Satellite soil moisture data assimilation impacts on modeling weather and ozone in the southeastern US - part I: an overview

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Abstract. This study evaluates the impact of satellite soil moisture data assimilation (SM DA) on regional weather and ozone (O₃) modeling over the southeastern US during the summer. Satellite SM data are assimilated into the Noah land surface model using an ensemble Kalman filter approach within National Aeronautics and Space Administration’s Land Information System framework, which is semicoupled with the Weather Research and Forecasting model with online Chemistry (WRF-Chem, standard version 3.9.1.1). The SM DA impacts on WRF-Chem performance of weather states and energy fluxes show strong spatiotemporal variability, and many factors such as dense vegetation, complex terrain, and unmodeled water use from human activities may have impacted the effectiveness of the SM DA. The changes in WRF-Chem weather fields due to the SM DA modified various model processes critical to its surface O₃ fields, such as biogenic isoprene and soil nitric oxide emissions, photochemical reactions, as well as dry deposition. The SM DA impacted WRF-Chem upper tropospheric O₃ partially via altering atmospheric transport and in-situ chemical production of O₃ from lightning and other emissions. It is shown that WRF-Chem upper tropospheric O₃ response to the SM DA has comparable magnitudes with its response to the estimated US anthropogenic emission changes within two years. As reductions in US anthropogenic emissions would be beneficial for mitigating European O₃ pollution, our analysis highlights the important role of SM in quantifying pollutants’ transport from the US to Europe. It also emphasizes that using up-to-date anthropogenic emissions is necessary for accurately assessing the SM DA impacts on the model performance of O₃ and other pollutants over a broad region. Additionally, this work demonstrates that the SM DA impact on WRF-Chem O₃ performance at various altitudes is complicated by not only the model’s emission input but also other factors such as the model representation of stratosphere-troposphere exchanges. This work will be followed by a Noah-Multiparameterization (with dynamic vegetation) based study over the southeastern US, in which selected processes including photosynthesis and O₃ dry deposition will be the foci.
1 Introduction

Tropospheric ozone (O$_3$) is a central component of tropospheric oxidation chemistry with atmospheric lifetimes ranging from hours within polluted boundary layer to weeks in the free troposphere (Stevenson et al., 2006; Cooper et al., 2014; Monks et al., 2015). Ground-level O$_3$ is a US Environmental Protection Agency (EPA) criteria air pollutant which harms human health and imposes threat to vegetation and sensitive ecosystems, and such impacts can be strongly linked or/and combined with other stresses, such as heat, aridity, soil nutrients, diseases, and non-O$_3$ air pollutants (e.g., Harlan and Ruddell, 2011; Avnery et al., 2011; World Health Organization, 2013; Fishman et al., 2014; Lapina et al., 2014; Cohen et al., 2017; Fleming et al., 2018; Mills et al., 2018a, b). Across the world, various metrics have been used to assess surface O$_3$ impacts (Lefohn et al., 2018). In October 2015, the US primary (to protect human health) and secondary (to protect public welfare including vegetation and sensitive ecosystems) National Ambient Air Quality Standards for ground-level O$_3$, in the format of the daily maximum 8 h-average (MDA8), were revised to 70 ppbv (US Federal Register, 2015). Understanding the connections between weather patterns and surface O$_3$ as well as their combined impacts on human and ecosystem health under the changing climate is important to developing strong-enough anthropogenic emission control to meet targeted O$_3$ air quality standards (Jacob and Winner, 2009; Doherty et al., 2013; Coates et al., 2016; Lin et al., 2017).

Ozone aloft is more conducive to rapid long-range transport to influence surface air quality in downwind regions (e.g., Zhang et al., 2008; Hemispheric Transport of Air Pollution, HTAP, 2010, and the references therein; Huang et al., 2010, 2013, 2017a; Doherty, 2015). In the upper troposphere/ lower stratosphere regions, O$_3$ as well as water vapor is particularly important to climate (Solomon et al., 2010; Shindell et al., 2012; Stevenson et al., 2013; Bowman et al. 2013; Intergovernmental Panel on Climate Change, 2013; Rap et al., 2015; Harris et al., 2015). Ozone variability in the free troposphere can be strongly affected by stratospheric air, transport of O$_3$ that is produced at other places of the troposphere, as well as in-situ chemical production from O$_3$ precursors including nitrogen oxides (NO$_x$, namely nitric oxide, NO, and nitrogen oxide, NO$_2$), carbon monoxide (CO), methane, and non-methane volatile organic compounds (VOCs). Mid-latitude cyclone is a major mechanism of venting boundary layer constituents, including O$_3$ and its precursors, to the mid- and upper troposphere. It is active throughout the year and relatively weaker during the summer. Convection, often associated with thunderstorms and lightning, is a dominant mechanism of exporting pollution in the summertime (e.g., Dickerson et al., 1987; Hess, 2005; Brown-Steiner and Hess, 2011; Barth et al., 2012). During North American summers, anticyclones established in the upper troposphere trap convective outflows and promote in-situ O$_3$ production from lightning and other emissions (e.g., Li et al., 2005; Cooper et al., 2006, 2007, 2009).

On a wide range of spatial and temporal scales, atmospheric weather and composition interact with land surface conditions (e.g., soil and vegetation states, topography, and land use/cover, LULC), which can be altered by various human activities and/or natural disturbances such as urbanization, deforestation, irrigation, and natural disasters (e.g., Betts, 1996; Kelly and Mapes, 2010; Taylor et al., 2012; Collow et al., 2014; Guillod et al., 2015; Tuttle and Salvucci, 2016; Cioni and Hohenegger,
2017; Fast et al., 2019; Schneider et al., 2019). As a key land variable, soil moisture (SM) influences the atmosphere via evapotranspiration. The SM-atmosphere coupling strengths are overall strong over transitional climate zones (i.e., the regions between humid and arid climates) where evapotranspiration is moderately high and constrained by SM (e.g., Koster et al., 2004, 2006; Seneviratne et al., 2010; Dirmeyer, 2011; Miralles et al., 2012; Gevaert et al., 2018). The southeastern US includes large areas of transitional climate zones, whose geographical boundaries vary temporally (e.g., Guo and Dirmeyer, 2013; Dirmeyer et al., 2013). Soil moisture and other land variables are currently measurable from space. It has been shown in a number of scientific and operational applications that satellite SM data assimilation (DA) impacts model skill of atmospheric weather states and energy fluxes (e.g., Mahfouf, 2010; de Rosnay et al., 2013; Santanello et al., 2016; Yin and Zhan, 2018). An effort began recently to evaluate the impacts of satellite SM DA on short-term regional-scale air quality modeling. Based on case studies in East Asia, such effects are shown to vary in space and time, and can be complicated by other sources of model error, such as the uncertainty of the models’ chemical inputs including emissions and chemical initial/lateral boundary conditions (Huang et al., 2018).

This study extends the work by Huang et al. (2018) to the southeastern US during intensive field campaign periods in the summer convective season. Modified from the approach used in Huang et al. (2018), we assimilate satellite SM into the Noah land surface model (LSM) within National Aeronautics and Space Administration (NASA)’s Land Information System (LIS), which is semicoupled with the Weather Research and Forecasting model with online Chemistry (WRF-Chem). The term “semicoupled” here is similar to “weakly-coupled”, as opposed to “fully-” or “strongly-” coupled, which indicates that the SM DA within LIS influences WRF-Chem’s land initial conditions. Atmospheric states and energy fluxes from the no-DA and DA cases are compared with surface, aircraft, and satellite observations during selected field campaign periods. The WRF-Chem results are also compared with the chemical fields of the Copernicus Atmosphere Monitoring Service (CAMS), which serves as the chemical initial/lateral boundary condition model of WRF-Chem. Other sources of errors in WRF-Chem simulated $O_3$ are identified by a WRF-Chem emission sensitivity simulation and the stratospheric $O_3$ tracer output from the Geophysical Fluid Dynamics Laboratory (GFDL)’s Atmospheric Model, version 4 (AM4). The modeling and SM DA approaches as well as evaluation datasets are first introduced in Section 2. Section 3 starts with an overview of the synoptic and drought conditions during the study periods (Section 3.1), followed by discussions on the model responses to satellite SM DA. The SM DA impacts on $O_3$ export from the US and the potential impacts on European surface $O_3$ are included in the discussions. Results during a summer 2016 field campaign and a summer 2013 campaign are covered in Sections 3.2-3.5 and Section 3.6, respectively. Section 4 summarizes key results from its previous sections, and includes implications and suggestions on future work.

