Simulations of Lightning-Generated NOx for Parameterized Convection in the WRF-Chem model

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ABSTRACT: Production of nitrogen oxides (NO_x) by lightning is an important precursor for ozone in the upper troposphere. In this study, the prediction of lightning flash rates and lightning-generated NO_x in the Weather and Research Forecasting model coupled with Chemistry (WRF-Chem) is evaluated using data from the Deep Convective Clouds and Chemistry (DC3) field campaign. The WRF-Chem simulations are performed at grid spacings of 15 km where convection is parameterized. Thus, lightning flash rate is predicted using the Price and Rind (1992) parameterization, which is based on cloud-top height and is predicted by the level of neutral buoyancy determined in the convective parameterization. By comparing the predicted flash rate to the Oklahoma Lightning Mapping Array data for specific DC3 case studies, we found for the May 29, 2012 severe storm in northern Oklahoma that the lightning parameterization needed to be adjusted by limiting the flash rate location to regions with high cloud condensate content, in order to better match the horizontal spatial distribution and magnitude of observed flash rates. Comparison of predicted NO_x mixing ratios in the anvil region of the storm showed that the predicted NO_x is 1 to 1.5 times greater than aircraft observations. However, comparison of predicted concentrations to aircraft data collected in the convective outflow (over western North Carolina) 20-22 hours after active convection showed that modeled NO_x had similar values to observations.

INTRODUCTION

Thunderstorms affect the distribution of chemical constituents in the troposphere by several processes. Rapid vertical transport in convective storm cores brings boundary layer air rich in carbon monoxide (CO), and volatile organic compounds (VOCs) from both anthropogenic and biogenic sources to the upper troposphere (UT). Combining this convective outflow air with elevated mixing ratios of nitrogen oxides (NO_x = NO + NO_2) produced by lightning allows for ozone production to occur in the upper troposphere where ozone is a radiatively-active gas. In order to predict UT ozone and its climate impact, it is important to be able to simulate the transport, lightning-generated NO_x (LNO_x) and UT ozone production in chemistry transport models. In this study, we focus on the production of NO_x from lightning and the downwind UT production of ozone.

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The lightning flash rate, the vertical and horizontal location of the NO source from lightning, and the amount of NO produced per flash are needed in order to predict LNO_x. Prediction of the lightning flash rate is often based on one or a combination of storm parameters (e.g. Barthe et al., 2010). For cases where the deep convection is represented using a cloud-resolving model (i.e. at grid spacing < 4 km), storm parameters, such as maximum updraft velocity, precipitation ice mass (Deierling et al., 2008), ice water path (Petersen et al., 2005), updraft volume (Deierling and Petersen, 2008), precipitation and non-precipitation ice mass flux product (Deierling et al., 2008), mid-level graupel mass flux (McCaul, 2009), and cloud top height (Williams, 1985), can be used to predict the flash rate in the storm. However, many of these parameters are not available (or erroneously represented) in model configurations that parameterize convection. When convection is parameterized, the flash rate can be predicted by storm parameters such as cloud top height, the upward cloud mass flux (Allen and Pickering, 2002), the convective precipitation rate (Meijer et al., 2001), and a combination of updraft velocity and cloud thickness (Grewe et al., 2001). These storm parameters must be obtained from the convective parameterization that is used.

Here, we evaluate the prediction of lightning flash rate in a regional-scale chemistry transport model that parameterizes convection and predicts flash rate based on the commonly used cloud top height method (Pickering et al., 1998). The May 29, 2012 Deep Convective Clouds and Chemistry (DC3) case is used for the evaluation. This severe storm in northern Oklahoma was observed by ground-based radar and lightning mapping arrays (LMAs), as well as weather balloon radio-soundings and balloon-borne electric field monitors. Three aircraft, the NASA DC-8, NSF/NCAR GV, and DLR Falcon, sampled the inflow and UT convective outflow regions to obtain the chemical composition of these regions.

MODEL DESCRIPTION AND CONFIGURATION

Model Description and Configuration

The Weather Research and Forecasting model (Skamarock et al., 2008) coupled with Chemistry (Grell et al., 2005) version 3.5.1 is used to simulate the meteorology and chemistry over most of North America (Figure 1) from 1200 UTC 29 May to 0000 UTC 31 May 2012. There are 415 x 325 grid points in the west-east and south-north directions, respectively, for the 15 km horizontal grid spacing domain. The vertical coordinate has 39 levels from the surface to 50 hPa. The vertical grid spacing near the surface is ~60 m, for 1-3 km altitudes it is 200-400 m, and for 5-13 km it is 550-600 m.

