The Deep Convective Clouds and Chemistry (DC3) field campaign provided a unique set of observations to further investigate the role lightning and lightning-generated nitrogen oxides (LNO\(_x\)) have on the composition of the upper troposphere. With the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem), a cloud-resolved simulation of the 29-30 May 2012 severe supercell system investigated 18 flash rate parameterization schemes (FRPSs), the mean LNO\(_x\) production flash\(^{-1}\), and the transport and distribution of other trace gases.

Most of the observed storm’s meteorological and chemical conditions were well represented when the model included convective damping and lightning data assimilation techniques. Newly-developed FRPSs based on DC3 radar observations and Lightning Mapping Array (LMA) data are implemented in the model, along with previously developed schemes from the literature. The schemes are based on relationships between lightning and various kinematic, structural, and microphysical thunderstorm characteristics available in the model. The results suggest the simulated graupel and
snow/ice hydrometeors require scaling factors to more closely represent proxy observations. The model flash rates generated over the simulation period are compared with LMA observations. Thirteen FRPSs overpredicted flashes by > 100%. Generally, FRPSs based on storm kinematics and structure (particularly updraft volume) perform slightly better than schemes based on hydrometeors. However, the upward cloud ice flux FRPS best represents the observed lightning.

The 10 WRF-Chem simulations included one run with no LNO$_x$ and nine runs with different LNO$_x$ production scenarios. The simulated CO and O$_3$ are within 1% and 3% of aircraft observations, respectively, when compared with one model layer lower, which suggests the model slightly underestimates the convective transport. A LNO$_x$ production scenario of 82 moles flash$^{-1}$ best represents the observed NO$_x$ mixing ratios in anvil outflow when combined with the observed flash channel vertical profiles and intracloud to cloud-to-ground ratios. This estimate is smaller than the mean 250 moles NO flash$^{-1}$ suggested for a typical thunderstorm, but within the lower end of the estimated range (33-660 moles fl$^{-1}$). Analysis of the convective outflow using observations made 12-24 hours downwind indicates the mean daytime photochemical O$_3$ production rate is about 1.6 ppbv hour$^{-1}$. 
AN INVESTIGATION OF THE PARAMETERIZED PREDICTION OF LIGHTNING IN CLOUD-RESOLVED CONVECTION AND THE RESULTING CHEMISTRY

by

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Dissertation submitted to the Faculty of the Graduate School of the University of Maryland, College Park in partial fulfillment of the requirements for the degree of Doctor of Philosophy

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<td>°C</td>
<td>degrees Celsius</td>
</tr>
<tr>
<td>2D</td>
<td>two-dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>three-dimensional</td>
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<tr>
<td>35EV</td>
<td>35 dBZ echo volume</td>
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<tr>
<td>45WS</td>
<td>45&lt;sup&gt;th&lt;/sup&gt; Weather Squadron</td>
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<tr>
<td>ACTIVE</td>
<td>Aerosol and Chemical Transport in Tropical Convection</td>
</tr>
<tr>
<td>AMMA</td>
<td>African Monsoon Multidisciplinary Analysis</td>
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<tr>
<td>AMU</td>
<td>Applied Meteorology Unit</td>
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<tr>
<td>CAPE</td>
<td>convective available potential energy</td>
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<tr>
<td>CCAFS</td>
<td>Cape Canaveral Air Force Station</td>
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<td>CG</td>
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<td>CO&lt;sub&gt;2&lt;/sub&gt;</td>
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<td>Colorado State University</td>
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<td>cloud top height</td>
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<tr>
<td>DART</td>
<td>Data Assimilation Research Testbed</td>
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<td>dBZ</td>
<td>decibels of reflectivity</td>
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<tr>
<td>DMSP</td>
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<tr>
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<td>GFS</td>
<td>Global Forecasting System</td>
</tr>
<tr>
<td>GLM</td>
<td>Geostationary Lightning Mapper</td>
</tr>
<tr>
<td>GOCART</td>
<td>Goddard Chemistry Aerosol Radiation and Transport</td>
</tr>
<tr>
<td>GOES-R</td>
<td>Geostationary Operational Environmental Satellite R-Series</td>
</tr>
<tr>
<td>GV</td>
<td>Gulfstream-V</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>H₂O₂</td>
<td>hydrogen peroxide</td>
</tr>
<tr>
<td>HNO₃</td>
<td>nitric acid</td>
</tr>
<tr>
<td>HYSPLIT</td>
<td>Hybrid Single-Particle Lagrangian Integrated Trajectory</td>
</tr>
<tr>
<td>hPa</td>
<td>hectoPascals</td>
</tr>
<tr>
<td>HRRR</td>
<td>High-Resolution Rapid Refresh</td>
</tr>
<tr>
<td>IC</td>
<td>intracloud</td>
</tr>
<tr>
<td>IC:CG</td>
<td>intracloud to cloud-to-ground ratio</td>
</tr>
<tr>
<td>ICEFLUX</td>
<td>upward cloud ice flux</td>
</tr>
<tr>
<td>IMFP</td>
<td>ice mass flux product</td>
</tr>
<tr>
<td>IOP</td>
<td>intensive operational period</td>
</tr>
<tr>
<td>ISCCP</td>
<td>International Satellite Cloud Climatology Project</td>
</tr>
<tr>
<td>ISS</td>
<td>International Space Station</td>
</tr>
<tr>
<td>IWP</td>
<td>ice water path</td>
</tr>
<tr>
<td>KPP</td>
<td>Kinetic PreProcessor</td>
</tr>
<tr>
<td>KSC</td>
<td>Kennedy Space Center</td>
</tr>
<tr>
<td>LCL</td>
<td>lifting condensation left</td>
</tr>
<tr>
<td>LDA</td>
<td>lightning data assimilation</td>
</tr>
<tr>
<td>LDAR</td>
<td>Lightning Detection and Ranging</td>
</tr>
<tr>
<td>LF</td>
<td>low frequency</td>
</tr>
<tr>
<td>LINET</td>
<td>lightning detection network</td>
</tr>
<tr>
<td>LIS</td>
<td>Lightning Imaging Sensor</td>
</tr>
<tr>
<td>LMA</td>
<td>lightning mapping array</td>
</tr>
<tr>
<td>LNOₓ</td>
<td>lightning-generated nitrogen oxides</td>
</tr>
<tr>
<td>LNOM</td>
<td>Lightning Nitrogen Oxides Model</td>
</tr>
<tr>
<td>LSM</td>
<td>land surface model</td>
</tr>
<tr>
<td>LTG3</td>
<td>McCaul blended lightning threat method</td>
</tr>
<tr>
<td>M</td>
<td>third body</td>
</tr>
<tr>
<td>MCS</td>
<td>mesoscale convective system</td>
</tr>
<tr>
<td>MGAUS</td>
<td>Mobile GPS Advanced Upper-Air Sounding System</td>
</tr>
<tr>
<td>MLCAPER</td>
<td>mixed-layer convective available potential energy</td>
</tr>
<tr>
<td>MOZART</td>
<td>Model for Ozone and Related chemical Tracers</td>
</tr>
<tr>
<td>MSFC</td>
<td>Marshall Space Flight Center</td>
</tr>
<tr>
<td>MYJ</td>
<td>Mellor-Yamada-Janjic</td>
</tr>
<tr>
<td>N</td>
<td>nitrogen</td>
</tr>
<tr>
<td>NAM-ANL</td>
<td>North American Mesoscale Analysis</td>
</tr>
<tr>
<td>NARR</td>
<td>North American Regional Reanalysis</td>
</tr>
<tr>
<td>NASA</td>
<td>National Aeronautics and Space Administration</td>
</tr>
<tr>
<td>NCAPE</td>
<td>normalized convective available potential energy</td>
</tr>
<tr>
<td>NCAR</td>
<td>National Center for Atmospheric Research</td>
</tr>
<tr>
<td>NCEP</td>
<td>National Centers for Environmental Prediction</td>
</tr>
<tr>
<td>NEXRAD</td>
<td>Next Generation Radar</td>
</tr>
<tr>
<td>NLDN</td>
<td>National Lightning Detection Network</td>
</tr>
<tr>
<td>N₂</td>
<td>molecular nitrogen</td>
</tr>
<tr>
<td>NO</td>
<td>nitric oxide</td>
</tr>
<tr>
<td>NO₂</td>
<td>nitrogen dioxide</td>
</tr>
<tr>
<td>NOₓ</td>
<td>nitrogen oxides</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
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<tr>
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</tr>
<tr>
<td>NOAA</td>
<td>National Oceanic and Atmospheric Administration</td>
</tr>
<tr>
<td>NOXP</td>
<td>NOAA X-band polarimetric</td>
</tr>
<tr>
<td>NSSL</td>
<td>National Severe Storms Laboratory</td>
</tr>
<tr>
<td>O₂</td>
<td>molecular oxygen</td>
</tr>
<tr>
<td>O₃</td>
<td>ozone</td>
</tr>
<tr>
<td>OH</td>
<td>hydroxyl radical</td>
</tr>
<tr>
<td>OMI</td>
<td>Ozone Monitoring Instrument</td>
</tr>
<tr>
<td>ONERA</td>
<td>Office Nationale d’Etudes et de Recherches Aerospatiales</td>
</tr>
<tr>
<td>OTD</td>
<td>Optical Transient Detector</td>
</tr>
<tr>
<td>PAN</td>
<td>peroxycetyl nitrate</td>
</tr>
<tr>
<td>PBL</td>
<td>planetary boundary layer</td>
</tr>
<tr>
<td>PIM</td>
<td>precipitation ice mass</td>
</tr>
<tr>
<td>ppbv</td>
<td>parts per billion volume</td>
</tr>
<tr>
<td>pptv</td>
<td>parts per trillion volume</td>
</tr>
<tr>
<td>R</td>
<td>organic group</td>
</tr>
<tr>
<td>RH</td>
<td>hydrocarbon</td>
</tr>
<tr>
<td>RO₂</td>
<td>organic peroxy radical</td>
</tr>
<tr>
<td>RRTMG</td>
<td>Rapid radiative transfer model for General Circulation Models</td>
</tr>
<tr>
<td>SCOUT-O3</td>
<td>Stratospheric-Climate Links with Emphasis on the Upper Troposphere and Lower Stratosphere</td>
</tr>
<tr>
<td>SIP</td>
<td>State Implementation Plan</td>
</tr>
<tr>
<td>SMART</td>
<td>Shared Mobile Atmospheric Research Teaching</td>
</tr>
<tr>
<td>STEPS</td>
<td>Severe Thunderstorm Electrification and Precipitation Study</td>
</tr>
<tr>
<td>STERAO-A</td>
<td>Stratospheric-Tropospheric Experiment: Radiation, Aerosols and Ozone</td>
</tr>
<tr>
<td>TELEX</td>
<td>Thunderstorm Electrification and Lightning Experiment</td>
</tr>
<tr>
<td>TRMM</td>
<td>Tropical Rainfall Measuring Mission</td>
</tr>
<tr>
<td>TROCCINOX</td>
<td>Tropical Convection, Cirrus and Nitrogen Oxides Experiment</td>
</tr>
<tr>
<td>UAH</td>
<td>University of Alabama in Huntsville</td>
</tr>
<tr>
<td>UTC</td>
<td>Coordinated Universal Time</td>
</tr>
<tr>
<td>UV</td>
<td>updraft volume</td>
</tr>
<tr>
<td>UVS</td>
<td>UV for supercells</td>
</tr>
<tr>
<td>VHF</td>
<td>very high frequency</td>
</tr>
<tr>
<td>VII</td>
<td>vertically integrated ice</td>
</tr>
<tr>
<td>VLF</td>
<td>very low frequency</td>
</tr>
<tr>
<td>vts</td>
<td>snow fall speed</td>
</tr>
<tr>
<td>w</td>
<td>vertical velocity</td>
</tr>
<tr>
<td>w_{max}</td>
<td>maximum vertical velocity</td>
</tr>
<tr>
<td>WRF</td>
<td>Weather Research and Forecasting</td>
</tr>
<tr>
<td>WRF-AqChem</td>
<td>Weather Research and Forecasting model coupled with a simple gas and aqueous chemistry module</td>
</tr>
<tr>
<td>WRF-Chem</td>
<td>Weather Research and Forecasting model coupled with Chemistry</td>
</tr>
<tr>
<td>WSR-88D</td>
<td>Weather Surveillance Radar-1988 Doppler</td>
</tr>
<tr>
<td>YSU</td>
<td>Yonsei University</td>
</tr>
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</table>
CHAPTER 1: INTRODUCTION

1.1 Motivation

Lightning prediction is desirable in weather forecasting models and is necessary in chemistry and climate models. Prior to the 1970s the lack of adequate detection techniques made it difficult to analyze global lightning activity or determine relationships between lightning and storm parameters that could be employed in prediction schemes; however, lightning detection instrumentation has evolved over time. The first optical sensor that orbited Earth could only observe lightning at night (Turman, 1978; Orville and Henderson, 1986). Over the next forty years advancements in detection technology (e.g., optical, magnetic direction finding, and time-of-arrival sensors) allowed for improvements in detection efficiency, spatial accuracy, the ability to distinguish between cloud-to-ground (CG) and intracloud (IC) lightning, and three-dimensional (3D) mapping of total lightning activity (Rison et al., 1999; Krehbiel et al., 2000; Christian et al., 2003; Thomas et al., 2004; Cummins and Murphy, 2009; Heckman and Liu, 2010; Liu and Heckman, 2011).