2 Methods

2.1 Modeling and SM DA approaches
This study focuses on a summer southeastern US deployment (16-28 August 2016) of the Atmospheric Carbon Transport (ACT)-America campaign (https://act-america.larc.nasa.gov). One goal of this campaign is to study atmospheric transport of trace gases. Three WRF-Chem full-chemistry simulations (i.e., base, “assim”, and “NEI14” in Table 1) were conducted on a 63 vertical layer, 12 km × 12 km (209×139 grids) horizontal resolution Lambert conformal grid centered at 33.5°N/87.5°W (Figure 1a-c). Trace gases and aerosols were simulated simultaneously and interactively with the meteorological fields using the standard version 3.9.1.1 of WRF-Chem (Grell et al., 2005).

Version 3.6 of the widely-used, four-soil-layer Noah LSM (Chen and Dudhia, 2001) within LIS (Kumar et al., 2006) version 7.1rp8 served as the land component of the used modeling/DA system. This version of Noah is similar to Noah version 3.3 (Huang et al., 2017b, 2018), except that snow physics is based on the University of Arizona scheme (Wang et al., 2009). An offline Noah simulation was performed within LIS prior to all WRF-Chem simulations for equilibrated land conditions, covering the period of 1999-2019. The “mean-state” approach (Rodell et al., 2005) was adopted to initialize Noah after cycling the model twice during this entire period. The 1/8° North American Land Data Assimilation System Phase 2 (NLDAS-2, https://ldas.gsfc.nasa.gov/nldas/v2/forcing) was used as the meteorological forcing for this spin-up. Consistent model grids and geographical inputs of the Noah LSM were used in the offline LIS and all WRF-Chem simulations.

Specifically, topography, time-varying green vegetation fraction, LULC type, and soil type inputs were based on the SRTM30 version 2.0, Copernicus Global Land Service, the International Geosphere-Biosphere Programme-modified Moderate Resolution Imaging Spectroradiometer (Figure 1a-c), and the State Soil Geographic (Figure S1, left, Miller and White, 1998) datasets, respectively.

Version 2 of the 9 km “enhanced” morning SM retrievals (produced using the baseline retrieval algorithm) from NASA’s Soil Moisture Active Passive (SMAP, Entekhabi et al., 2010) L-band polarimetric radiometer were assimilated into Noah within LIS. SMAP provides global coverage of surface (i.e., the top 5 cm of the soil column) SM within 2-3 days along its morning orbit (~6 am local time crossing) with the ground track repeating in 8 days. Compared to its predecessors that take measurements at higher frequencies, SMAP has a higher penetration depth for SM retrievals and lower attenuation in the presence of vegetation. According to SMAP Product Specification Document (https://nsidc.org/data/smap/technical-references), only successful retrievals that are no smaller than the valid minimum value of 0.02 m3 m-3 and of recommended quality (i.e., the retrieval quality flag has “0” values for bits 0, 1, 2) were used. Evaluation of SMAP data over North America with in-situ and LSM output suggests better data quality over flat and less forested regions (Pan et al., 2016), and previous studies have demonstrated that the SMAP DA improvements on weather variables are more distinguishable over regions with sparse vegetation (e.g., Huang et al., 2018; Yin and Zhan, 2018). Before the DA, SMAP data were re-projected to the model grid and bias correction was applied via matching the means and standard deviations of the Noah LSM and SMAP data for each grid (de Rosnay et al., 2013; Huang et al., 2018; Yin and Zhan, 2018) during August of 2015-2019. Such bias correction reduced the dynamic ranges of SM from the original SMAP retrievals. The Global Modeling and
Assimilation Office (GMAO) ensemble Kalman filter approach embedded in LIS was applied, with the ensemble size of 20. Perturbation attributes of state variables (Noah SM) and meteorological forcing variables (radiation and precipitation) were based on default settings of LIS derived from Kumar et al. (2009).

All WRF-Chem cases were started on 13 August 2016. Atmospheric meteorological initial/lateral boundary conditions were downscaled from the 3-hourly, 32 km North American Regional Reanalysis (NARR) which is used to derive most forcing fields of the NLDAS-2 and is generally drier and warmer than observations (e.g., Royer and Poirier, 2010; Kennedy et al., 2011). Consistent with NARR, the WRF-Chem model top was set at 100 hPa, slightly above the climatological tropopause heights for the study region/month. The 0.083°×0.083° National Centers for Environmental Prediction (NCEP) daily sea surface temperature (SST) reanalysis product was used as an additional WRF forcing. Chemical initial/lateral boundary conditions for major chemical species were downscaled from the 6-hourly, 0.4°×0.4°×60-level CAMS. Surface O$_3$ from CAMS is positively biased over the eastern US referring to various observations, but major chemical species in the free troposphere is overall successfully reproduced (e.g., Huijnen et al., 2020; Wang et al., 2020). As WRF-Chem has only tropospheric chemistry, the lack of dynamic chemical upper boundary conditions is expected to introduce biases in the modeled O$_3$ throughout the troposphere, and such biases depend on the distribution of model vertical layers as well as the length of the simulation. We used GFDL’s AM4 and its stratospheric O$_3$ tracer (3-hourly, 1°×1.25°×49-level) to determine how this limitation of WRF-Chem affects its O$_3$ performance. The used AM4 is modified from Zhao et al. (2018), and has been applied to other O$_3$ studies (e.g., Zhang et al., 2019). Atmospheric meteorological and land fields were reinitialized every day at 00 UTC with NARR and the previous-day no-DA or DA LIS outputs, respectively. Each day’s simulation was recorded hourly at 00:00 (minute:second) through the following 30 hours, forced by temporally constant SST as the diurnal variation of the sea surface is typically smaller than land on large scales. Each day’s WRF-Chem meteorological outputs served as the forcings of the no-DA and DA LIS runs, which produced land initial conditions for next day’s WRF-Chem simulations. Since the second day of the simulation period, chemical initial conditions were cycled from the chemical fields of the previous-day simulation. The model output >6 hours since each day’s initialization was analyzed for the period of 16-28 August 2016.

In all WRF-Chem simulations, key physics options applied include: the local Mellor–Yamada–Nakanishi–Niino planetary boundary layer (PBL) scheme along with its matching surface layer scheme (Nakanishi and Niino, 2009), the Rapid Radiative Transfer Model short-/long-wave radiation schemes (Iacono et al., 2008), the Morrison double-moment microphysics, which predicts the mass and number concentrations of hydrometeor species (Morrison et al., 2009), and the Grell–Freitas scale-aware cumulus scheme (Grell and Freitas, 2014), which has also been implemented in the GMAO GEOS-Forward Processing system (https://gmao.gsfc.nasa.gov/news/geos_system_news/2020/GEOS_FP_upgrade_5_25_1.php). Chemistry related configurations are: the Carbon-Bond Mechanism version Z (Zaveri and Peters, 1999) gas phase chemical
mechanism and the eight-bin sectional Model for Simulating Aerosol Interactions and Chemistry (Zaveri et al., 2008), including aqueous chemistry for resolved clouds. Both aerosol direct and indirect effects were enabled in all simulations.

Daily biomass burning emissions came from the Quick Fire Emissions Dataset (Darmenov and da Silva, 2015) version 2.5r1, and plume rise with a recent bug fix (suggested by Ravan Ahmadov, NOAA/ESRL, in August 2019) was applied. Emissions of biogenic VOCs and soil NO were computed online (i.e., driven by the WRF meteorology) using the Model of Emissions of Gases and Aerosols from Nature (MEGAN, Guenther et al., 2006). It has been shown that MEGAN may overpredict biogenic VOC emissions and tends to underpredict soil NO emissions especially in high-temperature (i.e., >30 °C) agricultural regions (e.g., Oikawa et al., 2015; Huang et al., 2017b, and the references therein). One possible source of uncertainty is that the SM influences on these emissions are not well understood and represented in MEGAN. Cloud-top-height-based lightning parameterization was applied (Wong et al., 2013). The intra-cloud to cloud-to-ground flash ratio was based on climatological (Boccioppio et al., 2001), and lightning NO was distributed using curves in Ott et al. (2010). For both intra-cloud and cloud-to-ground flashes, 125 moles of NO were emitted per flash, close to the estimates in several studies for the US (e.g., Pollack et al., 2016; Bucsela et al., 2019). Anthropogenic emissions in the base and “assim” simulations (Table 1) were based on US EPA’s National Emission inventory (NEI) 2016 beta, and in a third simulation “NEI14”, NEI 2014 was used. The differences between NEI 2016 beta and earlier versions of NEIs, such as NEI 2014 and NEI 2011, are summarized at: http://views.cira.colostate.edu/wiki/wiki/10197/inventory-collaborative-2016beta-emissions-modeling-platform, for various chemical species. Anthropogenic emissions of O₃ precursors are lower in NEI 2016 beta than in NEI 2014 (by <20% for key species) as well as NEI 2011, in which NOₓ emissions may be positively biased for 2013 (Travis et al., 2016). These differences are qualitatively consistent with the observed trends of surface air pollutants (https://www.epa.gov/air-trends).

