values over the continental U.S. (<http://www.ncdc.noaa.gov/monitoring-references/maps/us-climate-divisions.php>). For isoprene, the highest emission regions in Texas are East Texas ($1.20 \pm 0.53 \text{ mg m}^{-2} \text{ h}^{-1}$ for case GOES_UAH), South Central Texas ($0.61 \pm 0.26 \text{ mg m}^{-2} \text{ h}^{-1}$), and North Central Texas ($0.60 \pm 0.29 \text{ mg m}^{-2} \text{ h}^{-1}$). For monoterpenes, the top three highest emission regions are East Texas ($0.41 \pm 0.09 \text{ mg m}^{-2} \text{ h}^{-1}$ for case GOES_UAH), North Central Texas ($0.15 \pm 0.04 \text{ mg m}^{-2} \text{ h}^{-1}$), and South Central Texas ($0.14 \pm 0.03 \text{ mg m}^{-2} \text{ h}^{-1}$). The west-to-east gradients for both isoprene and monoterpene emissions are similar, with the lowest emission rates in West Texas, followed by moderate emission rates over South Texas and peaks in East Texas.

Figure 4. Comparison of episode-average isoprene and monoterpene emission rates ($\text{mg m}^{-2} \text{h}^{-1}$) as well as daytime (8:00 a.m.–6:00 p.m. local standard time) mean hourly PAR inputs either from WRF or GOES retrievals over Texas climate divisions during September 2013.

Replacing the base WRF radiation data with the UAH GOES satellite retrievals led to a 20% average reduction in the estimated isoprene emissions by MEGAN over Texas. The use of cloud assimilation in WRF had less of an effect, with only a 2% average reduction compared to the base WRF case. These reductions correspond well with the decrease in PAR between each case as shown in Table 2. Due to its high fraction of vegetation cover for broadleaf evergreen trees, the day-by-day variation in isoprene emissions over East Texas is significantly larger than the rest of the state. The impact of satellite PAR on monoterpene emissions over Texas is relatively small (on average 5% reduction over Texas) since MEGAN shows terpenes to be less sensitive to PAR than to temperature (Guenther et al., 2012). Replacing the default MEGAN v2.10 land use (PFT16v2011 and 2011 LAIv) and BVOC emission factor database (EFvE2011) with higher resolution land cover database (PFT16v2015 and 2013 LAIv) and aircraft BVOC flux measurements constrained emission factor led to a 12% and 33% average reduction in the estimated isoprene and monoterpene emissions by MEGAN over Texas.

3.4. CAMx Simulation Using Different MEGAN Outputs With Satellite PAR

Spaceborne formaldehyde column concentration can serve as a proxy to constrain the spatial distribution of biogenic isoprene emissions since oxidation of isoprene is the leading contributor of formaldehyde in remote areas (Millet et al., 2008; Palmer et al., 2006). We computed HCHO vertical column densities (VCD) from the three CAMx simulations and compared them with different satellite retrieval products to examine how well

Figure 5. Comparison of the daily mean formaldehyde (HCHO) vertical column density between CAMx simulations, OMI, and GOME2 retrievals during 1–15 September 2013 over Texas climate divisions.

Table 3

Statistics for CAMx Daily Mean Ozone and Isoprene Performance Over Texas CAMS Sites in September 2013 With Different PAR as Well as Land Use and Emission Factor Inputs in MEGAN

Case		OBS ^a (ppbV)	SIM ^b (ppbV)	R ^c	RMSE ^d (ppbV)	MB ^e (ppbV)	NMB ^f	NME ^g
Ozone	WRF_base	31.6	38.1	0.75	14.3	6.0	26%	40%
	WRF_assim	31.6	36.9	0.77	13.7	5.2	23%	39%
	GOES_UAH	31.6	38.0	0.75	14.3	6.0	26%	40%
Isoprene	WRF_base	0.29	0.57	0.30	0.69	0.32	132%	160%
	WRF_assim	0.29	0.52	0.31	0.58	0.26	107%	140%
	GOES_UAH	0.29	0.39	0.60	0.42	0.14	68%	104%

^aMean observation. ^bMean simulation. ^cCorrelation coefficient. ^dRoot-mean-square error. ^eMean bias. ^fNormalized mean bias. ^gNormalized mean error. ^hIndex of agreement.