The initial conditions for the meteorology variables are from the Data Assimilation Research Testbed (DART) used during the DC3 field campaign. Boundary conditions are provided by the NCEP GFS analysis (http://rda.ucar.edu/datasets/ds083.2/), which has a 6 hourly time resolution and 1° x 1° spatial resolution. Winds, potential temperature, pressure, water vapor, and condensed water (i.e., cloud particles), tracer variables, and chemistry species are integrated forward in time using a Runge-Kutta integration method. The moisture variables, tracers, and chemistry species are advected using a monotonic scheme (Wang et al., 2009).

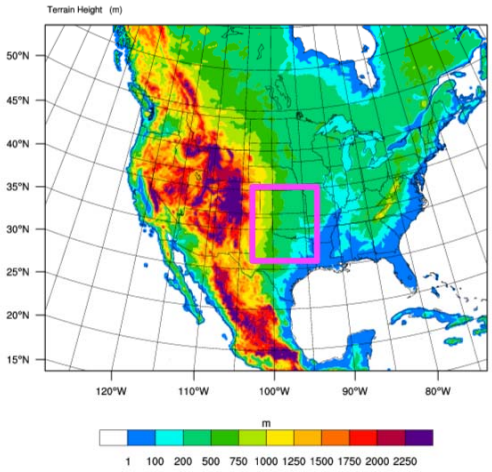

Figure 1. Model domain for the WRF-Chem simulations displaying the terrain height over the continental U.S. The magenta box marks the region for the location of the 29 May 2012 DC3 storm case shown in the subsequent figures.

Cloud physics are computed with the Morrison et al. (2008) double moment parameterization. This scheme predicts both mass mixing ratios and number concentrations for cloud water, rain, cloud ice, snow, and graupel. The graupel category has hail characteristics for this case study of a severe convective storm. The Grell-3 convective parameterization known as G3, which is an improved version of the parameterization described by Grell and Devyeni (2002), is used to represent subgrid convection, convective transport of tracers and chemical constituents, and wet deposition from subgrid convection. The planetary boundary layer parameterization used in the simulation is the Mellor-Yamada-Janjic scheme (Janjic, 2002). At the surface, the NOAH land surface model (Chen and Dudhia, 2001) is employed. For heating rates, the Rapid Radiative Transfer Model scheme (Chou and Suarez, 1994) is used for both short wave and long wave radiation.

Lightning flash rates are predicted using the scheme outlined by Wong et al. (2013) who follow Price and Rind (1992). This scheme uses the level of neutral buoyancy (LNB), determined in the G3 convective parameterization, to find the cloud top of the storm. Wong et al. (2013) set the cloud top height to be the LNB minus 2 km, but we simply use the LNB as cloud top height. The lightning flash rate is found from the cloud top height above ground level using a power-law relation with the power of 4.9 (Price and Rind, 1992). Then the total flash rate is adjusted based on the grid spacing. Wong et al. (2013) found that predicted flash rates using a grid spacing of 36 km compared well with NLDN observations that were scaled via the Boccippio et al. (2001) intracloud to cloud-to-ground flash ratio, but predicted flash rates using a 12 km grid spacing matched NLDN observations only when the prediction was scaled by $(12)^2/(36)^2$. The NO emission is set to 500 moles per flash and is placed vertically following the distributions prescribed by Ott et al. (2010). Wong et al. (2013) evaluated the flash rates using the parameterized convection scheme over the continental U.S. for the summer of 2006. They found that the integrated flash count is consistent with observations when model biases in convection are taken into account. However, their evaluation was focused over the central U.S. (30°-45°N and 80°-105°W), comparing flash counts between NLDN observations and model results, and did not assess the ability of the flash rate scheme for individual convection events.