The availability of high-detection-efficiency flash data, together with radar observations or model data, has allowed the development of flash rate parameterization schemes (FRPSs; relationships between lightning activity and thunderstorm characteristics) to estimate lightning flash rates and location. Currently lightning threat forecasts (McCaul et al., 2009; 2011) are being run in operational models to predict lightning flash rate densities in short-range weather forecasts (i.e., 12-72 hours). These models include the National Severe Storms Laboratory (NSSL) Weather Research and
Forecasting (WRF) model (McCaul et al., 2011), the National Oceanic and Atmospheric Administration (NOAA)/National Centers for Environmental Prediction (NCEP) High-Resolution Rapid Refresh (HRRR) model (Wong et al., 2013), the National Center for Atmospheric Research (NCAR) ensemble forecast (Schwartz et al., 2015), and the United Kingdom (UK) Met Office UK-variable resolution (UKV) model (Wilkinson and Bornemann, 2014). Giannaros et al. (2016) evaluated operational lightning forecasts in Central-South Europe using the WRF model with a convective parameterization and FRPS based on cloud top height (Price and Rind, 1992). Such forecasts are beneficial from an operations and public safety perspective for those individuals who are required or plan to spend an extended amount of time outdoors (e.g., construction, lawn care, airports, rocket launch preparations, and recreational activities). In addition to forecasting future lightning activity, FRPSs may be used to reproduce flash rates from past convective events to verify their performance against lightning observations (Barthe et al., 2010; Cummings et al., 2017a), generate model-simulated flash counts in areas where observed lightning data are unavailable, or use observed total lightning activity to estimate storm parameters that are not routinely measured or observed in real-time (e.g., cloud top height, updraft volume, and ice water path). Evaluating FRPS performance through case studies may reveal that some schemes are more representative of a particular latitude band, region, type of convection (e.g., airmass, multicell, and supercell), or time of year than others. If true, models will benefit from capturing the spatial and temporal variation of lightning through the use of FRPSs.

Additionally, FRPSs play a key role in calculating the production of lightning-generated nitrogen oxides (LNOₓ) and provide a means for the LNOₓ production trend to
vary in time within a model. An accurate model replication of the observed flash rate as a function of time would provide researchers with additional details on the chemical influence of LNO$_x$ within and downwind of a thunderstorm. As one of the largest natural sources of nitrogen oxides (NO$_x$ = nitric oxide (NO) + nitrogen dioxide (NO$_2$)), lightning accounts for roughly 5±3 Tg (N) yr$^{-1}$, or 10-15%, of the total NO$_x$ budget (Schumann and Huntrieser, 2007). Other major sources of tropospheric NO$_x$ include fossil fuel combustion, biomass burning, and microbial activity in soils (Schumann and Huntrieser, 2007). While the lower troposphere is mainly dominated by surface emissions, especially those due to human activity (Zhang et al., 2003), lightning is the largest source of NO$_x$ in the upper troposphere, where most LNO$_x$ is present above an altitude of 7 km (Martin et al., 2007). In this portion of the atmosphere, NO$_x$ has a longer lifetime and a large influence on ozone (O$_3$) (e.g., Allen et al., 2010), a significant greenhouse gas (Lacis et al., 1990), with implications for indirectly having a positive radiative forcing on the climate. Following a convective event, enhancements in O$_3$ can be found downwind within the thunderstorm outflow (DeCaria et al., 2005; Ott et al., 2010; Martini et al., 2011). The enhancements in O$_3$ influence its radiative forcing, which maximizes near the tropopause. Nitrogen oxides are also important because they increase the hydroxyl radical (OH) concentration, which is known as the “detergent of the atmosphere” because of its ability to react with and remove various trace gas species (e.g., carbon monoxide (CO), carbon dioxide (CO$_2$), hydrocarbons, and NO$_2$) from the atmosphere. If a future climate features more lightning, the resulting greater OH will decrease the methane (CH$_4$) lifetime (Fiore et al., 2006), and have a negative forcing on tropospheric radiative forcing of climate.
Many factors affect the uncertainty of LNO\textsubscript{x} production, including the variation in the type, length, energy, peak current, and number of lightning flashes (Price et al., 1997), as well as the location and strength of the convection. Although other natural and anthropogenic NO\textsubscript{x} sources may have uncertainty ranges that are similar to or greater than that associated with lightning, the potential feedback mechanisms between lightning and surface temperatures makes narrowing the uncertainty range of LNO\textsubscript{x} critical (Schumann and Huntrieser, 2007). In addition, a better understanding of the global LNO\textsubscript{x} budget would be beneficial for properly modeling variations and trends in NO\textsubscript{x} and O\textsubscript{3} and in analyzing the influence of other NO\textsubscript{x} sources, such as the injection of stratospheric NO\textsubscript{x} and aircraft emissions (Bond et al., 2001; Zhang et al. 2000).

Therefore, model-simulated lightning flash rates have the ability to enhance our knowledge of the role of LNO\textsubscript{x} in global climate-chemistry models (e.g., Banerjee et al., 2014; Liaskos et al., 2015) and regional air quality models (e.g., Allen et al., 2012). Incorporation of these FRPSs in past and future model simulations is also valuable for furthering our understanding of the potential impacts of climate change on convection and the resulting lightning activity (Reeve and Toumi, 1999; Petersen and Rutledge, 2001; Williams, 2005; Price, 2009; Romps et al., 2014; Magi, 2015).

For FRPSs to be truly helpful to the atmospheric chemistry, lightning, and modeling communities, it is important to understand if there is variability in scheme performance by latitude zone, region, and storm type, and how schemes perform at different resolutions (e.g., cloud-resolved and global). To do this, thunderstorms from different environments and of differing updraft strength, size, and severity must be analyzed. In a study of storms over northern Alabama, Mecikalski and Carey (2017)
showed that the altitude and reflectivity where flashes initiate and propagate vary as a function of storm type (i.e., multicell, mesoscale convective systems, and supercell), thereby showing the importance of differentiating between various storm types when performing lightning-related studies. Barthe and Barth (2008) and Barthe et al. (2010) emphasize the need for modeling numerous convective case studies. Without understanding these variations, the true potential of the relationships between model storm parameters and total lightning activity will not be fully understood and the community will not be able to expand our knowledge of the impact of lightning in other areas (e.g., LNO$_x$, air quality, and climate).

By building on the successes of previous experiments, the Deep Convective Clouds and Chemistry (DC3) field campaign made simultaneous observations of the microphysics, dynamics, chemistry, and lightning within convective systems, which was something that had been lacking in prior field experiments (Barthe and Barth, 2008), in addition to post-convection observations of the outflow plume (Barth et al., 2015). The availability of this large, cohesive dataset provides the necessary ground and upper air measurements required for my further analysis of the electrical and chemical relationships within thunderstorms.

1.2 Objectives

The objectives of my research are to evaluate previously published and recently developed FRPSs in a cloud-resolved WRF model simulation of the 29-30 May 2012 Oklahoma severe supercell system (Bela et al., 2016; DiGangi et al., 2016; Pollack et al., 2016; Li et al., 2017) observed during DC3 (Barth et al., 2015) and to determine which scheme or schemes perform the best in representing the observed lightning flashes. To
address how LNO$_x$ and other trace gases are influenced by convective transport and lightning flash rates, additional cloud-resolved simulations will be run using the WRF model coupled with Chemistry (WRF-Chem). The scientific questions that will be addressed include:

1. How does FRPS performance vary between schemes based on the model-simulated total flashes and flash rates?
2. Can a microphysically-based FRPS produce realistic predictions of flash rate in a cloud-resolved model?
3. How do observed versus default model vertical distributions of flash channel lengths and IC:CG ratios affect the model-simulated LNO$_x$ and other trace gases in the anvil outflow?
4. Does LNO$_x$ production per flash in a high flash rate Oklahoma storm vary from other midlatitude storms?
5. How do flash extent and flash energy relate to flash rate for an Oklahoma severe supercell system in comparison to other observed storms?
6. Is there a relationship between flash rate and LNO$_x$ production per flash?
7. By how much is the upper tropospheric chemistry (e.g., O$_3$) in convective outflow affected by LNO$_x$?

Chapter 2 will discuss the processes involved in generating lightning, how lightning detection instrumentation has evolved over time, and how models can be used to predict lightning. The formation of LNO$_x$ will be reviewed in Chapter 3, along with a
description of the available parameterization schemes and the chemical interactions that involve NO\textsubscript{x}. An overview of the DC3 field experiment and the 29-30 May 2012 Oklahoma severe supercell system is provided in Chapter 4, including the available instrumentation and WRF model preparation. Chapter 5 will describe the WRF-Chem model set-up used to simulate the observed 29-30 May convective event and the modifications made to the model (e.g., convective damping, observation-based LNO\textsubscript{x} placement, etc.). Chapter 6 reviews the methodologies and analyses used to investigate the model’s performance in simulating the observed meteorological features and predicting lightning flash rates with FRPSs. The observed and model-simulated trace gases will be analyzed in Chapter 7 with a specific focus on the best LNO\textsubscript{x} production scenario that represents the case study, as well as the relationships between lightning characteristics and LNO\textsubscript{x} production. Chapter 8 will investigate how the trace gases observed by the aircraft in the storm anvil evolved in the outflow plume between the anvil and a flight approximately 24 hours downwind. Chapter 9 summarizes the key findings and Chapter 10 will provide a discussion of future work.

Chapters 2 and 6, along with introductory material from Chapters 1, 4, and 5 form the Cummings et al. (2017a) paper that has been submitted to the *Journal of Geophysical Research – Atmospheres*. The Cummings et al. (2017b) paper in preparation will contain the results in Chapters 7 and 8.
CHAPTER 2: LIGHTNING

2.1 Lightning formation

Lightning typically occurs in association with deep convective clouds, called cumulonimbi, where the cloud top height is at an altitude greater than the freezing level. Due to the tendency for thunderstorms to exhibit cold cloud characteristics, a mixed-phase region often develops, which contains both supercooled droplets and ice particles (Wallace and Hobbs, 2006). Lightning has occasionally been observed in warm clouds whose vertical development does not reach the freezing level.

Currently, there are two theories that attempt to explain the electrical charge distribution within a thunderstorm. According to the precipitation theory, as heavier precipitation, such as graupel and hail, forms and falls through the cloud, collisions occur with the smaller droplets and particles. Upon colliding and rebounding, the smaller and larger hydrometeors exhibit opposite polarities. Generally, graupel and hail gain a negative charge, while a positive charge is given to small droplets and particles. However, the charge received by particles is also dependent on factors such as temperature and riming rate (MacGorman and Rust, 1998; Uman, 2001; MacGorman et al., 2005; Mansell et al., 2005; Lund et al., 2009). Charge separation is achieved as updrafts, downdrafts, and gravity transport the cloud and precipitation particles within the cloud. Although the precipitation theory is more widely accepted, some researchers believe the convection theory is responsible for a thunderstorm’s charge structure. Based on this theory, positive charge is transported from the earth’s surface to the cloud’s interior via updrafts and negative charge is carried by downward motion of the cloud.
boundary from the negative screening layer at the cloud top, along the cloud’s sides, and into the lower cloud interior (MacGorman and Rust, 1998; Uman, 2001).