the model replicated the observed HCHO spatial pattern. We exclude the North Central Texas and Upper Coast regions, where anthropogenic emissions from major metropolitan areas could confound relationships between HCHO columns and BVOC emissions. Figure 5 shows the daily mean HCHO VCD over the rest eight climate divisions of Texas for the three CAMx simulations, OMI, and GOME-2 for September 2013. CAMx-MEGAN simulations and the satellite retrievals generally agree on the rankings of HCHO column densities between most climate divisions except over the southern part of Texas (South Texas and Lower Valley). The model did a reasonable job at reproducing the observed mean column densities in West Texas but underestimated them in South Texas and overestimated them in East Texas. Therefore, the modeled HCHO west-to-east spatial gradient in Texas is larger than the observed value. GOME-2 retrievals observe less HCHO than OMI. The CAMx model agrees better with the GOME-2 retrievals, with overall model error of 17%–24% compared to 27%–30% for OMI. The lower ends of these ranges were achieved by using satellite PAR retrievals in MEGAN.

Figure 6. Diurnal patterns of (top) photosynthetically active radiation, (middle) isoprene emissions, and (bottom) isoprene mixing ratios in each simulation.

Figure 7. Comparison of vertical concentration profiles of isoprene between P-3B flight measurements and three CAMx runs during the DISCOVER-AQ campaign (the flights took place between 14 and 22 UTC each day with spirals above locations near Conroe, West Houston, Channelview, Moody Tower, Deer Park, Manvel Croix, Smith Point, and Galveston; see the flight route in Figure S8). The markers show the median values, and the error bars show the 25th and 75th percentiles.

We also compared the CAMx-MEGAN simulations against hourly ground-level isoprene concentrations observed at 18 CAMS sites. Incorporation of the GOES PAR data significantly improved the model performance for ground-level isoprene concentrations in terms of increasing the correlation from 0.31 for the WRF_base case to 0.60 while reducing the NMB from 107% to 68% (Table 3). We plot the diurnal profiles between PAR inputs, MEGAN isoprene emission estimates, and CAMx isoprene concentration simulation at the three CAMS sites far away from metropolitan centers (the sites marked with star in Figure 1) to study their correlations (Figure 6). The average diurnal isoprene concentration profiles produced by the simulation cases WRF_base and WRF_assim at those CAMS sites are consistently 1.07–1.3 times higher than observed values during daytime. The diurnal profiles simulated using the WRF predicted insolation fields show a small peak around 0.8 ppbV near early morning (8 a.m. local time) and a large peak around 1.3 ppbV near sunset (7 p.m. local time), while the measurements show that the concentration peaks shortly after sunrise (around 8 am) and then steadily decreases during daytime. By contrast, the diurnal pattern simulated using GOES PAR data generally replicates the measurement trend (with $R = 0.60$; see Table 3). The different diurnal patterns predicted by the three simulations may be due to the combined impact from MEGAN's formulation with different PAR inputs. The GOES_UAH case has lower isoprene emission rates due to lower PAR inputs. Therefore, on average, it simulated lower ground-level isoprene concentrations than the two WRF cases. By assimilating clouds in WRF, the average cloud cover increased across the domain through the time period. Thus, the downwelling shortwave radiation reaching the surface was reduced. This resulted in lower isoprene emissions during the middle of the day. However, incorporating satellite observations (case GOES_UAH) only reduced but did not eliminate the tendency of CAMx to overestimate ground-level isoprene concentrations.

Notice that most of the CAMS sites that measure isoprene concentrations are located in clearings and are clumped near just a few urban environments (see Figure 1). Therefore, they may not capture the full impact of improved PAR fields in MEGAN.

The impacts of assimilated clouds and satellite-retrieved PAR on simulations of mean daily maximum 8 h ozone (MDA8) over 38 Texas CAMS sites are illustrated in Table 3 and Figure S7. Assimilation of GOES-based clouds into WRF influences MDA8 ozone by 2–5 ppbV near the DFW region and 1–2 ppbV near the greater Houston area. However, replacement of WRF PAR with GOES retrievals influences ozone simulations by less than 1 ppbV. Note that cloud assimilation in WRF affects multiple drivers of ozone production (e.g., photolysis rates and temperature) whereas satellite PAR only modifies BVOC emissions. That allows assimilation to have a larger influence on ozone simulations, even though direct use of PAR retrievals more strongly influences BVOC emissions. Cloud assimilation increases correlation with observations of hourly ozone from 0.75 to 0.77 and decreases bias from 26% to 23% (Table 3), with the most pronounced improvement over the DFW area (Figure S8).