The chemistry mechanism used in the simulations is the Model for Ozone and Related chemical Tracers (MOZART) version 4 (Emmons et al., 2010) for gas-phase chemistry and the GOCART mass

mixing ratios for aerosols (Pfister et al., 2011). The fast Tropospheric Ultraviolet-Visible scheme (Tie et al., 2003) is used to calculate photolysis rates. The chemical initial and boundary conditions are from the global chemistry transport model MOZART-4 (Emmons et al., 2010). Anthropogenic emissions are for a typical summertime weekday based on the 2011 National Emission Inventory from the Environmental Protection Agency. The Model for Emissions of Gases and Aerosols from Nature (MEGANv2.04; Guenther et al., 2006) describes the biogenic emissions based on local temperature and solar radiation as well as climatological soil moisture, leaf area index, and vegetation speciation. Fire emissions are produced with the Fire Inventory of NCAR (FINN) model (Wiedinmyer et al., 2011), which uses fire count data from MODIS. The fire emissions are distributed vertically using a plume rise algorithm (Freitas et al., 2007).

RESULTS

Storm Morphology and Lightning Flash Rate

Although the WRF-Chem simulation parameterized convection, cloud particle mixing ratios for the predicted hydrometeors of cloud water, rain, ice, snow, and hail also depicted the storm of interest. Therefore, the simulated radar reflectivity can be computed and compared to the observed reflectivity from the NEXRAD radars (Figure 2). The storm initiated at 2115 UTC 29 May and by 0000 UTC 30 May developed into a multicell severe storm. The observed maximum reflectivity at 0100 UTC 30 May shows a line of several intense storm cells with an extensive forward anvil in which additional storm cells developed (Figure 2a). At this time, a left-moving convective storm that initiated over the Red River to the south (Oklahoma-Texas border) was beginning to merge with the north Oklahoma storm. Note, that the convection south of 34.8°N is not included in the observed composite reflectivity. The WRF-Chem

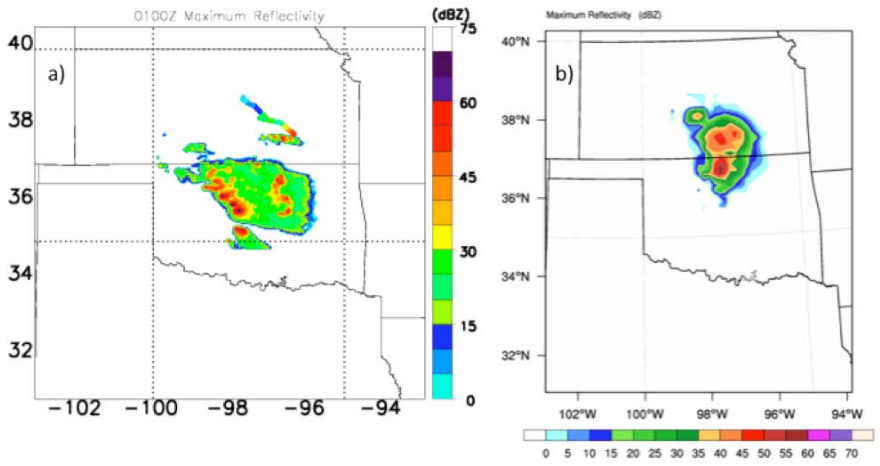

Figure 2. a) Observed maximum radar reflectivity from NEXRAD radars and b) simulated maximum radar reflectivity at 0100 UTC 30 May 2012. The observed composite radar reflectivity (courtesy Cameron Homeyer) is restricted to the 34.8 to 38.5°N region.

simulation produced a storm along the Oklahoma-Kansas border (Figure 2b). At 0100 UTC 30 May, the simulated storm is further north of the observed storm, and does not have as extensive of an anvil region. Nevertheless, the simulated storm is representative of the observations in terms of similar storm size, similar reflectivities of ~50 dBZ in the storm cores, and similar evolution moving from northern Oklahoma to southeast Oklahoma by 0600 UTC 30 May.

The flash rate prediction is compared to observations from the Oklahoma lightning mapping array (LMA), which measures total lightning VHF signals. The predicted flash rates using the Wong et al. (2013) approach are spread over a much wider region (Figure 3) than the main locations of the storms (Figure 2) and the flash rate magnitude is very low compared to observations. In order to restrict the lightning flash rates to the storm locations, an additional condition that the maximum total condensate in the grid column must be greater than 0.5 g kg^{-1} was implemented (Figure 3c). Further, the flash rate prediction was increased by a factor of 5 in order to match the magnitude of flashes measured for the 29 May storm. These changes allowed the predicted flash rate to be on the same order as observed by both the Oklahoma LMA and NLDN flash rates adjusted from the measured CG flashes to a total flash rate based on the Boccippio et al. (2001) climatology (Figure 3d).