Following either theory, the electric charge distribution in a thunderstorm generally exhibits a positive dipole structure with a negative charge center in the lower region of the convective cloud and a positive charge center in the upper portion (Figure 1a; MacGorman and Rust, 1998). Sometimes the thunderstorm may display a positive tripole structure, where a second, but smaller, positively charged region is also present near the base of the cloud (Figure 1b). Although atypical, thunderstorms may also exhibit an inverted-polarity structure, where the altitudes of the negative and positive charge regions reverse within the cloud (Figure 1c and 1d; Rust et al., 2005).

Figure 1. Schematic of a (1a) dipole, (1b) tripole, (1c) inverted dipole, and (1d) inverted tripole charge structure within a thunderstorm (from Kuhlman et al., 2006).

The charge separation continues until the air can no longer maintain the strength of the electric field in the storm. The typical electric field within a thunderstorm is less than 200 kV m\(^{-1}\) with a mean of 50 kV m\(^{-1}\) and a maximum of 400 kV m\(^{-1}\) (Price et al., 1997; Stolzenburg et al., 2007). When the critical threshold is reached, a lightning flash occurs. This threshold is dependent on air density and decreases with altitude (Gurevich
and Zybin, 2005). Lightning flashes occur between cloud and ground (CG flashes), between different portions of the cloud (IC flashes), between clouds (cloud-to-cloud flashes), or between cloud and air (Schumann and Huntrieser, 2007). Researchers initially suggested the global lightning flash rate was roughly 100 flashes s\(^{-1}\), but this estimate has decreased in recent years (~46 flashes s\(^{-1}\)) due to satellite observations (Cecil et al., 2014).

Approximately 44,000 thunderstorms occur each day around the globe (Huntrieser et al., 1998), with most lightning occurring over the land versus the ocean (Figure 2). Two theories support this observation. The thermal hypothesis suggests the land surface, which is hotter than the ocean, generates strong lifting necessary to produce a deep mixed-phase region. Over the ocean, clouds contain fewer droplets, but they are larger than in continental clouds. This reduces cloud buoyancy, which decreases updraft strength and limits the vertical development of the mixed-phase region. The aerosol hypothesis suggests the air over land contains more aerosols, which act to reduce cloud droplet size, suppress precipitation, and increase the mixed-phase region (Cooray, 2003; Williams, 2005; Schumann and Huntrieser, 2007).

Thunderstorms form almost every day in the tropics, unlike other regions of the globe (Figure 3; Huntrieser et al., 2011), with the majority of the earth’s lightning occurring within the tropical belt between ±30° latitude (Cooray, 2003; Schumann and Huntrieser, 2007). In the midlatitudes, thunderstorms primarily occur in the spring and summer. With longer days and a higher angle of incoming solar radiation, the land surface is hotter and the overlying air can become unstable. Therefore, lightning is most common in the Northern Hemisphere where a greater percentage of earth’s surface is
composed of land, unlike the Southern Hemisphere, which is largely ocean (Cooray, 2003; Schumann and Huntrieser, 2007). Due to these land surface differences, lightning occurs roughly 1.2 times more often in the Northern Hemisphere summer versus winter (Schumann and Huntrieser, 2007). In the United States, lightning occurs most frequently in the southeast during summer (Zhang et al., 2003). Lightning is not as common during the winter because lifting is primarily at the synoptic scale and there is not as much water vapor available to fully develop the mixed-phase region (Cooray, 2003).

**Figure 2.** Contribution of lightning flashes over land to the total mean flash frequency (land and ocean) by latitude (from Schumann and Huntrieser, 2007). Observations were taken from the OTD from April 1995 to March 2000.

**Figure 3.** Mean annual flash rate detected by LIS and OTD on a high resolution $0.5^\circ \times 0.5^\circ$ grid (from Cecil et al., 2014).
2.2 Evolution of lightning instrumentation

Prior to the 1970s the lack of adequate detection techniques made it difficult to analyze global lightning activity or determine relationships between lightning and storm parameters that could be employed in prediction schemes; however, lightning detection instrumentation has evolved over time. Lightning observations improved spatially with the development of the Defense Meteorological Satellite Program (DMSP). The first optical sensor that orbited Earth onboard DMSP satellite 8531 could only observe lightning at night (Turman, 1978; Orville and Henderson, 1986). Over the next forty years advancements in detection technology (e.g., optical, magnetic direction finding, and time-of-arrival sensors) allowed for improvements in detection efficiency, spatial accuracy, the ability to distinguish between CG and IC lightning, and 3D mapping of total lightning activity (Rison et al., 1999; Krehbiel et al., 2000; Christian et al., 2003; Thomas et al., 2004; Cummins and Murphy, 2009; Heckman and Liu, 2010; Liu and Heckman, 2011).

Observations were first collected for CG, IC, and cloud-to-cloud lightning between ±75° latitude, both day and night, with the launch of the Optical Transient Detector (OTD) on the MicroLab-1 satellite in April 1995 (Christian et al., 2003). Before the OTD mission ended in March 2000, the Lightning Imaging Sensor (LIS) was launched in November 1997 aboard the Tropical Rainfall Measuring Mission (TRMM) satellite. While both OTD and LIS observed lightning based on changes in the optical scene, LIS could observe lightning flashes at a storm-scale resolution, but only between ±38° latitude (Blakeslee et al., 2014; Buechler et al., 2014).
Two-dimensional (2D) ground-based observations are available from several sources. The National Lightning Detection Network (NLDN) was established in 1989 and has gone through several upgrades over the last 25 years. More than 100 sensors make up the network, which uses magnetic direction finding and time-of-arrival techniques to detect the low frequency (LF) and very low frequency (VLF) emissions released by flashes occurring over the continental United States and several hundred kilometers off the coast (LaJoie and Laing, 2008; Orville, 2008; Vaisala, 2014). The NLDN CG flash detection efficiency is ~95%, and approximately 50% of IC flashes are detected, although network improvements are increasing this value (Nag et al., 2011; Holle et al., 2014). The data provides information regarding the time and location of the flash, as well as its polarity, strength, the number of return strokes (multiplicity), 50% location error ellipse, and several other parameters.

The Earth Networks Total Lightning Network (ENTLN) also uses a time-of-arrival method; its sensors use a broad frequency range (1 Hz to 12 MHz) to detect both CG and IC strokes (Liu et al., 2015). The network has over 1,200 sensors deployed globally (Earth Networks, 2017), with the best coverage over the United States. The CG and IC detection efficiency is generally greater than 90% and 50% across the United States, respectively. The CG detection efficiency exceeds 95% east of the High Plains, and the IC detection efficiency increases up to 65% in the West and 95% over portions of the Midwest and East Coast (Liu and Heckman, 2011; Saunders, 2012; Liu et al., 2015). Flashes are generated by grouping strokes that are within 700 ms and 10 km of each other. If the cluster contains a return stroke, it is considered to be a CG flash. The observed data also provide information about polarity and peak current (Liu et al., 2015).
If the detection efficiency for IC flashes is too uncertain, a rough estimate of the number of total lightning flashes observed by a network may be calculated by:

\[
\text{total flashes} = CG \text{ flashes } \times \left(\frac{1}{DE}\right) \times [\text{IC:CG ratio } + 1], \quad (1)
\]

where \( DE \) is a network’s CG detection efficiency and the \( \text{IC:CG ratio} \) is the ratio of intracloud to cloud-to-ground flashes, which may be based on the gridded climatological mean IC:CG ratios over the United States (Boccippio et al., 2001). However, IC:CG ratios vary considerably from storm to storm and during a particular storm.

In the mid-1970s a 3D total lightning location mapping system, called the Lightning Detection and Ranging (LDAR) system, was developed at NASA Kennedy Space Center (KSC) and installed in and around KSC and Cape Canaveral Air Force Station (CCAFS; Starr et al., 1998). The LDAR system was used as a model by lightning researchers at New Mexico Tech as they began designing a new generation of permanent and mobile lightning mapping arrays (LMAs) in the mid-1990s. Currently, LMAs are located in 11 regions across North America: central New Mexico, northeast Colorado, west Texas, Oklahoma, Houston, northern Alabama, northern Georgia, Kennedy Space Center (KSC), Washington D.C., Wallops Island, and Toronto, Canada (Padula and Goodman, 2016). Each network includes multiple stations, which use time-of-arrival sensors to detect the very high frequency (VHF) electromagnetic pulses emitted by a lightning flash. The result is a 3D map of total lightning activity, although the sensors mainly detect IC flashes and the upper segments of CG flashes (Stano et al., 2010). After data processing, the LMA data can provide information about the VHF source density,
flash extent density, flash initiation density, average flash area, and the vertical
distribution of flash channel lengths.

In a continuing effort to improve lightning observations and extend the length of
historical records, the first Geostationary Lightning Mapper (GLM) was launched in
November 2016 onboard the Geostationary Operational Environmental Satellite R-Series
(GOES-R; renamed GOES-16 by NOAA). With the addition of future satellites from the
GOES-R series, continuous monitoring of CG, IC, and cloud-to-cloud lightning flashes
will be provided over the Western Hemisphere from New Zealand to the west coast of
Africa at a spatial resolution of roughly 8 km (Chronis et al., 2008; Goodman et al., 2013;
Buechler et al., 2014). The increased coverage over land and ocean locations will allow
for the quantity, intensity, and variation of lightning activity to be examined with greater
detail, especially areas where lightning monitoring is sparse. In addition, a duplicate of
the LIS instrument was installed on the International Space Station (ISS) in late February
2017. The ISS LIS provides coverage to much higher latitudes (±54° latitude; Blakeslee
et al., 2014) than TRMM LIS (±38° latitude), along with the ability to sample 98% of the
lightning that occurs annually across the globe. The ISS LIS observes lightning at a
given location only during an overpass and with the same field of view as TRMM LIS
(600 km × 600 km). However, the data collected by ISS LIS will be used to help
improve the global lightning climatology and LNO\textsubscript{x} estimates, in addition to many other
scientific applications (Blakeslee and Koshak, 2016).

2.3 Flash rate parameterization schemes
Cloud-resolved models may incorporate explicit electrical schemes to study lightning
activity in thunderstorms (e.g., Helsdon et al., 1992; Mansell et al., 2002; Barthe et al.,
2005; Fierro et al., 2013). The difficulties with using explicit schemes for simulating lightning flashes include the complexity of the electrical activity and the computational cost of modeling the intricate behavior (McCaul et al., 2009). To avoid these difficulties, FRPSs based on storm parameters output by models is a useful way to replicate a thunderstorm’s electrification. However, the schemes are only as good as the model’s ability to predict the location and strength of the convection and the distribution of hydrometeors (Fierro et al., 2013). If the kinematic and microphysical characteristics are inaccurate, the non-inductive charging, which is believed to be the main mechanism for cloud electrification (Takahashi, 1978; Jayaratne et al., 1983; Saunders et al., 1991; Latham et al., 2007; Barthe et al., 2010; Rakov, 2016), will not be properly represented by the proxy parameters (e.g., updraft volume and graupel echo volume). This charging mechanism usually occurs where a strong updraft coincides with the mixed-phase region of the cloud (Zipser and Lutz, 1994; Deierling and Petersen, 2008; Deierling et al., 2008). Here graupel and ice crystals collide and rebound in the presence of supercooled liquid water and are transported by updrafts and gravity to achieve charge separation and eventually lightning initiation (Takahashi, 1978; Saunders et al., 1991; MacGorman and Rust, 1998; Deierling and Petersen, 2008; Basarab et al., 2015). Described below are eighteen FRPSs for predicting total lightning. The schemes are evaluated in our study at a cloud-resolving scale and include those developed prior to and after the DC3 field experiment. The earliest FRPSs were based on kinematic and structural characteristics of thunderstorms, while more recent schemes evolved toward the use of microphysical variables. Table 1 lists each FRPS equation and Table 2 highlights the type of criteria threshold required by each scheme.
Table 1. Flash rate parameterization schemes tested in WRF cloud-resolved simulation of 29-30 May 2012 Oklahoma case study, where f is total flash rate in flashes min⁻¹, FD is flash density in flashes km⁻² day⁻¹, FD_l is flash density over land in flashes m_grid-cell⁻² s⁻¹, and FD_LTG3 is flash density in flashes km⁻² 5-min⁻¹.