Chemical loss via dry deposition (i.e., dry deposition velocity multiplied by surface concentration) was calculated based on the widely-used Wesely scheme (Wesely, 1989). This scheme defines dry deposition velocity as the reciprocal of the sum of aerodynamic resistance, quasi-laminar resistance, and surface resistance. Over land, its major component surface resistance is classified into stomatal and mesophyll resistance, cuticular resistance, in-canopy resistance, and ground resistance. Surface resistance is usually strongly affected by its stomatal resistance component which in the Wesely scheme is expressed as seasonal- and LULC-dependent constants (subject to large uncertainty) being adjusted by surface temperature and radiation. This contrasts with some other approaches which also account for the influences of SM, vapor pressure deficit and vegetation density, or couple stomatal resistance with photosynthesis. For calculating the nonstomatal surface resistance components, prescribed seasonal- and LULC-dependent constants are used in the Wesely scheme, adjusted by environmental variables such as wetness and radiation, whereas in other existing schemes, impacts of friction velocity and vegetation density are also considered (e.g., Charusombat et al., 2010; Park et al., 2014; Val Martin et al., 2014; Wu et al., 2018; Mills et al., 2018b; Anav et al., 2018; Wong et al., 2019; Clifton et al., 2020, and the references therein). Aerodynamic resistance and quasi-laminar resistance are both sensitive to surface properties such as surface roughness.
This paper also briefly discusses in Section 3.6 some results from two WRF-Chem simulations (i.e., “SEACf” and “SEACa” in Table 1) during the 2013 Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC4RS, Toon et al., 2016, https://espo.nasa.gov/home/seac4rs/content/SEAC4RS) campaign. SEAC4RS studies the attribution and quantification of pollutants and their distributions as a result of deep convection. These simulations were conducted on a 27 vertical layer, 25 km×25 km (99×67 grids) horizontal resolution Lambert conformal grid also centered at 33.5°N/87.5°W. Their LSM and inputs, WRF physics and chemistry configurations were the same as those used in the 12 km cases described above. In “SEACa”, we assimilated successfully-retrieved, daily SM from version 04.5 of the European Space Agency Climate Change Initiative project (ESA CCI) SM product (Gruber et al., 2019), developed on a 0.25°×0.25° horizontal resolution grid based on measurements from passive satellite sensors. The assimilated CCI SM data were re-projected to the model grid and bias-corrected based on the climatology of Noah and CCI SM during August of 1999-2018. These simulations were evaluated with SEAC4RS aircraft chemical observations, which were richer than those collected during ACT-America in terms of the diversity of measured reactive chemical compounds (Section 2.2.1). Such comparisons help evaluate the emissions of O₃ precursors from various (e.g., NEI 2014 anthropogenic, lightning, and biogenic) sources as well as how the model representation of land-atmosphere interactions affects such emission assessments.

The model horizontal resolutions of 12 km and 25 km were set to be close to the assimilated satellite SM products to minimize the horizontal representation errors. At these resolutions, land surface heterogeneity and fine-scale processes (e.g., cloud formation and turbulent mixing) may not be realistically represented. Cloud-top-height-based lightning emissions and SM-precipitation feedbacks can be highly dependent on convective parameterizations (e.g., Hohenegger et al., 2009; Wong et al., 2013; Taylor et al., 2013). Addressing shortcomings of convective parameterizations in simulations at these scales is still in strong need. Performing convection-permitting simulations with assimilation of downscaled microwave SM or/and high-resolution thermal infrared based SM (e.g., 2-8 km from the Geostationary Operational Environmental Satellite) for cloudless conditions should also be experimented in the future.

2.2 Evaluation datasets

2.2.1 Aircraft in-situ measurements during ACT-America and SEAC4RS

During the 2016 ACT-America deployment, the NASA B-200 aircraft took meteorological and trace gas measurements in the southeastern US from the surface to ~300 hPa on nine days. Different line colors in Figure 1d denote individual flight paths during this period. These flights were conducted under different weather conditions during the daytime (i.e., within 14-23 UTC, local time+6), with durations of 4-9 hours (https://www-air.larc.nasa.gov/missions/ACT-America/reports.2019/index.html). Fights on 16, 20, 21 of August 2016 sampled the air under stormy weather conditions, whereas the other flights were conducted under fair weather conditions. We used meteorological as well as collocated O₃ and CO measurements collected on the B-200 to evaluate our WRF-Chem simulations. The O₃ mixing ratio measurements using the differential ultraviolet absorption has a 5 ppbv uncertainty (Bertschi and Jaffe, 2005), and CO mixing ratio was measured...
with an uncertainty of 10 ppbv, using a Picarro analyzer which is based on wavelength-scanned cavity ring down spectroscopy (Karion et al., 2013). We used the weather and trace gas observations averaged in 1-minute intervals (released in September 2018) for model evaluation, as they represent atmospheric conditions on comparable spatial scales to the model. Ozone and CO measurements with O₃/CO>1.25 mole mole⁻¹ (Travis et al., 2016) are assumed to be influenced by fresh stratospheric intrusions and were excluded in our analysis. This approach, however, was rather arbitrary and may not have excluded air that had an aged stratospheric origin.

Aircraft (NASA DC-8) in-situ measurements of CO, NO₂ and formaldehyde (HCHO) from the surface to ~200 hPa during six SEAC⁴RS daytime (i.e., within 13-23 UTC, local time+6), 8-10-hour science flights in August 2013 were compared with our WRF-Chem simulations. The CO mixing ratio was measured using the tunable diode laser spectroscopy technique, with an uncertainty of 5% or 5 ppbv. The NO₂ measurements were made by two teams, based on thermal dissociation laser induced fluorescence and chemiluminescence methods, with the uncertainty of ±5% and (0.030 ppbv+7%), respectively. Two other teams took the HCHO measurements, using a compact atmospheric multispecies spectrometer and the laser-induced fluorescence technique, with the uncertainty of ±4% and (0.010 ppbv±10%), respectively. Aircraft data averaged in 1-minute intervals (released in November 2018) were used, with the biomass burning affected samples (acetonitrile >0.2 ppbv) and CO from fresh-stratospheric-intrusion-affected air (O₃/CO>1.25 mole mole⁻¹) excluded.