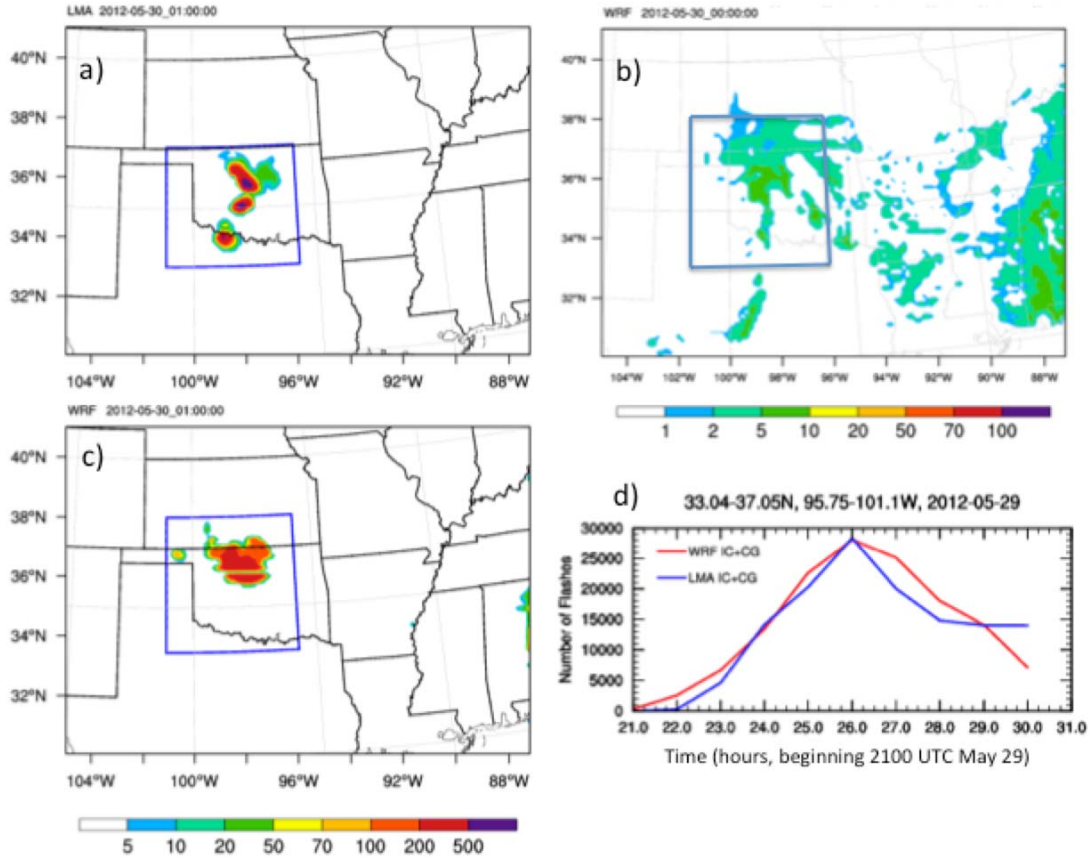

Figure 3. Hourly flash rate for 0100 UTC from a) the LMA observations, b) the WRF-Chem simulation as described in Wong et al. (2013), and c) the WRF-Chem simulation where flash rates are restricted to regions where the

maximum total condensate in the grid column exceeds 0.5 g kg^{-1}. In c) the flash rate has also been increased by a factor of 5. d) Summation of flash rates in the areas marked by the boxes in a-c) as a function of time. LMA data courtesy of Eric Bruning and Don MacGorman.