<table>
<thead>
<tr>
<th>Flash Rate Parameterization Scheme</th>
<th>Flash Rate Equation (reference)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum vertical velocity (w_max)</td>
<td>( f = 5 \times 10^{-6} \times (w_{\text{max}})^{4.5} ) (Price &amp; Rind, 1992)</td>
</tr>
<tr>
<td>Cloud top height (CTH)</td>
<td>( f = 3.44 \times 10^{-5} \times H^{4.9} ) (Price &amp; Rind, 1992)</td>
</tr>
<tr>
<td>Updraft volume (UV)</td>
<td>( f = 6.75 \times 10^{-11} \times w_{5} - 13.9 ) (Deierling &amp; Petersen, 2008)</td>
</tr>
<tr>
<td>Ice water path (IWP)</td>
<td>( \text{FD} = 33.33 \times \text{IWP} - 0.17 ) (Petersen et al., 2005)</td>
</tr>
<tr>
<td>Precipitation ice mass (PIM)</td>
<td>( f = 3.4 \times 10^{-8} \times p_{m} - 18.1 ) (Deierling et al., 2008)</td>
</tr>
<tr>
<td>Ice mass flux product (IMFP)</td>
<td>( f = 9.0 \times 10^{-15} \times (f_{p} \times f_{np}) + 13.4 ) (Deierling, 2006; Deierling et al., 2008)</td>
</tr>
<tr>
<td>CSU graupel echo volume (CSU GEV)</td>
<td>( f = 7.0 \times 10^{-2} \times \text{GEV} ) (Basarab et al., 2015)</td>
</tr>
<tr>
<td>CSU 35dBZ echo volume (CSU 35EV)</td>
<td>( f = 7.2 \times 10^{-2} \times 35EV ) (Basarab et al., 2015)</td>
</tr>
<tr>
<td>CSU precipitation ice mass (CSU PIM)</td>
<td>( f = 1.2 \times 10^{-7} \times \text{PIM} ) (Basarab et al., 2015)</td>
</tr>
<tr>
<td>UAH graupel echo volume (UAH GEV10)</td>
<td>See Carey et al. (2015)</td>
</tr>
<tr>
<td>UAH graupel echo volume (UAH GEV5)</td>
<td>See Carey et al. (2015)</td>
</tr>
<tr>
<td>UAH updraft volume (UAH UV)</td>
<td>See Carey et al. (2015)</td>
</tr>
<tr>
<td>UAH graupel echo volume for supercells (UAH GEV10S)</td>
<td>See Carey et al. (2015)</td>
</tr>
<tr>
<td>UAH graupel echo volume for supercells (UAH GEV5S)</td>
<td>See Carey et al. (2015)</td>
</tr>
<tr>
<td>UAH updraft volume for supercells (UAH UVS)</td>
<td>See Carey et al. (2015)</td>
</tr>
<tr>
<td>Upward cloud ice flux (ICEFLUX)</td>
<td>( \text{FD}<em>{1} = 6.58 \times 10^{-7} \times \phi</em>{\text{ice}} ) (Finney et al., 2014)</td>
</tr>
<tr>
<td>OK 35dBZ echo volume (OK 35EV)</td>
<td>( f = 0.0111 \times 35EV + 1.6619 ) (CSU/T. Davis)</td>
</tr>
<tr>
<td>Blended lightning threat (LTG3)</td>
<td>( \text{FD}_{\text{LTG3}} = (0.95 \times \text{graupe} \text{l flux}) + (0.05 \times \text{VII}) ) (McCaul et al., 2009)</td>
</tr>
</tbody>
</table>

* Units for each storm parameter are: \( w_{\text{max}} \) in (m s⁻¹); CTH in (km); UV in (m³); IWP in (kg m⁻²); PIM and CSU PIM in (kg); IMFP in (kg² m⁻² s⁻¹); every GEV and 35EV are in (km³); UAH UV and UVS in (km³); ICEFLUX in (kg ice m_cloud⁻² s⁻¹); graupel flux in (m s⁻¹ g kg⁻¹) and VII in (kg kg⁻¹)
<table>
<thead>
<tr>
<th>Flash Rate Parameterization Scheme</th>
<th>Reflectivity (dBZ)</th>
<th>Temperature (°C)</th>
<th>Vertical Velocity (m s(^{-1}))</th>
<th>Hydrometeor (g kg(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(_{\text{max}})</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CTH +</td>
<td>&gt; 20</td>
<td>&lt; 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UV</td>
<td>&lt; -5</td>
<td>&gt; 5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IWP</td>
<td>&gt; 25</td>
<td>&lt; -10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PIM *</td>
<td>&lt; -5</td>
<td>w &lt; vts</td>
<td>snow &gt; 0.25 graupel &gt; 0.5</td>
<td></td>
</tr>
<tr>
<td>IMFP *</td>
<td>&lt; -5</td>
<td>Non-precip: w &gt; vts Precip: w &lt; vts</td>
<td>ice &gt; 0 snow &gt; 0.25 graupel &gt; 0.5</td>
<td></td>
</tr>
<tr>
<td>CSU GEV</td>
<td>&gt; 35</td>
<td>-40 &lt; T &lt; -5</td>
<td>graupel &gt; 0.5</td>
<td></td>
</tr>
<tr>
<td>CSU 35EV</td>
<td>&gt; 35</td>
<td>-40 &lt; T &lt; -5</td>
<td>graupel &gt; 0.5</td>
<td></td>
</tr>
<tr>
<td>CSU PIM</td>
<td>&gt; 35</td>
<td>-40 &lt; T &lt; -5</td>
<td>graupel &gt; 0.5</td>
<td></td>
</tr>
<tr>
<td>UAH GEV10</td>
<td>-40 &lt; T &lt; -10</td>
<td>graupel &gt; 0.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UAH GEV5</td>
<td>-40 &lt; T &lt; -5</td>
<td>graupel &gt; 0.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UAH UV</td>
<td>-40 &lt; T &lt; -10</td>
<td>&gt; 5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UAH GEV10S</td>
<td>-40 &lt; T &lt; -10</td>
<td>graupel &gt; 0.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UAH GEV5S</td>
<td>-40 &lt; T &lt; -5</td>
<td>graupel &gt; 0.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UAH UVS</td>
<td>-40 &lt; T &lt; -10</td>
<td>&gt; 5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ICEFLUX *</td>
<td></td>
<td>w &lt; vts</td>
<td>ice &gt; 0 snow &gt; 0.25</td>
<td></td>
</tr>
<tr>
<td>OK 35EV</td>
<td>&gt; 35</td>
<td>-40 &lt; T &lt; -5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LTG3</td>
<td>T = -15</td>
<td>graupel &gt; 0.5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* indicates the highest altitude where both criteria are met.

* indicates the storm vertical velocity (w) and snow fall speed (vts) are both required.

### 2.3.1 Cloud top height and maximum vertical velocity

Early research investigated correlations between lightning flash rate and either cloud top height (CTH) or maximum vertical velocity (w\(_{\text{max}}\)). Williams (1985) indicated a non-linear relationship existed between total lightning and CTH, as well as CTH and w\(_{\text{max}}\), based on thunderstorms observed in New England, Florida, and New Mexico (i.e., continental, midlatitude convection). Using these same data, Price and Rind (1992) further developed the relationships with the intent that they could be used at a coarse
resolution to predict global lightning patterns. For use in cloud-resolved models, such as WRF, the CTH (km) is represented by the maximum height of the 20 dBZ radar reflectivity where the temperature is below freezing (0 °C). Since updraft velocities play an important role in cloud electrification, Price and Rind (1992) used additional field measurements to investigate the differences in the relationships between $w_{\text{max}}$ and CTH for thunderstorms over land and water. The results show there is a positive correlation between the two storm parameters and that when CTHs are similar, the $w_{\text{max}}$ tends to be stronger for continental versus marine convection. This supported conclusions previously made by researchers regarding why lightning activity may vary given certain convective cloud characteristics. By combining the two equations, which link lightning flash rate (flashes min$^{-1}$) with CTH and CTH with $w_{\text{max}}$, a non-linear relationship between lightning activity and $w_{\text{max}}$ (m s$^{-1}$) was defined. The horizontal resolution that is suggested as most appropriate for applying either FRPS is an area that is as wide as the storm is tall (Williams, 1985; Pickering et al., 1998).

2.3.2 Updraft volume

The updraft volume (UV) scheme (Deierling and Petersen, 2008) was developed on a storm scale using ground-based dual-polarimetric and dual-Doppler radar data and total lightning data from 11 convective events, which include single cell, multicell, and supercell thunderstorms. The events were observed in northern Alabama in 2005 and in Kansas and Colorado during the Stratospheric-Tropospheric Experiment: Radiation, Aerosols and Ozone (STERAO-A) and Severe Thunderstorm Electrification and Precipitation Study (STEPS) field campaigns. Total lightning data were provided by the Northern Alabama LMA and by the Office Nationale d’Etudes et de Recherches
Aerospatiales (ONERA) lightning interferometer (in STERAO-A and STEPS). Deierling and Petersen (2008) indicate there is a strong correlation ($r = +0.93$) with total lightning when UV is computed within the mixed-phase region (i.e., temperature $<-5\, ^\circ\text{C}$) where vertical velocities $> 5\, \text{m\,s}^{-1}$. It is also suggested that this combination of criteria required for developing the scheme creates a robust relationship that is at least applicable in the two different regional environments in which the above thunderstorm events were observed. Negative flash rates are generated when $\text{UV} < 2.06\times10^{11}\, \text{m}^3$ because the linear relationship between UV and total lightning activity (flashes min$^{-1}$) has a non-zero y-intercept.

### 2.3.3 Ice mass flux product and precipitation ice mass

Ice mass flux product (IMFP) and precipitation ice mass (PIM) (Deierling, 2006; Deierling et al., 2008) are examples of flash rate-storm parameter relationships involving ice-phase hydrometeors. The IMFP and PIM schemes were both developed using the same thunderstorm cases and observed data as the UV scheme (Deierling and Petersen, 2008). The storm parameters were calculated at temperatures $<-5\, ^\circ\text{C}$, where PIM (kg) is a summation of only the graupel mass and IMFP (kg$^2$ m$^2$ s$^{-2}$) involves the vertical motion of both the precipitation and nonprecipitation (suspended) ice masses through each grid point.

Hydrometeor types were derived from polarimetric radar data using fuzzy logic algorithms (Vivekanandan et al., 1999). The hydrometeor categories used by Deierling et al. (2008) to define precipitation ice included hail, hail/rain mixture, graupel/small hail/rain mix, and graupel/small hail. Nonprecipitation ice was classified as dry snow and ice crystals that were either irregular or horizontally oriented. Using the dominant
hydrometeor identified at each radar grid point, Deierling et al. (2008) used the reflectivity (Z) – mass content (M) relationships to calculate the ice mass (Heymsfield and Palmer, 1986; Heymsfield and Miller, 1988). The precipitation ice mass flux calculated by Deierling et al. (2008) used the precipitation ice terminal fall speed, while Barthe et al. (2010) indicated this could be replaced by the difference between vertical wind velocity and precipitation ice fall speed. Barthe et al. (2010) also suggested nonprecipitation ice mass flux may be determined using the difference between vertical wind velocity and nonprecipitation ice fall speed instead of horizontal divergence.

Both FRPSs indicate a linear relationship exists on a storm scale between the independent (IMFP or PIM) and dependent (total lightning activity) variables (Deierling et al., 2008). However, the y-intercepts are non-zero. This means lightning is produced (flashes min\(^{-1}\)) when IMFP is zero and negative flash rates occur when PIM < \(5.32 \times 10^8\) kg.

For our WRF simulation, precipitation ice includes graupel/hail and snow, while nonprecipitation ice includes snow and cloud ice. Precipitation (nonprecipitation) snow is considered to occur at model grid points where the snow terminal fall speed determined by the microphysics scheme is greater (less) than the updraft velocity. Nonprecipitation ice is identified at model grid points where cloud ice exists and the vertical velocity > \(0 \text{ m s}^{-1}\). Model-simulated graupel/hail at any grid point is assumed to be precipitation.