### 2.2.2 Ground-based measurements

WRF-Chem results were evaluated by various surface meteorological and chemical observations. These include: 1) surface air temperature (T2), relative humidity (RH, derived from the original dew point and air temperature data), and wind speed (WS) from the NCEP Global Surface Observational Weather Data (doi: 10.5065/4F4P-E398); 2) half-hourly or hourly latent and sensible heat fluxes measured using the eddy covariance method at eight sites within the FLUXNET network. Latent and sensible heat fluxes from this network exhibited mean errors of -5.2% and -1.7%, respectively (Schmidt et al., 2012). We only analyzed the modeled energy fluxes at the sites where the model-based LULC classifications are realistic. A 0.5°×0.5° daily FLUXCOM product was also utilized, which merges FLUXNET data with machine learning approaches, remote sensing and meteorological data. Over North America, it is estimated that latent and sensible heat fluxes from this FLUXCOM product are associated with ~12% and ~13% of uncertainty, respectively (Jung et al., 2019); and 3) hourly O₃ at the US EPA Air Quality System (AQS, mostly in urban/suburban regions) and the Clean Air Status and Trends Network (CASTNET, mostly in nonurban areas) sites. Hourly AQS and CASTNET O₃ are US sources of the Tropospheric Ozone Assessment Report database, the world’s largest collection of surface O₃ data supporting analysis on O₃ distributions, temporal changes and impacts. Measurements of NO₂ and HCHO are also available at some of the AQS sites. It is highly possible that these measurements are biased due to the interferences of other chemical species and therefore they were not used in this work.
2.2.3 Precipitation products

The WRF-Chem precipitation fields were also qualitatively compared with two precipitation data products: 1) the 4 km, hourly NCEP Stage IV Quantitative Precipitation Estimates (Lin and Mitchell, 2005), which is a widely-used, national radar and rain gauge based analysis product mosaicked from 12 River Forecast Centers over the contiguous US, and its quality partially depends on the manual quality control done at the River Forecast Centers; and 2) the 0.1°×0.1°, half-hourly calibrated rainfall estimates from version 6B of the Integrated Multi-satellite Retrievals for the Global Precipitation Measurement (GPM) constellation final run product (Huffman et al., 2019). Compared with single-platform based precipitation products, multisensor based precipitation datasets have reduced limitations and therefore have become popular in scientific applications. Nevertheless, these datasets may be associated with region-, season-, and rainfall-rate dependent uncertainties (e.g., Tan et al., 2016; Nelson et al., 2016, and the references therein).

3 Results and discussions

3.1 Synoptic and drought conditions during the study periods

In August 2016, several states in the southern US experienced moderately-to-extremely moist conditions according to major drought indexes such as the Palmer Hydrological Drought Index (Figure S2, left). These were largely due to the influences of passing cold fronts and tropical systems from the Gulf of Mexico (https://www.ncdc.noaa.gov/sotc/synoptic/201608). Temperatures were consequently lower than normal in these regions. Contrastingly, controlled by the Bermuda High, more frequent air stagnation, warmer-, and drier-than-normal conditions affected multiple Atlantic states. Opposite hydrological anomalies were recorded during August 2016 and August 2013 for the southern Great Plain and Atlantic regions (Figure S2, left).

The anomalies in synoptic patterns and drought conditions in August of 2016 and 2013, as well as the day-to-day weather changes, can be closely linked to regional O₃ variability in the southeastern US. Based on the pressure gradients along the western edges of the Bermuda High (Zhu and Liang, 2012; Shen et al., 2015), the influences of the Bermuda High on southeastern US surface O₃ enhancements may be stronger in August 2016 than in August 2013 (Figure S2, middle). Lightning intensities and emissions respond to climate change (Romps et al., 2014; Murray, 2016; Finney et al., 2018), therefore affecting the probability of fires ignited by lightning. Based on satellite detections which are subject to cloud contamination, fire activities associated with emissions of heat and O₃ related pollutants were stronger in drier regions in the southern US in August of 2016 and 2013. The variable synoptic and drought conditions also controlled biogenic VOC and soil NO emissions as well as O₃-related chemical reaction and deposition rates, and the resulting impacts on O₃ depended on the changing anthropogenic NOₓ emissions (Hudman et al., 2010; Hogrefe et al., 2011; Coates et al., 2016; Lin et al., 2017). In the upper troposphere, troughs bumping into the anticyclone above the southeastern US in August 2016 helped shape the
pollution outflows differently than in August 2013 when the North American monsoon anticyclone was built over the southwestern US and the central-eastern US was controlled by a strong cool trough (Figure S2, right).

Studies have shown that the variations in land-atmosphere coupling strength are connected with SM interannual variability and the local spatiotemporal evolution of hydrologic regime (e.g., Guo and Dirmeyer, 2013; Tuttle and Salvucci, 2016). Therefore, over the southern Great Plain and Atlantic regions, SM-atmosphere coupling strengths in August 2016 and August 2013 may have diverged from the climatology in opposite directions. For example, in August 2016, the overall potential impacts of SM on surface water/energy fluxes and atmospheric states may be higher than normal over the Atlantic regions whereas below the average in the southern Great Plain. In August 2013, the land-atmosphere coupling may be stronger than normal and abnormally weak over the southern Great Plain and the Atlantic regions, respectively.

3.2 SMAP DA impacts on weather states and surface energy fluxes

The weather states and energy fluxes during 16-28 August 2016 from the WRF-Chem base simulation are illustrated in Figure 2 (for SM and T2), Figure 3 (for RH, WS, and PBL height, PBLH), Figure 4 (for precipitation), Figures 5 and S2 (for energy fluxes and their partitioning), together with the SMAP DA impacts on these variables.

The highest daytime (13-24 UTC, local times+5 or +6) average T2 were observed in several states in the Atlantic region that were undergoing drought conditions (Figure S2, left; Figure 2c), The daily T2 maxima occurred during noon-early afternoon in most places, consistent with the findings from Huang et al. (2016). The Lower Mississippi River regions were influenced by high humidity (Figure 3c). Under the influence of the BH, surface winds were overall mild to the east of Texas. Strongest rainfall affected Texas, Arkansas, Kentucky, Tennessee, and near the border of Kansas and Missouri (Figure 4a-b), which belonged to the wetter-than-normal regions according to August 2016 drought indexes. Rainfall in most areas peaked in the late afternoon or evening after the times of peak T2 (Figure 4e-f). The observed diurnal cycles of rainfall and T2 indicate that, for the study area/period, convection was mainly due to the thermodynamic response to surface temperature. However, land-sea interactions, fronts, topography, as well as aerosol loadings may also have come into play.

The dry and wet anomalies in the southeastern US based on the modeled SM (Figure 2a) are shown consistent with weekly (not shown in figures) and monthly drought indexes (e.g., Figure S2, left). The modeled SM values in various soil layers are near the model-based soil wilting points and field capacities (Figure S1, middle and right) over drought-influenced and wet regions, respectively. The WRF-Chem base simulation overall captured the observed patterns of T2, RH, and WS across the domain, with its daytime PBLH spatially correlated with the T2 patterns (Figures 2b and 3a;e;i). Referring to the Stage IV and GPM rainfall data, the WRF-Chem base case also overall fairly well reproduced the diurnal cycles of rainfall during the study period, but the rainfall “hotspots” simulated by the model appear west to those in the Stage IV and GPM products (Figure 4c). Dirmeyer et al. (2012) found that models’ rainfall performance more strongly depended on the distinctive
treatment of the model physics than on the model resolution. Our WRF-Chem performance for rainfall diurnal cycle in this region is similar to previous convection-permitting WRF-Chem simulations (e.g., Barth et al., 2012). Additionally, the WRF-Chem predicted mean rainfall rates over low-precipitation regions (e.g., several Atlantic states) are higher than those based on the Stage IV and GPM rainfall products, which tend to overestimate precipitation at the low end (e.g., Nelson et al., 2016; Tan et al., 2016). Such positive model biases for low-precipitation regions have also been reported in Barth et al. (2012).

Overall, the SMAP DA broadly reduced surface SM at the model initial times (i.e., 00 UTC each day), except the coastal Texas regions and parts of Ohio and Florida (Figure 2e). Such changes in SM are consistent with the modeled daytime RH responses (Figure 3b), and are anti-correlated with the model responses in its averaged daytime T2 and PBLH fields (Figure 2f;3j), as well as their daily amplitudes (not shown in figures). In places, the daily maxima of WRF-Chem T2 were delayed by an hour or two when the SMAP DA was enabled (Figure 2h). The changes in WRF-Chem temperature gradients due to the SMAP DA led to slight WS enhancements over many of the model grids (Figure 3f). On the 13-day timescale, the SMAP DA had less discernable impacts on rainfall, consistent with findings from Koster et al. (2010, 2011) and Huang et al. (2018). The SMAP DA impacts on mean rainfall rate and diurnal cycles show noisy patterns (Figure 4d;g;h), and positive and negative SM-precipitation relationships are both found. The spatial and temporal variability in these model sensitivities reflects the impacts of local hydrological regimes and their anomalies as well as moisture advection.