Chemistry near the Storm

To produce O_3 in the aging convective outflow plume, chemical reactions involving NO_x, hydrogen oxides, which are produced by carbon monoxide (CO), methane (CH_4), formaldehyde (CH_2O), and hydrogen peroxide (H_2O_2), and sunlight (and H_2O) must occur. Thus, the convective transport of all these chemical constituents should be evaluated. The production of NO_x from lightning can be assessed by comparing WRF-Chem predicted NO_x in the inflow and outflow regions of the storm to the aircraft observations. The NASA DC-8 aircraft sampled the air within and just above the boundary layer to the southeast and east of the storm. Mixing ratios of NO were measured using a chemiluminescence technique (Ryerson et al., 2000) and NO_2 mixing ratios were measured using thermo dissociation-laser induced fluorescence (TD-LIF) (Wooldridge et al., 2010) on the DC-8. The NSF/NCAR GV aircraft sampled NO and NO_2 by chemiluminescence (Ridley and Grahek, 1990; Ridley et al., 1992) in the upper troposphere convective outflow. The DC-8 also sampled in the convective outflow of the storm. In the boundary layer, the predicted NO_x mixing ratios are 200-700 pptv, which agrees well with observations (Figure 4a). Predicted NO_x mixing ratios at 11 km altitude (Figure 4b) reach 2-5 ppbv in the storm outflow. To the north of the storm, NO_x mixing ratios are ~200 pptv (an order of magnitude smaller than in the convective outflow) and to the south of the storm NO_x mixing ratios are less than 200 pptv. The aircraft observations of NO_x have similar magnitudes as to what is predicted, although the WRF-Chem simulation may be overestimating peak NO_x values. Other species in the convective outflow region show that CO is ~20 ppbv too high because the boundary layer CO mixing ratios are also too high. WRF-Chem formaldehyde

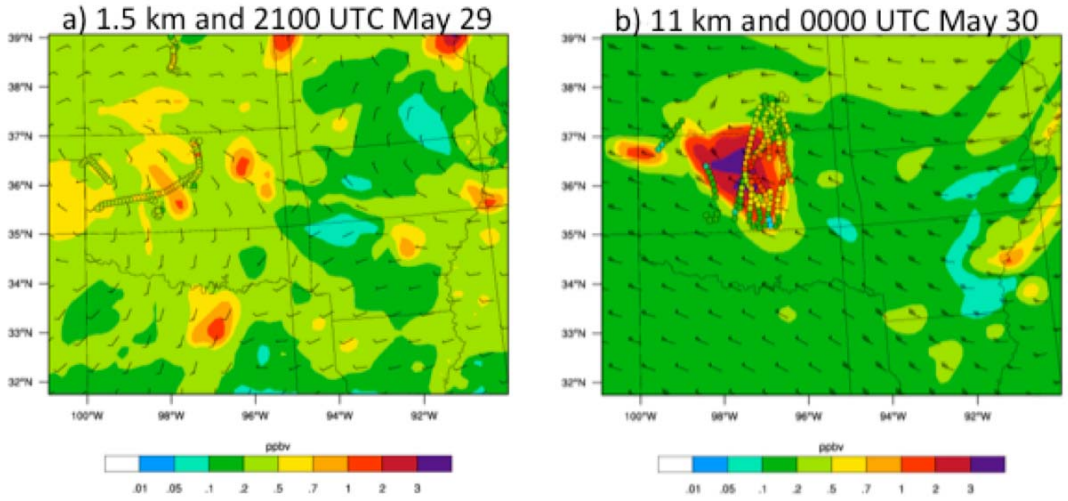

Figure 4. a) Model predicted (color shading) and observed (filled circles) NO_x mixing ratios. The model results are instantaneous results at a) 1.5 km, 2100 UTC 29 May and b) 11 km altitude, 0000 UTC 30 May. The observations are from the DC-8 and GV aircraft obtained for a) below 2 km altitude and b) within one hour of 0000 UTC and within 1 km of 11 km altitude. Observations courtesy of Ryerson, Pollack, Peischl (all NOAA/ESRL), Cohen, Nault (UC-Berkeley), and Weinheimer, Montzka, Flocke (NCAR).

mixing ratios of 200-1000 pptv were predicted for in the convective outflow, while 500-2000 pptv were measured. Ozone mixing ratios in the convective outflow region were predicted to be 60-90 ppbv and were observed to be 70-90 ppbv. In summary, the transport and production of NO_x from lightning produces mixing ratios similar or slightly higher than the NO_x measured by the aircraft, but CO is overpredicted and formaldehyde is underpredicted. The NO_x, CO and CH_2O will affect the ozone production in the convective outflow plume as it travels downwind.