### 2.3.4 Ice water path

The ice water path (IWP) scheme is another example of a FRPS based on hydrometeors and was developed using data from the LIS and Precipitation Radar instruments onboard the TRMM satellite during the 1998-2000 warm seasons (Petersen et al., 2005). Data
points used in developing this relationship represent IWP (kg m\(^{-2}\)) and flash density (flashes km\(^{-2}\) day\(^{-1}\)) over 0.5\(^\circ\) × 0.5\(^\circ\) (~50 km × 50 km) grid cells between ±35\(^\circ\) latitude. In our cloud-resolved WRF simulation IWP was calculated by integrating the precipitation and nonprecipitation ice mass at all points within a column where radar reflectivity > 18 dBZ and temperature < -10 °C (Petersen et al., 2005; Barthe et al., 2010). However, the column area is scaled down to the smaller WRF processor area (~18 km × 19 km) and the lightning flash density within the processor is converted to flash rate (flashes min\(^{-1}\)). While this scheme is linear, the y-intercept is negative. Therefore, a negative flash rate is generated when the IWP < 5.10×10\(^{-3}\) kg m\(^{-2}\). The model-simulated hydrometeors included in the IWP storm parameter calculation are cloud ice, snow, and graupel/hail. Barthe et al. (2010) found that this FRPS scheme is sensitive to the radar reflectivity threshold used to evaluate the IWP. In their cloud-resolved simulation they adjusted for the overprediction in anvil reflectivity by increasing the reflectivity limit, so IWP is integrated over a smaller region. This caused IWP to increase for their simulated storm.

2.3.5 **Upward cloud ice flux**

Developed from data over a similar area (±38° latitude) as the IWP scheme, the upward cloud ice flux (ICEFLUX; kg\(_{ic} m_{cloud}^{-2} s^{-1}\)) scheme defines a linear relationship using suspended ice data from the ERA-Interim global atmospheric reanalysis provided by the European Centre for Medium-Range Weather Forecasting (ECMWF) and lightning flash density data observed by LIS on 2.5\(^\circ\) × 2.5\(^\circ\) (~270 km × 250 km) grid cells (Finney et al., 2014). In our model the calculated flash density (flashes m\(_{grid\_cell}^{-2} s^{-1}\)) was converted to flash rate (flashes min\(^{-1}\)) by accounting for the model domain’s horizontal resolution.
Our analysis represents the first time this scheme is tested at cloud-resolved resolution. Finney et al. (2014) suggest ICEFLUX be evaluated at 440 hPa, since it is the cloud top pressure criterion for deep convective clouds specified by the International Satellite Cloud Climatology Project (ISCCP) (Rossow et al., 1996). Finney et al. (2014) also assessed this scheme at 440±100 hPa to test its sensitivity to pressure. They found lower correlations at higher pressures and similar correlations at lower pressures, confirming that 440 hPa was a good choice.

2.3.6 McCaul lightning threat methods

Lightning threat methods developed by McCaul et al. (2009, 2011) forecast flash rate density (flashes km\(^{-2}\) 5-min\(^{-1}\)) using either graupel flux at -15 °C or the gridded vertically integrated ice (VII). The graupel flux is a product of the upward vertical velocity (m s\(^{-1}\)) and graupel mixing ratio (g kg\(^{-1}\)), while the VII focuses on the graupel, snow, and cloud ice mixing ratios (kg kg\(^{-1}\)) within the grid column. Seven convective events observed over northern Alabama were analyzed with WRF at cloud-resolved scales. Over the lifetime of each event, the maximum LMA flash origin density per 5-min and maximum model-simulated storm parameter were identified within the domain and used to create linear relationships between lightning and ice hydrometeors. The slope of each line was then used to calibrate their respective equation. The graupel flux and VII methods capture the temporal variability and areal coverage of lightning activity, respectively, with a weighted summation of the two methods (0.95 graupel flux and 0.05 VII) providing the best prediction of flash rate density (McCaul et al., 2009). The weighted summation is referred to as the blended lightning threat (LTG3). Initially, the resulting flash rate densities determined by graupel flux and VII were only used when they
exceeded a threshold of 0.01 and 0.40 flashes km\(^{-2}\) 5-min\(^{-1}\), respectively. However, additional techniques were developed to acknowledge specific concerns. These include (1) increasing the graupel flux method threshold (1.5 flashes km\(^{-2}\) 5-min\(^{-1}\)) to address winter stratiform weather, (2) forcing VII to have the same peak flash rate density as graupel flux to avoid deviation of individual lightning threat methods during high flash rate events, and (3) assigning a flash rate density threshold to the blended method for a more accurate depiction of areal coverage (McCaul et al., 2011; Eugene McCaul, personal communication, January 13, 2017). Our case study will only focus on the LTG3 method and will also represent the first time it is evaluated using the Morrison two-moment microphysics and Yonsei University (YSU) planetary boundary layer (PBL) schemes.

2.3.7 Newly-developed FRPSs from DC3

Observations from the DC3 field campaign were included in the creation of new total lightning-storm parameter relationships. Total lightning flash data collected by LMA and radar data within the northeast Colorado and northern Alabama DC3 study regions allowed for the development of additional FRPSs by Colorado State University (CSU) and the University of Alabama in Huntsville (UAH), respectively (Basarab et al., 2015; Carey et al., 2015). Data used in FRPS development for these regions were from the DC3 period as well as other years. Our study will evaluate the performance of these newly-developed schemes for the first time in a model at cloud-resolved resolution.

2.3.7.1 Colorado FRPSs

Nine of the 11 isolated storms (i.e., single cell and supercell with varying severity) used by Basarab et al. (2015) in developing new FRPSs were from DC3, while the other two
events were from summer 2013. All events were objectively identified using a cell-tracking algorithm (Fuchs et al., 2015). The average and maximum total flash rates associated with the observed convection dataset are 53.9 flashes min\(^{-1}\) and 287.8 flashes min\(^{-1}\), respectively. In addition to LMA data, the polarimetric radar data were gridded at 0.5 km\(^3\) resolution and fuzzy logic algorithms (Dolan et al., 2013) were applied to the radar data to identify the dominant hydrometeor type per grid. Basarab et al. (2015) used the Colorado convective events dataset to modify previously developed FRPSs from the literature (e.g., PIM; kg). These schemes were not properly tuned to capture the higher flash rate Colorado storms and were also developed using a different hydrometeor identification algorithm.

In addition, graupel echo volume (CSU GEV; km\(^3\)) and 35 dBZ echo volume (CSU 35EV; km\(^3\)), which are similar to PIM and have previously shown strong correlations to lightning (Carey and Rutledge, 1996; Wiens et al., 2005; Liu et al., 2012), were also used to develop FRPSs for Colorado storms. To calculate the storm parameters, data points were restricted to the mixed-phase region of convective clouds (i.e., -5 °C > temperature > -40 °C and reflectivity > 35 dBZ). The linear relationships between total lightning and the CSU PIM, GEV, and 35EV resulted in a better fit to the data than the prior existing schemes in the literature. The CSU 35EV was the most successful storm parameter for estimating total lightning flash rates in Colorado. Basarab et al. (2015) also suggest this scheme may be robust enough to be used in different environments and regions based on its exceptional performance when used to examine thousands of isolated convective events from four areas (i.e., Colorado, Oklahoma, northern Alabama, and Washington, D.C.). This scheme performed best when the
environment had low normalized convective available potential energy (NCAPE < 0.1 m s⁻²), moderate warm cloud depth (1-2 km), and moderate vertical wind shear (10-20 m s⁻¹).

### 2.3.7.2 Northern Alabama FRPSs

Carey et al. (2015) developed FRPSs using 32 convective cells observed over northern Alabama, which ranged in storm type and severity (i.e., multicell, supercell and one quasi-linear convective system). Five of the events occurred during DC3. Unlike the CSU approach, which used a cell-tracking algorithm to identify and track isolated convective cells (Fuchs et al., 2015), UAH (Carey et al., 2015) used both objective and subjective approaches for tracking. The manual approach was necessary for the multicell events observed during DC3 to avoid any influence from nearby storms. Based on the LMA data, this dataset had an average total flash rate of 12.5 flashes min⁻¹ and a maximum of 102 flashes min⁻¹. Polarimetric and Doppler radar data were also available and fuzzy logic algorithms were utilized to determine the dominant hydrometeor types (Vivekanandan et al., 1999). Both datasets were gridded at 1 km resolution in the horizontal and vertical. Of the 17 storm parameters Carey et al. (2015) tested for the northern Alabama region, the linear relationships between total lightning (flashes min⁻¹) and graupel echo volume between -10 °C > temperature > -40 °C (UAH GEV10; km³), graupel echo volume between -5 °C > temperature > -40 °C (UAH GEV5; km³), and updraft volume between -10 °C > temperature > -40 °C and vertical velocities > 5 m s⁻¹ (UAH UV; km³) appeared to work best based on the normalized median and mean bias errors. Based on these storm parameters, three additional FRPSs were developed for supercell events (UAH GEV10S, GEV5S, and UVS).
2.3.7.3 Tailored FRPS for 29-30 May 2012 convective event

Since the objective of our study was to evaluate FRPSs in a simulation of an Oklahoma thunderstorm observed during DC3, it was desirable to include a scheme based on data from this region. According to Basarab et al. (2015), the 35EV was the most robust storm parameter used in their analysis for estimating lightning flash rates based on how well it performed when tested using thousands of isolated storms in multiple regions of the continental United States. Therefore, CSU developed a version of this scheme using data from the Weather Surveillance Radar-1988 Doppler (WSR-88D) at Oklahoma City (KTLX) and the central Oklahoma LMA during the 29-30 May 2012 event. The observed 35EV (km³) and total lightning flash rates (flashes min⁻¹) resulted in a linear relationship based on convection located north of Oklahoma City (35.49 °N) in the Oklahoma domain. This Oklahoma 35EV (OK 35EV) scheme applied the same mixed-phase region temperature criteria as the CSU 35EV scheme (-5 °C > temperature > -40 °C). A similar relationship was found in two cells within a mesoscale convective system (MCS) observed in Oklahoma during the Thunderstorm Electrification and Lightning Experiment (TELEX) in 2004, where lightning initiation typically occurred within the 35 dBZ reflectivity contour in the presence of graupel (Lund et al., 2009).

2.4 Previous FRPS evaluation with cloud-resolved models

Barthe et al. (2010) simulated an isolated severe storm observed during STERAO-A and an airmass thunderstorm over northern Alabama using WRF. An evaluation of six FRPSs using model output suggests the flash rates and trends are best represented by $w_{\text{max}}$ and CTH for the severe and airmass storms, respectively. Their research differs from previous work because it was the first time flash rate-storm parameter relationships
developed from field experiment observations were tested in a cloud-resolved model. Cummings et al. (2013) used the WRF Aqueous Chemistry (WRF-AqChem; Barth et al., 2007) model to run a cloud-resolved simulation of a deep convective storm that occurred during the Stratospheric-Climate Links with Emphasis on the Upper Troposphere and Lower Stratosphere (SCOUT-O3)/Aerosol and Chemical Transport in Tropical Convection (ACTIVE) field campaigns near Darwin, Australia. The performance of FRPSs in tropical island convection was assessed for the first time by Cummings et al. (2013) and initial results suggested $w_{\text{max}}$ and CTH were good predictors of the observed flash trend at the cloud-resolved scale. Since models do not perfectly replicate the features of an observed storm, a better representation of the observed flashes is produced using the regression between the observed and model-simulated storm parameters to adjust the FRPSs (Barthe et al., 2010) or by scaling the model-simulated flash rates. In my case study reported here, I scale the over or underprediction of specific aspects of a storm parameter (e.g., graupel, snow) within a FRPS.
A thunderstorm may affect the chemical composition of the environment in several ways. Precipitation cleanses the atmosphere by washing out soluble pollutants, such as nitric acid (HNO₃), and depositing them on the ground. Updrafts lift polluted air from the surface to higher altitudes, where it can disperse within the upper troposphere. However, downdrafts transport cleaner air from the free troposphere or lower stratosphere to the boundary layer. Production and destruction of trace gases, such as NOₓ and O₃, occurs during an active thunderstorm or downwind following the convective event. Lightning produces NOₓ, which in large enough quantities may lead to O₃ loss within a storm cloud. As the NOₓ is diluted in the upper tropospheric storm outflow, it leads to efficient photochemical O₃ production downwind of a storm.