The inclusion of the SMAP DA did not dominantly improve or degrade the overall T2, RH and WS performance of WRF-Chem (e.g., Figures 2g;3d;3h, based on the root-mean-square error (RMSE) metric): i.e., improvements on T2, RH, and WS occurred in 47%, 51% and 52% of the model grids where observations are available, and the domain-wide mean RMSE changes for T2, RH, and WS are \(-0.024\) K, \(-0.005\) ms\(^{-1}\), respectively. This is qualitatively consistent with the findings in Huang et al. (2018) and Yin and Zhan (2018) for dense vegetation regions (i.e., green vegetation fraction >0.6), based on RMSE and other evaluation metrics. Additionally, as discussed in Huang et al. (2018), unrealistic model representations of terrain height can pose challenges for evaluating the modeled surface weather fields with ground-based observations. The 12 km model grid used in this work well represents terrain height (i.e., \(|\text{model-actual}|<15\) m) at over 70% of the model grids that have collocated observations, but at some locations the discrepancies between the model and actual terrain height exceed 100 m. Furthermore, human activities such as irrigation can significantly modify water budget and land-atmosphere coupling strength over agricultural regions (e.g., Lu et al., 2017), but these were unmodeled (i.e., not accounted for) in the used modeling system. Observations from SMAP and other satellites are capable of detecting the signals of irrigation over the southeastern US (e.g., the circled regions in Figure 1e based on Ozdogan and Gutman (2008) and Zaussinger et al. (2019)) and other regions of the world. How irrigation patterns and scheduling, depending in part on the weather conditions, affected our WRF-Chem performance as well as the effectiveness of the SMAP bias correction and DA are worth further investigations. In places, the changes in WRF-Chem rainfall patterns due to the SMAP DA are within
the discrepancies between the Stage IV and GPM rainfall products. A better understanding of the uncertainty associated with these two used rainfall products can benefit the assessment of SM DA impacts on the model’s precipitation performance.

The spatial patterns of evaporative fraction (defined as: latent heat/(latent heat+sensible heat)) follow those of SM and RH, with the maxima (>0.75) seen in the Lower Mississippi River region and smaller values (<0.65) in the dry Atlantic states and some parts of the southern Great Plains (Figure 5a-b). Note that the absolute latent and sensible heat fluxes can differ significantly at locations with similar evaporative fraction values (Figure S3). The WRF-Chem based evaporative fraction shows similar spatial gradients but is overall negatively biased (Figure 5c). The changes in WRF-Chem evaporative fraction due to the SMAP DA are spatially correlated with the surface moisture changes (Figure 2e;3b;5d). As a result, the model performance of evaporative fraction was only improved over some of the regions where it was increased by the SMAP DA.

It is found that the SMAP DA impacts on model performance are not universally consistent for energy fluxes and land/atmosphere states. This can be explained by the fact that this used modeling system has shortcomings in representing SM-flux coupling and/or the relationships between moisture/heat fluxes and the atmospheric weather which need to be clearly identified and corrected. Future efforts should be devoted to: evaluation of additional flux variables (e.g., runoff, radiation), applications using other LSMs (e.g., the Noah-Multiparameterization) together with multivariate land DA, and utilization of alternative WRF inputs and physics configurations.

The WRF-Chem modeled weather states were also evaluated with ACT-America aircraft observations at various altitudes. Along the flight paths, the observed air temperature and water vapor mixing ratios decrease with altitude. The modeled air temperature and humidity as well as their responses to the SMAP DA vary in space and time. In general, these responses are particularly strong near the surface. Under stormy weather conditions on 16, 20, 21 of August 2016, the maximum changes in air temperature and humidity in the free troposphere exceeded 2.5 °K and 2 g/kg, respectively (Figure 6c;f). Corresponding to these changes, the SMAP DA modified the RMSEs of WRF-Chem air temperature and/or water vapor by over 5% for several individual flights and overall reduced the RMSEs of these model variables by ~0.7% and ~1.6%, respectively (Figures 7).

3.3 SMAP DA impacts on surface \( \mathrm{O}_3 \) concentrations

The changes in the above-described meteorological variables (e.g., air temperature, RH, WS, PBLH) due to the SMAP DA alter various atmospheric processes which can have mixed impacts on surface \( \mathrm{O}_3 \) concentrations. For example, warmer environments promote biogenic VOC and soil NO emissions as well as accelerate chemical reactions. Faster winds and thickened PBL dilute air pollutants including \( \mathrm{O}_3 \) and its precursors, and therefore reduce \( \mathrm{O}_3 \) destruction via titration (i.e., \( \mathrm{O}_3 + \mathrm{NO} \rightarrow \mathrm{O}_2 + \mathrm{NO}_2 \)) as well as photochemical production of \( \mathrm{O}_3 \). The changes in wind vectors affect pollutants’ concentrations in downwind regions. Water vapor mixing ratios perturb \( \mathrm{O}_3 \) photochemical production and loss via affecting the HO\(_x\) cycle. Also, higher RH often has relevance with cloud abundance and solar radiation and therefore slow down the photochemical
processes (Camalier et al., 2007). Additionally, chemical loss via stomatal uptake may be slower under lower-SM/humidity, higher-temperature conditions, and nonstomatal uptake also varies with meteorology. These processes, however, may not be realistically represented by the Wesely dry deposition scheme (Section 2.1) used in this study.

Figure 8a-b compare the observed and WRF-Chem base case daytime surface $O_3$ during 16-28 August 2016, and the SMAP DA impacts on daytime surface $O_3$ are shown in Figure 8c. Low-to-moderate $O_3$ pollution levels are seen over most areas within the model domain, except the Atlantic states due to the influences of frequent air stagnation, warm and dry conditions. Period-mean daytime surface $O_3$ responses to the SMAP DA are overall slightly positive, but exceeded 2 ppbv in places. The $O_3$ changes show strong spatial correlations with those of T2 and PBLH (Figure 2f;3j), which are anti-correlated with the surface humidity responses (Figure 2e;3b). The maximum impacts of SMAP DA on daily daytime surface $O_3$ exceeded 4 ppbv on most of the days during 16-28 August 2016 (Figure 9a). On almost all days, the $O_3$ sensitivities are moderately correlated with the daytime T2 changes (blue text in Figure 9a). The period-mean WRF-Chem surface MDA8 and its response to the SMAP DA (Figure 10a-b) show similar spatial patterns to those of the modeled surface daytime $O_3$, but are of slightly higher magnitudes. Enhanced biogenic isoprene and soil NO emissions (Figure 3k-n and Figure S4), especially for the regions with elevated emissions (e.g., the Missouri Ozarks for isoprene and agricultural land for soil NO), as well as accelerated photochemical reactions were the major causes of such changes in surface daytime-average and MDA8 $O_3$. MEGAN’s limitations in representing biogenic VOC emission responses to drought may have had minor impacts on most of the high-isoprene-emission regions which were not affected by drought during this period. Uncertainty in the modeled soil NO emissions and their responses to the SMAP DA may be larger over high-temperature cropland regions which needs further investigations accounting for the influences of SM and fertilization conditions. The deposition velocities of $O_3$ and its related chemical species also responded to the SMAP DA, with the $O_3$ deposition velocity changes estimated to be the most important to the modeled $O_3$ concentrations according to previous studies (e.g., Baublitz et al., 2020). The modeled daytime $O_3$ deposition velocity responses to the SMAP DA (Figure 3o-p and Figure S4) are found anti-correlated with those in the surface temperature. Note that these deposition results are based on the Wesely scheme in which the SM influence on stomatal resistance is omitted. If a SM limitation factor (details in Figure S1 caption) was included in the calculations, the modeled deposition velocities would respond more strongly to the SMAP DA. Including such a SM limitation factor, however, would not necessarily improve the modeled deposition velocities in part due to the uncertainty in the model’s LULC input and the prescribed seasonal- and LULC-dependent constants in the used Wesely scheme.

The SMAP DA improved surface MDA8 at 42% and 51% of the model grids where AQS and/or CASTNET observations are available, respectively. The domain-wide mean MDA8 RMSE changes due to the SMAP DA are 0.058 ppbv and 0.007 ppbv referring to gridded AQS and CASTNET $O_3$ observations, respectively. As summarized in Table 2, after enabling the SMAP DA, the number of grids with $O_3$ exceedance false alarms (i.e., WRF-Chem MDA8 $O_3$ $>$ 70 ppbv but the observed MDA8 $O_3$ $<=$ 70 ppbv) remained the same, except that this number dropped on 18 August and increased on 26 August. Such
O₃ performance changes in response to the SMAP DA are overall less desirable than those in the weather fields. This can be explained by the fact that many other factors, such as the quality of the anthropogenic emission input of WRF-Chem, also affected the model’s surface O₃ performance. Figures 10c-f and 9b show that using NEI 2016 beta anthropogenic emissions instead of the outdated NEI 2014 resulted in notable reductions in surface daytime-average and MDA8 O₃ across the model domain. These reductions lowered the modeled surface O₃ biases by up to ~4 ppbv and reduced the number of grids with O₃ exceedance false alarms on 7 out of the 13 days (Table 2). Improving the modeled weather fields via the SMAP DA would more clearly improve the model’s O₃ performance if the uncertainty of NEI 2016 beta and other inputs as well as the model parameterizations (e.g., chemical mechanism, natural emission, photolysis and deposition schemes) is reduced.