Chemistry in the Downwind Plume

The NASA DC-8 and NSF/NCAR GV aircraft flew on the afternoon of 30 May 2012 to the same convective outflow plume that was sampled the previous day in Oklahoma. The downwind plume was located over eastern Tennessee and western North Carolina. Evidence of O_3 production during the 20 hours since the plume exited convection was seen by the high O_3 mixing ratios of over 90 ppbv (Figure 5). The WRF-Chem simulation extended to 00 UTC 31 May so that the O_3 production in the convective plume could be evaluated. At 2100 UTC 30 May, the WRF model places the convective outflow plume further west of the actual location (Figure 5). The modeled convective plume most directly connected to the 0000 UTC north Oklahoma region resided over eastern Tennessee (which can be compared with the observed plume over Tennessee-North Carolina). WRF-Chem O_3 mixing ratios over eastern Tennessee are 90-100, which are within 10 ppbv of observations. The WRF-Chem NO_x mixing ratios for the same region are ~1 ppbv and CO ~125 ppbv. Observations of NO_x and CO are 1-2 ppbv and 110 ppbv, respectively. Thus, WRF-Chem appears to reasonably represent the O_3 production in the convective outflow plume.

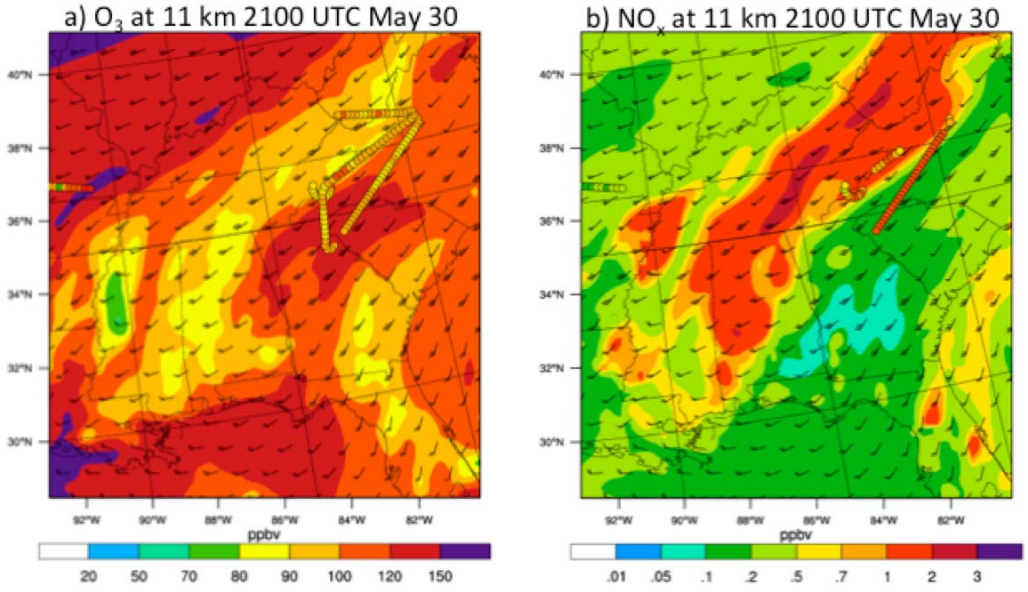

Figure 5. a) Ozone and b) NOx mixing ratios at 11 km altitude for 2100 UTC May 30, 2012 predicted by the WRF-Chem model. Dots are observations from the GV aircraft within 1 km of 11 km altitude.

CONCLUSIONS

WRF-Chem at parameterized convection scales (Δx = 15 km) successfully simulated the 29 May 2012 DC3 case study of a severe storm in northern Oklahoma. The lightning flash rate parameterization, implemented by Wong et al. (2013) and based on Price and Rind (1992), was evaluated for this case study. It was found that further refinement of the flash rate parameterization was needed. Specifically, the prediction of flash rate needed to be restricted to areas where the resolved total cloud particle mixing ratio was greater than 0.5 g kg^{-1}. The number of flashes also needed to be increased by a factor of 5 in order to match flash counts made by the Oklahoma lightning mapping array.

Evaluation of the convective transport and lightning-generated NO_x showed that NO_x in the convective outflow was well predicted, but CO mixing ratios were overpredicted because of high CO in the boundary layer. The chemical aging of the convective plume was simulated for another 24 hours and compared to aircraft observations taken over the southern Appalachia. The WRF simulation placed the convective plume 100-200 km west of the measurement region. By comparing the WRF-Chem convective plume composition to the aircraft measurements, it was found that the increase of O_3 from 70 ppbv in the storm outflow over Oklahoma to 90-100 ppbv over the southern Appalachia was reasonably represented by WRF-Chem.

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