Figure 7 compares the CAMx simulated isoprene vertical profiles with the available P-3B in situ flight measurements on September 4, 6, 11, and 13, 2013. Tracer gas vertical profiles at 8 spiral points near the HGB area were sampled approximately 0.3 to 4 km above ground level by 4 segments of flight trips from 9 am to 5 pm local time each day (see Figure S9). Isoprene was measured by online Proton Transfer Reaction Mass Spectrometry with the sampling times ranging from 3 to 10 s. The detection limit for isoprene concentration is a few pptV (Lindinger & Jordan, 1998; Anderson et al., 2014). The isoprene vertical profiles from in situ measurements for the 4 days were quite similar, with a mean concentration around 0.2 ppbV at 250 m decreasing almost monotonically with height to near zero above 2.75 km. The CAMx model simulations, however, have greater daily variability. During 4 and 13 September, the model overestimated concentrations aloft. However, on 6 and 13 September, the model underestimated concentrations aloft and simulated a deeper gradient above 0.75 km. The inability to better represent the vertical profile of isoprene from the WRF-MEGAN-CAMx modeling platform is due to the combined uncertainties in the dynamics, emission, chemical mechanism, and vertical mixing. Flynn et al. (2016) implemented the regional CMAQ model to simulate the observed ozone and NO₂ profile shapes during different DISCOVER-AQ campaigns and found that the model has limited capacity to represent the vertical profiles during 2013 Houston campaign. Nevertheless, the fact that case GOES_UAH had the best tendency to approach the observed values for all the evaluated days hints at the benefit of using satellite PAR information for future regional air quality applications.

4. Conclusions

This study used UAH's GOES insolation and cloud retrieval products to test the sensitivity BVOC estimates to cloud and PAR retrievals. It then used air quality simulations with the WRF-MEGAN-CAMx modeling platform to test the sensitivity of HCHO and ozone to those emission changes over Texas during the 2013 DISCOVER-AQ campaign.

Evaluation against surface pyranometer observations shows that satellite-retrieved PAR reduced the overestimation of insolation by the WRF meteorological model. This conclusion holds for all the evaluations conducted against different networks (i.e., SURFRAD and Texas local broadband radiation monitoring stations) and during different time periods (i.e., August 2006 and September 2013). This indicates that satellite-derived radiation data can be a preferred source of input for biogenic emission models. The UAH satellite PAR product also showed similar performance to the discontinued satellite retrieval product from UMD but at a higher spatial resolution.

Assimilation of GOES-based clouds into WRF was shown to significantly improve performance in simulating cloud locations and surface radiation. Unlike the direct use of satellite-based PAR retrievals, cloud assimilation has a broader impact on temperature, moisture, boundary layer development, and transport of pollutants in the models. Therefore, assimilating GOES cloud information into WRF and using it to drive chemical transport model can improve model performance for ground-level ozone, which is affected by many of these variables.

Incorporating satellite-based PAR reduced MEGAN estimates of isoprene emission rates by about 20% and terpene emissions by about 5% over the Texas simulation domain (D2; see Figure 1). The reduction in

isoprene emissions resulted in a better agreement with diurnal variation of ground-level concentrations at remote CAMS sites and a more reasonable spatial pattern when compared to satellite-observed formaldehyde columns. The CAMx vertical isoprene profiles using satellite PAR input had a better tendency to replicate the in situ flight measurements over different sampling days. However, the changes in BVOC emissions had only a small impact on ozone simulations during the simulated period. This highlights the non-linear nature of ozone production in the atmosphere.

Overall, the results show that incorporating satellite-based cloud data via either assimilation in the meteorological model or through direct use of satellite PAR can reduce isoprene simulation bias over Texas. Using the high-resolution land cover database and the best available BVOC emission factors constrained with campaign isoprene flux measurement (Yu et al., 2017) yielded the best comparisons with the ground and flight in situ measurements. Compared with the default MEGAN v2.10 land use and BVOC emission factor inputs, the update version yielded on average 12% decrease for isoprene emission estimates over Texas during September 2013. However, some overestimation of isoprene remained, suggesting other aspects of MEGAN and CAMx require closer examination.

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