It is noticed that daytime surface O₃ fields from the global CAMS and AM4 modeling systems are overall higher than those simulated by WRF-Chem (Figure 8b;d;e). One of the reasons is that stratosphere-troposphere exchanges are better represented in these two global models. According to AM4’s stratospheric tracer, during the study period, the stratospheric O₃ influences on daytime surface O₃ range from <2 ppbv in the southern Great Plains (storm-affected regions) to 6-7 ppbv around Kansas and the Atlantic Ocean. Note that although AM4 provides a broad overview of the areas strongly impacted by stratospheric air, fine-scale features associated with stratospheric intrusions may be missing from this coarse-resolution simulation (Lin et al., 2012; Ott et al., 2016). In the used WRF-Chem system, which has only tropospheric chemistry, the representation of stratospheric influences only depends on the quality of the model’s chemical LBCs. This representation may be improved by adding accurate, time-varying chemical upper boundary conditions, e.g., downscaled from a well-performed global model simulation. Such an update, however, is expected to increase the modeled surface O₃ (e.g., Figure 3 in Huang et al., 2013, based on a different regional air quality model). For regions where modeled surface O₃ is already positively biased, stronger efforts to address other sources of model errors would be needed to achieve desirable surface O₃ performance.

### 3.4 SMAP DA impacts on O₃ at various altitudes

The SMAP DA impacts on WRF-Chem modeled chemical fields are also investigated at a wide range of altitudes. Figure 6g-i compare the observed and WRF-Chem base case O₃ and CO concentrations along nine ACT-America flights in August 2016, as well as the SMAP DA impacts on WRF-Chem results at these sampling locations. The observed and modeled CO vertical profiles show strong day-by-day variability, with near-surface concentrations ranging from 60 to 170 ppbv and elevated concentrations aloft (<600 hPa) occurring on 16, 20, 21 of August when aircraft measurements were taken under stormy weather conditions. In general, the observed and modeled O₃ increase with altitude. WRF-Chem fairly well captured the magnitudes of the near-surface O₃ concentrations but underpredicted O₃ in the free troposphere. Overall, the modeled trace gas concentrations reacted to the SMAP DA most strongly near the surface. Under stormy weather conditions, the changes in modeled CO and O₃ approach 15 ppbv and 10 ppbv, respectively. The SMAP DA impacts on modeled CO and O₃ RMSEs are overall close to neutral (δRMSE<0.5%) but over 2% during selected flights (Figures 7). Similar to the
evaluation results for surface weather and O\textsubscript{3} fields, the O\textsubscript{3} performance changes by the SMAP DA are less desirable than those in the weather fields.

To help better understand SM controls on upper tropospheric O\textsubscript{3} chemistry, Figure 11 shows the period-mean (16-28 August 2016) daytime O\textsubscript{3}, CO, and NO\textsubscript{2} at ~400 hPa from the WRF-Chem base simulation, as well as the SMAP DA impacts on these model fields. The daily daytime O\textsubscript{3} responses to the SMAP DA at ~400 hPa are presented in Figure 9c. Elevated WRF-Chem O\textsubscript{3} concentrations (>70 ppbv) are seen near the center of the upper-tropospheric anticyclone (Figure S2, right), which circulated the lifted pollutants and promoted in-situ chemical production. The SMAP DA modified the period-mean daytime O\textsubscript{3} by up to >1 ppbv, and its impact on daytime O\textsubscript{3} on individual days during the study period occasionally exceeded 10 ppbv, which is larger than its maximum impact on the daily daytime surface O\textsubscript{3} (Figure 9a,c). As indicated by the modeled CO and NO\textsubscript{2} responses to the SMAP DA, O\textsubscript{3} distributions in the upper troposphere and their responses to the SMAP DA are partially controlled by atmospheric transport and rapid in-situ chemical production of O\textsubscript{3} from lightning NO and other emissions, both of which are sensitive to SM. Note that although CO and NO\textsubscript{2} are used here primarily as a tracer of transport and an indicator of lightning production, respectively, lightning emissions can modify CO lifetimes, and atmospheric transport can also affect NO\textsubscript{2}.

Similar to the O\textsubscript{3} conditions at the surface, at ~400 hPa, the WRF-Chem simulated daytime O\textsubscript{3} concentrations are lower than the global CAMS and AM4 results (Figure 11a-b) as well as the ACT-America aircraft measurements (Figure 6g-h), by up to tens of ppbv. The AM4 stratospheric tracer suggests 5-17 ppbv of stratospheric influences on period-mean O\textsubscript{3} at these altitudes (Figure 11c), which again helps identify the shortcoming of WRF-Chem in representing stratosphere-troposphere exchanges. Applying accurate, time-varying chemical upper boundary conditions in future works can help better assess the SMAP DA impact on O\textsubscript{3} performance in the upper troposphere and improve the understanding of upper tropospheric chemistry.

3.5 SMAP DA versus anthropogenic emission perturbation impacts on tropospheric O\textsubscript{3}

Perturbing anthropogenic emissions was a major approach implemented in the HTAP Phases 1 and 2 (HTAP1 and HTAP2) multi-model experiments to quantify how emission changes in one given region of the world affect air pollution in other regions of the world (Fiore et al., 2009; Huang et al., 2017a). Based on HTAP1 multi-model (at horizontal resolutions ranging from 1°×1° to 5°×5°) estimates for August 2001, European surface O\textsubscript{3} decreased by ~0.35 ppbv in response to a 20% reduction in North American anthropogenic emissions (Fiore et al., 2009). Using HTAP2 configurations, a 0.7°×0.7° Composition-Integrated Forecasting System (C-IFS, which is the forecast model of CAMS) estimated that, in August 2010, ~400 hPa and surface O\textsubscript{3} concentrations over the southeastern US were reduced by 0.7-1.5 ppbv and >2 ppbv, respectively, in response to a 20% reduction in North American anthropogenic emissions. Such an emission perturbation also reduced
European ~400 hPa and surface O\textsubscript{3} by 0.4-0.7 ppbv (i.e., ~1/3-1/2 of the 0.7-1.5 ppbv changes in the southeastern US due to dilution and chemical loss along the great transport distance) and 0.1-0.5 ppbv, respectively.

Based on our WRF-Chem base and “NEI14” simulations, we quantified the impact of updating anthropogenic emissions from NEI 2014 to NEI 2016 beta (<20% of change for most species as introduced in Section 2.1) on daytime O\textsubscript{3} export from the southeastern US. Although skewed to negative values, the O\textsubscript{3} changes related to the NEI emission update show comparable magnitudes with those due to the SMAP DA at ~400 hPa: i.e., mostly within ±10 ppbv and ±1.5 ppbv at daily and 13-day timescales, respectively (Figure 9c-d,11g;12b). This suggests that the SMAP DA and the US EPA estimated anthropogenic emission change from 2014 to 2016 over the southeastern US could have similar levels of impact on O\textsubscript{3} in Europe. Referring to the C-IFS HTAP2 sensitivity simulation results, at ~400 hPa, the impacts on European O\textsubscript{3} may be 1/3-1/2 of the O\textsubscript{3} changes in the southeastern US, and at the surface, the impacts may be within ±0.5 ppbv. Such estimations based on results from different modeling systems for different time periods need further evaluation.

This analysis highlights the important role of SM in quantifying pollutants’ source-receptor relationships between the US and Europe. It also emphasizes that using outdated anthropogenic emissions in WRF-Chem would lead to inaccurate assessments of the SMAP DA impacts on the model performance of O\textsubscript{3} and other air pollutants over a broad region.