3.1 Lightning-generated nitrogen oxides
A lightning flash is brief, but hot (~30,000 K). The high temperature partly dissociates molecular oxygen (O₂) and nitrogen (N₂) in and near the flash, which allows oxygen and nitrogen atoms to react and produce NO. The lightning channel quickly cools as it mixes with colder, ambient air over the course of a few seconds. During the cooling process the lightning-heated air reaches a “freeze-in” temperature, roughly 3,000 K (Hill et al., 1980; Schumann and Huntrieser, 2007), where the reactions which would normally create and destroy NO are no longer in chemical equilibrium. This leads to a large fraction of the initially generated NO to be saved (Chameides et al., 1977; Hill et al., 1980; Huntrieser et al., 1998; Rakov and Uman, 2003).
The lifetime of NO$_x$ varies as a function of altitude, with lifetimes on the order of a day or less near the earth’s surface to lifetimes as long as several days to a week in the upper troposphere (Ridley et al., 1996; Jaeglé et al., 1998; Huntrieser et al., 1998; Martin et al., 2007). The variation is mainly due to two mechanisms involving the production of HNO$_3$. The reaction between NO$_2$ and OH is temperature dependent, so the reaction rate slows as the temperature decreases in altitude between the surface and the tropopause. Nitrogen dioxide is also involved in the production of N$_2$O$_5$. However, the heterogeneous production of HNO$_3$ slows because the reaction between N$_2$O$_5$ and water occurs on aerosols, which there are fewer of in the upper troposphere. There is also a greater tendency for NO$_x$ to exist as NO (Jaeglé et al., 1998) in the upper troposphere due to other temperature dependent reactions that slow with altitude, such as those between NO and O$_3$ and between NO and HO$_2$.

Unfortunately, direct measurements of LNO$_x$ production are not possible, although cloud-resolving models and observations from satellites and aircraft have helped to slightly reduce the uncertainty. The best approximation for the contribution of lightning to the global NO$_x$ budget is 5±3 Tg (N) yr$^{-1}$ (Schumann and Huntrieser, 2007). The main areas of uncertainty include the production of NO per IC and CG flashes, the amount of NO produced per unit flash length, and the vertical profile of LNO$_x$ mass (Ott et al., 2010). The 5 Tg (N) yr$^{-1}$ translates to approximately 250 moles NO$_x$ flash$^{-1}$ or 3.5 kg (N) flash$^{-1}$. The conversion was completed in the literature survey (Schumann and Huntrieser, 2007) using the mass of nitrogen (14 g (N) mole$^{-1}$) and the assumption that every second roughly 44 flashes occur across the globe (Christian et al., 2003).
Analyses investigating types and lengths of lightning flashes indicate the amount of NO produced per meter flash channel length is less in IC versus CG flashes and that longer flash lengths produce more LNOx (Barthe and Barth, 2008). However, other cloud-resolved modeling constrained by aircraft observations (DeCaria et al., 2000, 2005) suggests that on average IC and CG flashes make similar amounts of NO per flash. For a “typical” thunderstorm the accepted LNOx production range is 33-660 moles NO flash⁻¹, with an average production rate of 250 moles NO flash⁻¹ (Schumann and Huntrieser, 2007). Previous model analyses of midlatitude thunderstorms suggest 200-500 moles NO flash⁻¹ is a reasonable estimate (DeCaria et al., 2000, 2005; Fehr et al., 2004; Ott et al., 2007) of the mean production rate. Simulations of five convective events taken from the midlatitudes and subtropics yielded a mean value of 500 moles NO flash⁻¹ (Ott et al., 2010). A simulation of a “Hector” thunderstorm over the Tiwi Islands of northwestern Australia indicated a NO production scenario of 500 moles flash⁻¹ was also appropriate for this tropical island convection; however, 600 moles NO flash⁻¹ was not an unreasonable upper limit (Cummings et al., 2013). Although the LNOx production from each of these analyses falls within the range of a “typical” thunderstorm, the variation indicates uncertainty still exists. In addition, Ott et al. (2010) suggest the amount of LNOx per unit flash length ranges from 1.7 to 22 × 10⁻³ moles NO m⁻¹ due to the influence of peak current and ambient pressure. Ideally, researchers would like to decrease the uncertainty range of the global LNOx budget to ±1 Tg (N) yr⁻¹ or 20%, but understand the difficulty in doing so (Schumann and Huntrieser, 2007).
3.2 LNO\textsubscript{x} parameterization schemes

When simulating the generation, distribution, and transport of LNO\textsubscript{x} within a convective cloud, several conditions must be defined. These include the number of total flashes, the fractional flash channel vertical distribution, and the number of moles NO per flash. Depending on the type of convective parameterization that is chosen, these selections may need to be partitioned into CG and IC lightning flashes. The dependence of LNO\textsubscript{x} production on pressure must also be accounted for when calculating the vertical profile of the NO\textsubscript{x} contribution from the fractional lightning channel (DeCaria et al., 2005) and LNO\textsubscript{x} mass (Ott et al., 2010) distributions. Several approaches for incorporating LNO\textsubscript{x} in the horizontal within the cloud also exist. The options for vertical and horizontal LNO\textsubscript{x} distributions are described below.

### 3.2.1 Vertical distribution of lightning flash channel lengths and NO\textsubscript{x}

A LNO\textsubscript{x} vertical distribution may be specified for either cloud-resolved or parameterized convection. The default distributions offered in WRF follow DeCaria et al. (2005) and Ott et al. (2010). However, observed lightning flash channel data can replace these vertical profiles in case study simulations, as discussed in Section 3.2.1.3.

#### 3.2.1.1 Cloud-resolved convection

When the vertical distributions of lightning flash channel lengths were first developed, observations from lightning mapping systems indicated that thunderstorm flash channels generally peaked at one or two layers (MacGorman and Rust, 1998). Based on these early data, DeCaria et al. (2000) suggested the vertical profiles for CG and IC lightning were best represented as unimodal and bimodal Gaussian distributions, respectively. Therefore, the lightning channels in cloud-resolved convection are set to maximize at
specified lower (CG and IC flashes) and upper (IC flashes) temperature levels, which correspond to a thunderstorm’s two main charge regions (Ott et al., 2010). For midlatitude storms, the channels are set to -15 °C and -45 °C, which is roughly 6 km and 10.5 km, respectively. The main negative charge region is typically located at -15 °C in the lower portion of the convective cloud (DeCaria et al., 2005). The upper temperature limit may be modified higher or lower based on cloud top height (Pickering et al., 2009; Ott et al., 2010). For instance, the upper mode isotherm was adjusted to a colder temperature (-60 °C or ~12.7 km) for a cloud-resolved simulation of a “Hector” thunderstorm (Cummings et al., 2013), which is typically very tall. Not only is the tropopause higher in the tropics, but the mean IC flash altitude was also higher than the assumption for midlatitude thunderstorms during the period when the simulated storm was observed. Adjustments in the upper temperature level may also be necessary to achieve better agreement between the altitude of aircraft-observed and model-simulated NOx mixing ratios (Ott et al., 2010).

3.2.1.2 Parameterized convection

At regional and global scales, LNOx production can be parameterized through the use of output from cloud-resolved simulations of observed convective events (DeCaria et al., 2000). Pickering et al. (1998) and Ott et al. (2010) simulated various types of thunderstorms (e.g., isolated and MCS) from across the globe (i.e., the central United States, south Florida, Germany, western Pacific, the region between Australia and New Guinea, the Atlantic off West Africa, and Brazil) using 2D and 3D cloud-scale chemical transport models. The resulting vertical profiles represent a combination of the CG and IC LNOx mass influenced by both production and convective transport. Pickering et al.
(1998) suggested the average LNO$_x$ vertical distributions were C-shaped with peaks in the upper troposphere and in the boundary layer, while Ott et al. (2010) showed the profiles resembled a backward C-shape with a single peak in the middle to upper troposphere. The updated vertical distributions are considered more realistic because a 3D model is used to distribute LNO$_x$ based on the VHF sources generated by observed CG and IC flashes, instead of using a 2D model to distribute the CG and IC LNO$_x$ between the -15 °C isotherm and the surface and cloud top, respectively. Therefore the single-mode Gaussian distributions defined by Ott et al. (2010) for midlatitude continental, subtropical, and tropical continental and marine environments are typically used for parameterized convection in larger scale models, such as GEOS-Chem, the NASA Global Modeling Initiative (GMI; Allen et al., 2010), and the GEOS-5 Chemistry and Climate Model (GEOS-CCM, Liaskos et al., 2015).

3.2.1.3 Observations

Observed vertical distributions of flash channel lengths may be constructed for specific convective events and used to replace the default Gaussian distributions for CG and IC lightning in thunderstorms at cloud-resolved scales (DeCaria et al., 2000). Within the coverage of a LMA network, a CG flash dataset (e.g., NLDN) is used to help identify and partition the LMA total lightning into CG and IC flashes. A method, such as the 3D convex hull volume (Bruning and Thomas, 2015), can then be used to derive the fraction of lightning channel lengths in the vertical. A vertical distribution may not be the same throughout a thunderstorm’s life cycle and it may also vary by region and between storms (DeCaria et al., 2000). With the installation of LMA networks across the United States, a
climatology of flash channel length vertical profiles could be used to update the default distributions or possibly provide location dependent options.

Another approach to calculating $\text{LNO}_x$ production is with the Lightning Nitrogen Oxides Model (LNOM) by Koshak et al. (2014). This model does not take into consideration any mixing of the $\text{LNO}_x$ within the atmosphere. It only provides vertical profiles of 10-meter flash channel segments (channel length) and $\text{LNO}_x$ production. The flash channel segment data come from LMA observations and the $\text{LNO}_x$ production per meter of channel length come from laboratory data and theoretical assumptions. Unlike the most recent research, which suggests average $\text{LNO}_x$ production for IC and CG flashes may be equal, Koshak (2014) indicates that on average a CG flash (604.3 moles) in northern Alabama may produce 16.6 times more $\text{LNO}_x$ than an IC flash (36.4 moles).

3.2.2 Horizontal distribution of $\text{LNO}_x$

Once a vertical distribution of the fraction of total $\text{LNO}_x$ in each layer is selected, the $\text{LNO}_x$ can be placed uniformly within each horizontal layer of the convective cloud given specified thresholds of reflectivity or hydrometeor mass mixing ratios. To determine the amount of NO that is incorporated into the horizontal area of the convection, the number of lightning flashes within the column, the frequency of lightning flash channel lengths, and the NO production scenario are each considered. Early studies limited the CG $\text{LNO}_x$ to radar reflectivities $> 20$ dBZ between the surface and -15 °C isotherm, while IC $\text{LNO}_x$ was restricted to every layer within the cloud boundary from the -15 °C isotherm to cloud top (Pickering et al., 1998; DeCaria et al., 2000). In the 3D models used by DeCaria et al. (2005) and Ott et al. (2010), all the $\text{LNO}_x$ was injected within the 20 dBZ contour. This method represents a situation where the $\text{LNO}_x$ is immediately dispersed within the
identified portion of the cloud. More recently, Mecikalski and Carey (2017) and Fuchs and Rutledge (2017, in press) have investigated the partitioning of lightning source and flash data by altitude and radar reflectivity for convective events observed in different regions of the United States. Both studies provide insight into how the radar reflectivity threshold for the horizontal placement of LNO\textsubscript{x} in this bulk approach may be modified for specific regions, storm types, and flash types.

A filament approach was also investigated, which tries to replicate the branching of a lightning flash within a predetermined area downwind of the maximum updraft (Ott et al., 2007; Barthe and Barth, 2008; Ott et al., 2010). This area represents the average horizontal flash extent and within each layer above this region the LNO\textsubscript{x} is randomly distributed among a specific number of points that are defined by the magnitude of the vertical distribution in that layer. This approach attempts to provide a more realistic representation of the LNO\textsubscript{x} production and transport by focusing on a smaller area of the cloud where a flash occurs. However, Ott et al. (2010) found this method resulted in a similar NO production per flash as simulations using the bulk approach and indicated that different analysis techniques and model set ups may have a greater influence on estimates of NO production.