### 3.6 Evaluation of NEI 2014 using WRF-Chem simulations and SEAC\textsuperscript{4}RS observations

We compared NO\textsubscript{2}, HCHO and CO from two 25 km WRF-Chem simulations (i.e., the “SEACf” and “SEACa” cases in Table 1) with aircraft observations during six SEAC\textsuperscript{4}RS flights in August 2013 (Figure S5). Such comparisons help evaluate the emissions of O\textsubscript{3} precursors from various (e.g., NEI 2014 anthropogenic, lightning and biogenic) sources as well as how the model representation of land-atmosphere interactions can affect such emission assessments. It is shown that in case “SEACf”, WRF-Chem reproduced the overall vertical gradients of the observed chemicals, except that at this resolution it had difficulty in capturing urban plumes (e.g., for where the observed NO\textsubscript{2} >4 ppbv). This suggests that emissions of major O\textsubscript{3} precursors are moderately well represented in the used WRF-Chem system. The strongest changes in modeled NO\textsubscript{2}, HCHO, and CO by assimilating the CCI SM are ~2 ppbv, ~3 ppbv, and ~25 ppbv, respectively, all occurring near the surface (>700 hPa). In the upper troposphere, the SM DA reduced the modeled NO\textsubscript{2} by up to ~0.5 ppbv (at ~400 hPa) and enhanced the modeled CO by up to ~6 ppbv (at ~200 hPa). These changes led to better model agreements with the observations, indicating that assimilating the CCI SM likely improved the model treatment of lightning production and convective transport. As the SM DA modified the mismatches between the modeled and the observed trace gas concentrations, it is suggested that accurate representations of land-atmosphere interactions can benefit more rigorous evaluation and improvement of emissions using observations. Additionally, aircraft observations show robustness in aiding the evaluation of the emissions of O\textsubscript{3} precursors from various sources, and therefore continuing to make rich and detailed observations like...
those would be helpful for evaluating and improving newer/future versions of emission estimates as well as the model representations of land-atmosphere interactions.

4 Summary and suggestions on future directions

This study focused on evaluating SMAP SM DA impacts on coupled WRF-Chem weather and air quality modeling over the southeastern US during the ACT-America campaign in August 2016. The impacts of SMAP DA on WRF-Chem modeled daytime RH as well as evaporative fraction were qualitatively consistent with the changes in the model’s initial SM states, which were anti-correlated with the modeled daytime surface T2 and PBLH changes. The DA impacts on WRF-Chem performance of weather states and energy fluxes showed strong spatiotemporal variability, and many factors such as dense vegetation, complex terrain, and unmodeled processes such as water use from human activities (e.g., irrigation) may have impacted the effectiveness of the DA. Overall, the modeled T2, RH, and WS performance was improved by the DA in 47%, 51% and 52% of the grids where observations were available. Referring to ACT-America aircraft observations on nine flight days, the DA reduced the RMSEs of WRF-Chem air temperature and water vapor by ~0.7% and ~1.6%, respectively. The overall DA impact on the modeled rainfall was less discernible, within the discrepancies between two rainfall evaluation products in places. The DA impacts on model performance were not consistent for energy flux partitioning and land/atmosphere states everywhere, suggesting that the used modeling system had shortcomings in representing SM-flux coupling and/or the relationships between moisture/heat fluxes and the atmospheric weather which need to be clearly identified and corrected. Future efforts should focus on: 1) evaluation of additional flux variables (e.g., runoff, radiation); 2) applications using other LSMs along with multivariate land DA; and 3) utilization of alternative LIS/WRF configurations, including adding irrigation processes to the modeling system and performing convection-permitting simulations with the assimilation of various kinds of high-resolution land products. Additionally, improving bias correction methods (e.g., also matching higher moments of the LSM and satellite SM climatology) and practicing the assimilation of SMAP Level 1 brightness temperature alone or in combination with atmospheric observations will be needed.

The SMAP DA impact on WRF-Chem surface daytime-average and MDA8 O3 were strongly correlated with the changes in daytime T2 and PBLH, which were anti-correlated with the daytime surface humidity changes. Such changes in surface O3 were mainly due to enhanced biogenic isoprene and soil NO emissions as well as accelerated photochemical reactions in response to the DA, and the changes in the modeled dry deposition fields also played a role. The SMAP DA impacts on modeled O3 along the ACT-America flight paths were particularly strong (i.e., approaching 10 ppbv) under stormy weather conditions. The WRF-Chem O3 performance change in response to the DA was overall less desirable than those in the weather fields. This in part was because many other factors, such as the model representations of anthropogenic emissions and stratosphere-troposphere exchanges, also affected the model’s surface O3 performance.
We showed that at ~400 hPa, elevated O\textsubscript{3} concentrations were modeled near the center of the upper tropospheric anticyclone. The modeled O\textsubscript{3} was negatively biased, mainly resulting from the poor representation of stratosphere-troposphere exchanges by WRF-Chem. The impact of SMAP DA on upper tropospheric O\textsubscript{3} was partially via altering atmospheric transport and in-situ chemical production of O\textsubscript{3} from lightning NO and other emissions. We also presented that the impacts of DA and an emission update from NEI 2014 to NEI 2016 beta on WRF-Chem modeled upper tropospheric O\textsubscript{3} had comparable magnitudes. As indicated by HTAP2 global model sensitivity simulations, a reduction in North American anthropogenic emissions would be beneficial for mitigating European O\textsubscript{3} pollution. Therefore, our analysis highlighted the important role of SM in quantifying the pollutants’ source-receptor relationships between the US and Europe. It also emphasized that using up-to-date anthropogenic emissions in WRF-Chem would be necessary for accurately assessing SM DA impacts on the model performance of O\textsubscript{3} and other air pollutants over a broad region. Continuing to improve NEI 2016 beta and any newer versions of emission estimates, as well as the parameterizations and other inputs of the models, is strongly encouraged. Such efforts can benefit from rich, detailed, high-accuracy observations, such as those taken during airborne field campaigns.

This study is a critical first step towards using satellite SM products to help improve the simulated weather and chemistry fields in models that are widely-used for air quality research and forecasting, as well as policy-relevant assessments. It is necessary to clarify that in this study the SMAP DA influenced the WRF-Chem modeled O\textsubscript{3} mainly via changing the model’s weather fields that drove its chemistry calculations online. The parameterizations for biogenic emissions and dry deposition in the standard WRF-Chem model were not modified in this study to realistically reflect the impacts of water availability. Ozone damage to vegetation was not modeled in this work, which was expected to only have minor impacts on these half-month-long simulations. Reducing these limitations in WRF-Chem and other models’ parameterizations (e.g., Hudman et al., 2012; Val Martin et al., 2014; Sadiq et al., 2017; Jiang et al., 2018; Clifton et al., 2020) are important to further improving the modeled chemical fields via applying the SM DA at various scales. Using dynamic vegetation models (available in the Noah-Multiparameterization LSM) along with additional process-based (e.g., chemical fluxes, stomatal behaviors) measurements and laboratory experiments would be necessary for improving some of these parameterizations, and these will be experimented in a follow-up study. Community efforts such as the ongoing Air Quality Model Evaluation International Initiative Phase 4 experiment (https://aqmeii.jrc.ec.europa.eu/phase4.html) would also be greatly beneficial. High-quality weather input is a requirement for rigorous evaluations of any set of these parameterizations.

**Code and data availability**

The standalone LIS is accessible at: https://lis.gsfc.nasa.gov. LIS/WRF-Chem coupling is facilitated in the NASA-Unified WRF system (https://nuwrf.gsfc.nasa.gov). The global C-IFS simulations for HTAP2 are available at the AeroCom database. Observations and observation-derived data products used in this work can be found at: https://nsidc.org/data/smap/smap-data.html; https://www.esa-soilmoisture-cci.org; https://www-air.larc.nasa.gov/index.html; https://www.epa.gov/aqs;
Author contributions

MH led the design and execution of the study as well as the paper writing. JHC, JPD, GRC, and KWB contributed to the field campaign data collection and/or analysis. GRC, KWB, SVK and XZ contributed to the modeling and/or DA work. All authors helped finalize the paper.

Competing interests

The authors declare that they have no conflict of interest.