3.3 Effects on other trace gases

Compared with the boundary layer, the lifetime of NO\textsubscript{x} is about 5-10 times longer in the upper troposphere, where the dominance of lightning as a global NO\textsubscript{x} source plays a key role in the production of O\textsubscript{3}. Because of its ability to absorb and emit longwave terrestrial radiation, O\textsubscript{3} is considered a significant greenhouse gas (Lacis et al., 1990). For O\textsubscript{3} production in the upper troposphere, time is required for photochemical reactions
to occur in the outflow following a convective event (Pickering et al., 1990; 1996; DeCaria et al., 2005; Choi et al., 2009; Apel et al., 2015). Whether NO\textsubscript{x} is generated by lightning or lofted with other surface pollutants (e.g., carbon monoxide (CO) and hydrocarbons) into the convective cloud by updrafts, tropospheric O\textsubscript{3} production occurs via photochemical oxidation reactions involving CO and hydrocarbons:

\[
\begin{align*}
\text{CO} + \text{OH} & \rightarrow \text{CO}_2 + \text{H} & (\text{R1}) \\
\text{H} + \text{O}_2 + \text{M} & \rightarrow \text{HO}_2 + \text{M} & (\text{R2}) \\
\text{HO}_2 + \text{NO} & \rightarrow \text{NO}_2 + \text{OH} & (\text{R3}) \\
\text{NO}_2 + \text{hv} & \rightarrow \text{NO} + \text{O} & (\lambda < 420 \text{ nm}) & (\text{R4}) \\
\text{O} + \text{O}_2 + \text{M} & \rightarrow \text{O}_3 + \text{M} & (\text{R5}) \\
\text{net: CO} + 2\text{O}_2 & \rightarrow \text{CO}_2 + \text{O}_3
\end{align*}
\]

\[
\begin{align*}
\text{RH} + \text{OH} & \rightarrow \text{R} + \text{H}_2\text{O} & (\text{R6}) \\
\text{R} + \text{O}_2 + \text{M} & \rightarrow \text{RO}_2 + \text{M} & (\text{R7}) \\
\text{RO}_2 + \text{NO} & \rightarrow \text{NO}_2 + \text{RO} & (\text{R8}) \\
\text{RO} + \text{O}_2 & \rightarrow \text{R'}\text{CHO} + \text{HO}_2 & (\text{R9}) \\
\text{HO}_2 + \text{NO} & \rightarrow \text{NO}_2 + \text{OH} & (\text{R3}) \\
2 (\text{NO}_2 + \text{hv} & \rightarrow \text{NO} + \text{O}) & (\lambda < 420 \text{ nm}) & (\text{R4}) \\
2 (\text{O} + \text{O}_2 + \text{M} & \rightarrow \text{O}_3 + \text{M}) & (\text{R5}) \\
\text{net: RH} + 4\text{O}_2 & \rightarrow \text{R'}\text{CHO} + \text{H}_2\text{O} + 2\text{O}_3
\end{align*}
\]
where RH is a hydrocarbon (e.g., CH₄), R is an organic group, RO₂ is an organic peroxy radical formed by hydrocarbon oxidation, and M represents a third body.

Ozone concentrations tend not to increase in the short-term within thunderstorms (DeCaria et al., 2005). However, in the 24-hours following a convective event LNOₓ leads to enhanced O₃ production in thunderstorm outflow (DeCaria et al., 2005; Ott et al., 2007). The concentration of NOₓ in the anvil dilutes as air flows downwind into the upper troposphere. This allows for O₃ production and enhancement, as NOₓ catalyzes O₃ more efficiently on a per molecule basis when concentrations are diluted (Pickering et al., 1990). DeCaria et al. (2005) computed an O₃ enhancement of 10 parts per billion volume (ppbv) day⁻¹ at 10.5 km in convective outflow, while Ott et al. (2007) found O₃ decreased at the same altitude, but increased 5 ppbv day⁻¹ at 5.5 km. A similar enhancement from lightning (up to 16 ppbv) was found in the upper troposphere during summer 2004 over the Gulf Coast, southeast United States, and western North Atlantic (Martini et al., 2011).

Yuan et al. (2012) used observations and model-simulations to investigate enhanced O₃ production in the upper troposphere due to increases in lightning and LNOₓ production associated with rises in aerosol loading from a volcanic eruption in 2005 and increased anthropogenic emissions since 1850. The pre-industrial environment was relatively clean compared to today’s; therefore, an increase in aerosols would make the impact on lightning activity, O₃, and its radiative forcing more pronounced than in today’s environment. Today, however, other processes, such as biomass burning and manmade emissions, which also produce O₃, mask the aerosol-lightning-ozone link, so the influence on O₃ radiative forcing due to lightning is not as strong. This change in lightning flashes is not accounted for in past climate modeling, indicating the aerosol-
lightning-ozone connection needs to be included to properly understand the changes in climate over time. It is also suggested that areas with higher pollution and larger flash rates may produce less O\textsubscript{3} than regions with pristine air and moderate flash rates (Ott et al., 2007) due to reduced O\textsubscript{3} production efficiency under high-NO\textsubscript{x} conditions. Due to a rule set by the Environmental Protection Agency (EPA), called the NO\textsubscript{x} State Implementation Plan (SIP), the eastern United States has observed substantial decreases in anthropogenic NO\textsubscript{x} emissions over the last decade. With this reduction in power plant emissions it has been shown that LNO\textsubscript{x} has a more pronounced influence on upper tropospheric O\textsubscript{3} production and its radiative impact than anthropogenic NO\textsubscript{x} emissions (Choi et al., 2009; Martini et al., 2011).

A single NO molecule produced by lightning can also generate three OH molecules by photochemical oxidation, creating an enhancement in OH concentrations:

\[
\text{HO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{OH} \quad (\text{R3})
\]

\[
\text{NO}_2 + h\nu \rightarrow \text{NO} + \text{O} \quad (\lambda < 420 \text{ nm}) \quad (\text{R4})
\]

\[
\text{O} + \text{O}_2 + M \rightarrow \text{O}_3 + M \quad (\text{R5})
\]

\[
\text{O}_3 + h\nu \rightarrow \text{O}_2 + \text{O}^{(1}\text{D}) \quad (\lambda < 320 \text{ nm}) \quad (\text{R10})
\]

\[
\text{O}^{(1}\text{D}) + \text{H}_2\text{O} \rightarrow 2 \text{OH} \quad (\text{R11})
\]

where O\textsuperscript{(1}D\textsuperscript{)} is the O atom in an excited singlet state. This reaction series is significant because it illustrates the direct affect NO\textsubscript{x} has on OH and shows how NO\textsubscript{x} is indirectly linked to changes in climate forcing by CH\textsubscript{4} through control of CH\textsubscript{4} lifetime by OH.
CHAPTER 4: DEEP CONVECTIVE CLOUDS AND CHEMISTRY FIELD EXPERIMENT

4.1 Background

The May-June 2012 DC3 field campaign provided a multi-faceted approach to study varying types of convection (e.g., midlatitude airmass, multicell, and supercell thunderstorms), their convective transport of trace gases (e.g., anthropogenic, biogenic, and wildfire emissions), and associated lightning occurrence and NO$_x$ production. Field experiments prior to DC3 had not investigated the influence of the environment and convection on the composition and chemistry of the upper troposphere with such a plethora of ground-based and airborne measurements of thunderstorms, the environment prior to and during convection, and the outflow downwind 12-48 hours post-convection.

The operations center was located in Salina, Kansas, which offered reasonable flight times for research aircraft to arrive at any of the three pre-determined sampling regions in northeast Colorado, central Oklahoma to west Texas, and northern Alabama. The three domains were selected based on the available instrumentation and type of convection associated with the region.

The three aircraft involved in the field campaign were the National Center for Atmospheric Research (NCAR) Gulfstream V (GV), National Aeronautics and Space Administration (NASA) DC-8, and the German DLR Falcon. The aircraft provided meteorological and chemical (i.e., trace gases and aerosols) observations of the storm inflow and outflow, in addition to background environmental conditions prior to storm development. Generally, the DC-8 focused on storm inflow, while the GV concentrated on the high-altitude outflow; however, both aircraft did sample higher and lower
altitudes, respectively, during a research flight. The Falcon also concentrated on high-altitude anvil outflow and often flew closer to the convective cores than the other aircraft.

During the campaign, meteorological and chemical tracer (e.g., LNO\textsubscript{x} and boundary layer) forecasts were provided daily to aid decision makers in selecting where research flights would occur. On downwind flight days, forward (i.e., Flexible Particle (FLEXPART) dispersion model) and backward (Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model) trajectories of the upper level air were analyzed to forecast the outflow plume location sampled the previous afternoon/evening. By the conclusion of the campaign, 26 intensive operational periods (IOPs) had occurred. Additional details regarding the DC3 field campaign may be found in Barth et al. (2015).

### 4.2 Forecast model preparation

During the DC3 experiment, the WRF model version 3.3.1 was run by NCAR at a 3-km horizontal resolution and initialized based on the 15-km Data Assimilation Research Testbed (DART) ensemble run. The model set-up included the following schemes: Morrison two-moment microphysics, Mellor-Yamada-Janjic (MYJ) PBL, Noah land surface model (LSM), the Rapid Radiative Transfer Model for General Circulation Models (GCMs) (RRTMG; Iacono et al., 2008), and no cumulus parameterization. While the WRF-Chem was not used, LNO\textsubscript{x} was included as a tracer in the WRF model and the UV FRPS (Deierling and Petersen, 2008) provided the flashes required for the LNO\textsubscript{x} parameterization scheme.

In order to select the FRPS to be used in the operational forecasting for DC3, I performed comparative analyses for two case study periods (i.e., 10-11 June 2010 and the DC3 test flight period from 1-15 May 2011) between flash rate observations and model
output from cloud-resolved WRF simulations using the $w_{\text{max}}$, CTH, and UV schemes. Both periods used the WRF model version 3.2.1 at a 3-km horizontal resolution with the Thompson microphysics and MYJ PBL schemes. Simulated total lightning flashes were determined for the convection during each case study period and compared against the total flashes estimated from the observed NLDN CG flashes using Eqn. 1 (see Chapter 2). Comparisons included: (1) the cumulative number of total flashes over the lifetime of each storm, (2) temporal correlations per 3-hour interval, and (3) spatial correlations per model processor region. The temporal and spatial correlations were used to determine how well the model simulated the timing and location of the convection.

Based on the four convective events (i.e., quasi-stationary, MCS, cold frontal system and single cell) examined during the 10-11 June 2010 case study (Cummings et al., 2012), flash rates were generally overestimated by the UV scheme and underestimated by the $w_{\text{max}}$ and CTH schemes (Table 3); however, estimates based on CTH were reasonable for events with strong forcing (i.e., quasi-stationary systems and MCS). The temporal correlation per 3-hour interval varied by storm type and FRPS (0.41-0.93), but each scheme showed the strongest correlation (> 0.75) for the MCS (Table 4). The spatial correlation per model processor region also varied by storm type and FRPS (0.26-0.69; Table 5). Generally, the FRPSs performed equally in terms of spatial correlation for storms with stronger forcing.
Table 3. Number of observed and model-simulated total flashes for four convective case studies during 10-11 June 2010. The observed total flashes are an estimate based on the NLDN CG flashes and Equation 1.

<table>
<thead>
<tr>
<th>Storm</th>
<th>Storm Type</th>
<th>Observed Flashes</th>
<th>Flash Rate Parameterization Scheme Model-Simulated Flashes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Quasi-Stationary System</td>
<td>256,535</td>
<td>50,054</td>
</tr>
<tr>
<td>2</td>
<td>MCS</td>
<td>130,502</td>
<td>14,903</td>
</tr>
<tr>
<td>3</td>
<td>Cold Front</td>
<td>222,011</td>
<td>74,768</td>
</tr>
<tr>
<td>4</td>
<td>Single Cell</td>
<td>11,548</td>
<td>146</td>
</tr>
</tbody>
</table>

Table 4. Temporal correlation between the observed and model-simulated total lightning flashes for four convective case studies during 10-11 June 2010. The strongest correlation for each storm type is identified in bold font.

<table>
<thead>
<tr>
<th>Storm</th>
<th>Storm Type</th>
<th>Flash Rate Parameterization Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$w_{\text{max}}$</td>
</tr>
<tr>
<td>1</td>
<td>Quasi-Stationary System</td>
<td>0.41</td>
</tr>
<tr>
<td>2</td>
<td>MCS</td>
<td>0.91</td>
</tr>
<tr>
<td>3</td>
<td>Cold Front</td>
<td>0.52</td>
</tr>
<tr>
<td>4*</td>
<td>Single Cell</td>
<td>---</td>
</tr>
</tbody>
</table>

* indicates storm 4 only contained two data points

Table 5. Spatial correlation between the observed and model-simulated total lightning flashes for four convective case studies during 10-11 June 2010. The strongest correlation for each storm type is identified in bold font.