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Table 1: Summary of WRF-Chem simulations conducted in this study.

| Case name | Horizontal/vertical resolutions | Analyzed period (field campaign) | Assimilated SM data (version; resolution) | Anthropogenic emission inputs for various chemical species |
|-----------|---------------------------------|----------------------------------|-------------------------------------------|----------------------------------------------------------|
| Base      | 12 km/63 layer                  | 16-28 August 2016 (ACT-America) | none                                      | NEI 2016 beta                                            |
| Assim     |                                 |                                  | SMAP enhanced passive (version 2; 9 km)   | NEI 2016 beta                                            |
| NEI14     |                                 |                                  | none                                      | NEI 2014                                                 |
| SEACf     | 25 km/27 layer                  | 12-24 August 2013 (SEAC4RS)      | none                                      | NEI 2014                                                 |
| SEACa     |                                 |                                  | ESA CCI passive (version 04.5; 0.25°)     | NEI 2014                                                 |

Acronyms: ACT: Atmospheric Carbon Transport; ESA CCI: European Space Agency Climate Change Initiative; NEI: National Emission Inventory; SEAC4RS: Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys; SM: Soil Moisture; SMAP: Soil Moisture Active Passive; WRF-Chem: Weather Research and Forecasting model with online Chemistry

Table 2: The number of model grids with surface MDA8 O₃ exceedance false alarms (i.e., WRF-Chem MDA8 O₃>70 ppbv but the observed MDA8 O₃<=70 ppbv) from the 12 km WRF-Chem simulations. Degradations and improvements from the base case are highlighted in red and green, respectively.

| Days of August 2016 | Referring to AQS observations | Referring to CASTNET observations |
|---------------------|-------------------------------|-----------------------------------|
|                     | Base | Assim | NEI14 | Base | Assim | NEI14 |
| 16                  | 0    | 0     | 0     | 0    | 0     | 0     |
| 17                  | 0    | 0     | 0     | 0    | 0     | 0     |
| 18                  | 1    | 3     | 4     | 0    | 0     | 0     |
| 19                  | 9    | 9     | 10    | 0    | 0     | 0     |
| 20                  | 4    | 4     | 13    | 0    | 0     | 1     |
| 21                  | 0    | 0     | 0     | 0    | 0     | 0     |
| 22                  | 0    | 0     | 0     | 0    | 0     | 0     |
| 23                  | 1    | 1     | 1     | 0    | 0     | 0     |
| 24                  | 1    | 1     | 2     | 0    | 0     | 0     |
| 25                  | 1    | 1     | 2     | 0    | 0     | 0     |
| 26                  | 6    | 5     | 9     | 1    | 0     | 1     |
| 27                  | 0    | 0     | 0     | 0    | 0     | 0     |
| 28                  | 6    | 6     | 14    | 0    | 0     | 0     |
Figures

Figure 1: (a) Terrain heights; (b) August 2016 green vegetation fraction; and (c) grid-dominant land use/cover categories used in the 12 km LIS/WRF-Chem simulations. (d) B-200 flight paths in the southeastern US during the 2016 ACT-America campaign. Cyan-blue circles in (c) denote the approximate locations of areas with high irrigation water use based on literature. Similar model domains, consistent sources of geographical inputs and meteorological forcings were used in 12 km and 25 km LIS/WRF-Chem simulations.

Figure 2: Period-mean (16-28 August 2016) WRF-Chem base case (a) surface soil moisture at initial times; (b) daytime 2 m air temperature (T); and (d) time of daily peak air T in US Central Standard Time (CST), as well as (c;f;h) the impacts of SMAP DA on these fields. Observed daytime 2 m air T and the impact of the SMAP DA on RMSEs of the daytime 2 m air T are shown in (c) and (g), respectively.
Figure 3: Period-mean (16-28 August 2016) WRF-Chem base case daytime (a) 2 m relative humidity (RH); (c) 10 m wind speed; (i) PBLH; biogenic emissions of (j) isoprene and (k) soil NO; and (l) O₃ deposition velocity, as well as (e;g;m;n;o;p) the impacts of SMAP DA on these model fields. Observed daytime 2 m RH and surface wind speed, as well as the impacts of the SMAP DA on RMSEs of these fields are shown in (b;f) and (d;h), respectively. Additional biogenic emissions and deposition results are shown in Figure S4.

Figure 4: Period-mean (16-28 August 2016) (a-d) rainfall rate and (e-h) time of peak rainfall in US Central Standard Time (CST) from (a;e) the national Stage IV Quantitative Precipitation Estimates product; (b;f) the Global Precipitation Measurement; and (c;g) WRF-Chem base case. Results from the WRF-Chem “assim” case are indicated in (d;h).
Figure 5: Period-mean (16-28 August 2016) daily evaporative fraction, defined as: daily latent heat/(daily latent heat+daily sensible heat), from (a) a FLUXCOM product; (b) selected FLUXNET sites; and (c) WRF-Chem base case. (d) shows the impact of the SMAP DA on WRF-Chem EF. Additional evaluation results for latent and sensible heat fluxes at the focused FLUXNET sites are presented in Figure S3.

Figure 6: Vertical profiles of (a) air temperature; (d) water vapor mixing ratio (H2O); (g) O3; and (j) carbon monoxide (CO) observed on the B-200 aircraft during the ACT-America 2016 campaign, based on a 1-minute averaged dataset. Their WRF-Chem counterparts from the base case and the impacts of the SMAP DA are shown in (b); (e); (h); and (c); (f); (i); (l), respectively. The different colors distinguish samples taken on various flight days, and the B-200 paths on these flight days are shown in Figure 1d. Flights on 16, 20, 21 of August 2016 were conducted under stormy weather conditions as highlighted in (a), whereas the B-200 flew under fair weather conditions during other flights.
Figure 7: Evaluation of WRF-Chem results with the B-200 aircraft observations during the ACT-America 2016 campaign: (a) the RMSEs of air temperature (T), water vapor mixing ratio (H2O), carbon monoxide (CO) and ozone of the model base case; and (b) the impacts of the SMAP DA on RMSEs of these variables. The B-200 flight paths by day are shown in Figure 1d.

Figure 8: Period-mean (16-28 August 2016) daytime surface O3 from (a) the EPA AQS (filled circles) and CASTNET (triangles) sites; (b) WRF-Chem base case; (d) CAMS; and (e) GFDL AM4. (c) shows the impact of the SMAP DA on WRF-Chem modeled daytime surface O3. (f) indicates stratospheric influences on daytime surface O3 based on the AM4 stratospheric O3 tracer output.
Figure 9: Box-and-whisker plots of WRF-Chem daytime O\(_3\) responses to (a;c) the SMAP DA; and (b;d) updating anthropogenic emissions from NEI 2014 to NEI 2016 beta. (a-b) and (c-d) show O\(_3\) changes at the surface (only for terrestrial model grids, 68% of all model grids) and at ~400 hPa (in all model grids), respectively. Blue text in (a) are spatial correlation coefficients between WRF-Chem daily daytime 2 m air temperature changes and O\(_3\) changes due to the SMAP DA. Note the different Y-axis ranges.

Figure 10: Period-mean (16-28 August 2016) daily maximum 8-h average (MDA8) surface O\(_3\) from (a) WRF-Chem base case and (d) the EPA AQS (filled circles) and CASTNET (triangles) sites. The impact of the SMAP DA on WRF-Chem MDA8 O\(_3\) and the associated RMSE changes are shown in (b) and (e), respectively. The benefit of using NEI 2016 beta instead of NEI 2014 is indicated in (c;f).
Figure 11: Period-mean (16-28 August 2016) daytime O$_3$ in the upper troposphere (i.e., the model levels close to 400 hPa) from (a) CAMS; (b) GFDL AM4; and (d) WRF-Chem base case. (g) shows the impact of the SMAP DA on WRF-Chem modeled daytime O$_3$ in the upper troposphere, and (c) indicates the stratospheric influences on O$_3$ at these altitudes based on the AM4 stratospheric O$_3$ tracer output. Period-mean daytime CO and NO$_2$ from WRF-Chem base case as well as their responses to the SMAP DA are shown in (e;h) and (f;i), respectively.
Figure 12: (a;e) \( \text{O}_3 \) and (b;d;f) impacts of emission changes on \( \text{O}_3 \) from: (a-b) WRF-Chem at ~400 hPa, during the daytimes of 16-28 August 2016; (c-d) the Composition-Integrated Forecasting System (C-IFS) at the surface, during all times of August 2010; and (e-f) the C-IFS at ~400 hPa, during all times of August 2010. These C-IFS simulations were performed at 0.7°×0.7° in support of the HTAP2 (Huang et al., 2017a). “NA” in (d) stands for “North American”.

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