<table>
<thead>
<tr>
<th>Storm</th>
<th>Storm Type</th>
<th>Flash Rate Parameterization Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$w_{\text{max}}$</td>
</tr>
<tr>
<td>1</td>
<td>Quasi-Stationary System</td>
<td>0.55</td>
</tr>
<tr>
<td>2</td>
<td>MCS</td>
<td>0.69</td>
</tr>
<tr>
<td>3</td>
<td>Cold Front</td>
<td>0.51</td>
</tr>
<tr>
<td>4</td>
<td>Single Cell</td>
<td>0.26</td>
</tr>
</tbody>
</table>
The 10 convective events analyzed from the May 2011 DC3 test flights were associated with a short wave trough, dryline, or cold front. Each forecast run, whether it occurred the day of or the day before each selected storm, generally underestimated the observed flashes over the storm’s lifetime using all three FRPSs. An example of the results for four storms is provided in Table 6. A comparison of the radar reflectivity for each of the 10 storms indicated a lack of sufficient storm intensity, which translated to substantial underestimates in the simulated flash rates. The simulated reflectivity generally forecasted shorter periods of intense convection and for about half of the storms the high reflectivities (> 50 dBZ) covered a smaller area than the observed reflectivity. Also, the forecast storms often missed the observed peak reflectivities, especially when the peak exceeded 65 dBZ. The UV scheme required the smallest scaling factor to match the observed flash rates for forecast runs 24 hours prior to and on the day the storm occurred. Temporal correlations between observed and model-simulated flashes per 3-hour interval varied by each storm and within each storm type (Table 7). Generally, the spatial correlation per processor region is weak between the observed and model-simulated flashes (Table 8). A visual analysis of the observed and model-simulated flash rates per model processor indicated the UV scheme did well capturing both the number of total flashes and their location. An example of one of the 10 convective events based on the 18 UTC run the day prior to the convection is shown in Figure 4. For forecasting 24 hours in advance, the UV scheme equally over- and underestimated the flash rates for a given convective event and provided a flash rate estimate that is closer to the observations than the other two FRPSs. Similar results were generated when model output from the day of the convection was used to predict flash rates.
Table 6. Number of observed and model-simulated total flashes for four convective case studies observed during the DC3 test flight on 3 May 2011. The observed total flashes are an estimate based on the NLDN CG flashes and Equation 1. The model output is based on the 18 UTC run on 2 May 2011, which is the day prior to the convective event.

<table>
<thead>
<tr>
<th>Storm</th>
<th>Storm Type</th>
<th>Observed Flashes</th>
<th>Flash Rate Parameterization Scheme Model-Simulated Flashes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>$w_{\text{max}}$</td>
</tr>
<tr>
<td>6</td>
<td>Shortwave trough</td>
<td>4,087</td>
<td>330</td>
</tr>
<tr>
<td>8</td>
<td>Shortwave trough</td>
<td>101,567</td>
<td>2,468</td>
</tr>
<tr>
<td>12</td>
<td>Shortwave trough</td>
<td>30,211</td>
<td>299</td>
</tr>
<tr>
<td>13</td>
<td>Shortwave trough</td>
<td>437,836</td>
<td>1,537</td>
</tr>
</tbody>
</table>

Table 7. Temporal correlation between the observed and model-simulated total lightning flashes for four convective case studies observed during the DC3 test flight on 3 May 2011. The strongest correlation for each storm type is identified in bold font. The model output is based on the 18 UTC run on 2 May 2011, which is the day prior to the convective event.

<table>
<thead>
<tr>
<th>Storm</th>
<th>Storm Type</th>
<th>Flash Rate Parameterization Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$w_{\text{max}}$</td>
</tr>
<tr>
<td>6</td>
<td>Shortwave trough</td>
<td>0.70</td>
</tr>
<tr>
<td>8</td>
<td>Shortwave trough</td>
<td>0.36</td>
</tr>
<tr>
<td>12</td>
<td>Shortwave trough</td>
<td>0.59</td>
</tr>
<tr>
<td>13</td>
<td>Shortwave trough</td>
<td>0.88</td>
</tr>
</tbody>
</table>

Table 8. Spatial correlation between the observed and model-simulated total lightning flashes for four convective case studies observed during the DC3 test flight on 3 May 2011. The model output is based on the 18 UTC run on 2 May 2011, which is the day prior to the convective event.

<table>
<thead>
<tr>
<th>Storm</th>
<th>Storm Type</th>
<th>Flash Rate Parameterization Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$w_{\text{max}}$</td>
</tr>
<tr>
<td>6</td>
<td>Shortwave trough</td>
<td>0.92</td>
</tr>
<tr>
<td>8</td>
<td>Shortwave trough</td>
<td>-0.02</td>
</tr>
<tr>
<td>12</td>
<td>Shortwave trough</td>
<td>0.35</td>
</tr>
<tr>
<td>13</td>
<td>Shortwave trough</td>
<td>0.16</td>
</tr>
</tbody>
</table>
Since the final DC3 model configuration used the Morrison two-moment versus Thompson microphysics scheme, an additional case study period evaluated flash rate performance using three storms that occurred during 19-20 May 2011. The WRF model output indicated the Morrison two-moment microphysics scheme developed more intense convection than the Thompson scheme and produced 1.4-2.4 times as many flashes. Similar to previous case study, the UV scheme required the smallest scaling factors to match the adjusted NLDN flashes (Eqn. 1). Based on the results from the three separate case studies, I recommended the UV FRPS be used to forecast flash rates during DC3.

Figure 4. Total lightning flashes per model processor region based on (a) adjusted NLDN flashes, (b) UV scheme, (c) \( w_{\text{max}} \) scheme, and (d) CTH scheme on at 03 UTC on 3 May 2011 during the DC3 test flights. The model output is based on the 18 UTC run on 2 May 2011, which is the day prior to the convective event.
4.3 Tracking active convection

Following the completion of the DC3 field campaign, I developed 3-hour moving spatial masks that tracked the active convection sampled by ground stations and the DC3 aircraft during 16 of the 26 IOPs. Generally, IOPs were excluded if they focused on (1) active convection not sampled by both the GV and DC8 aircraft, (2) aged convective outflow, or (3) boundary layer emission measurements under clear sky conditions. The bounding boxes were used by Bruning (2014a, 2014b) to generate LMA total flash statistics for the thunderstorm complexes within the 2D detection range of an LMA network. This data is publicly accessible in the Earth Observing Laboratory (EOL) DC3 field catalog and provides a high level statistical summary on the LMA sources, as well as flash initiation, footprint, extent, and energy.

4.4 The 29-30 May 2012 Oklahoma severe supercell system

On the morning of 29 May 2012 conditions were very unstable and favorable for convective development within the Oklahoma domain. The 12 UTC sounding from Norman, Oklahoma, indicated the wind profile generally had a westerly component with veering from the surface to 600 hPa. A dryline was located across the Texas panhandle and a cold front stretched across the Ohio River Valley from northeast-to-southwest, with the southern portion pushing northward as a warm front over Oklahoma and Kansas. By 21:10 UTC the front was quasi-stationary and two isolated cells developed to its south along the Kansas-Oklahoma border and ahead of the dryline. Over the next several hours both storms formed mid-level mesocyclones (DiGangi et al., 2016) and evolved into a line of supercells. The line continued in an east-southeast direction as new cells formed
behind it and underneath the anvil. The severe supercell system evolved into a multicell MCS by 03:00 UTC on 30 May and moved through central Oklahoma within the hour.

Meteorological data collected by ground-based instrumentation in the Oklahoma domain include radar data from the NSSL WSR-88D or Next Generation Radar (NEXRAD) located near Norman, Oklahoma, and the NSSL’s NOAA X-band polarimetric (NOXP) and C-band Shared Mobile Atmospheric Research and Teaching (SMART) radars. Lightning data are provided by ground-based facilities via the central Oklahoma LMA network and NLDN. The total lightning flash detection efficiency provided by the 11 stations in this LMA network is > 90% at a 200 km radius (Chmielewski and Bruning, 2016). The convection developed between the northern edges of the LMA network’s 2D and 3D lightning detection coverage (Figure 5). As the storm system progressed east-southeastward, it stayed within the 2D coverage of the network for the majority of its life (21:10-04:19 UTC) and was generally within the 3D coverage area between 23:40-03:00 UTC when the flashes were within roughly a 100 km radius. The NLDN CG flash detection efficiency is 90-95% over the continental United States (Cummins and Murphy, 2009).
Figure 5. Total lightning flashes observed by central OK LMA network from 21:10 UTC on 29 May to 04:20 UTC on 30 May 2012. The 3D and 2D lightning detection coverage is represented by the 100 km and 200 km radius from the center of the network, respectively. The network center is located at approximately 35.279°N, 97.918°W.

The observed total lightning flash rate time series was generated from a grid of LMA data with 1-min temporal and 1-km spatial resolution. Figure 6 shows that the maximum flash rate observed by the LMA occurred at 01:37 UTC (312 flashes min\(^{-1}\)). The CG flash rate time series was produced from the observed NLDN flash data with weak positive CG flashes (peak current < +15 kA) filtered out. The peak CG flash rate (94 flashes min\(^{-1}\); Figure 6) occurred roughly 15 minutes later (01:51 UTC).

Approximately 8,679 CG and 31,633 total flashes were observed over the lifetime of the convection with an average total flash rate of 75.5 flashes min\(^{-1}\). Roughly 15,060 total flashes occurred during the 5-hour period simulated in our case study (20:00-01:00 UTC observed time), with an average total flash rate of 68.5 total flashes min\(^{-1}\). The 1-min
data from both networks were binned into 10-min intervals (Figure 7) to match the output from the WRF model. The total flash rate time series shows several distinct peaks as the flash rate increased from 21:30 UTC to the maximum (~2,600 flashes 10-min\(^{-1}\)) at 01:40 UTC. These peaks occurred at 22:00 UTC, 22:50 UTC, 23:50 UTC, and 01:00 UTC with roughly 100, 300, 800, and 2,200 total flashes 10-min\(^{-1}\), respectively. Following the primary peak, the observed flash rate decreased at a faster rate than it increased. The 29-30 May 2012 convection contained high flash rate supercells with small flash extents (Barth et al., 2015). DiGangi et al. (2016) also showed the Kingfisher storm, which was within the southern portion of the convection analyzed in this case study, had an abundance of small flashes, especially during its mature phase, when flash rates were > 100 flashes min\(^{-1}\).

The 10-minute time evolving intracloud to cloud-to-ground (IC:CG) flash ratios were calculated over the life of the storm using the observed NLDN CG and LMA total lightning flash data (Figure 8). The LMA data was partitioned into IC and CG flashes by matching the timing and location of the NLDN CG and LMA total flash data. The mean time varying IC:CG ratio over the storm lifetime is 2.73±2.51, while the mean for the 5-hour simulation period is slightly higher (3.93±2.22).

During this mission the DC8 focused on storm inflow and outflow, while the GV concentrated on high-altitude outflow. The 1-sec DC8 and GV aircraft data is averaged over 5 sec and 4 sec, respectively, to correspond with the 1 km × 1 km horizontal resolution of the model data. \(\text{NO}_x\) measurements were not available for the Falcon for this research flight. The NSSL Mobile GPS Advanced Upper-Air Sounding System (MGAUS) provided upper air data in the vicinity of the storm. Three mobile soundings
were deployed at 20:29 UTC (35.667 °N, 98.341 °W) and 22:55 UTC (35.854 °N, 98.066 °W) on 29 May and 00:21 UTC (35.595 °N, 97.859 °W) on 30 May (Ziegler, 2013b). The 22:55 UTC sounding lost data as the radiosonde passed through the anvil and is spliced with data from the 20:29 UTC sounding above 435 hPa, since the upper air profile likely changes more slowly in the upper versus lower troposphere (Conrad Ziegler, personal communication, April 18, 2017). Visible satellite imagery from the Geostationary Operational Environmental Satellite-13 (GOES-13) was used to estimate the anvil area of the observed storm system from 21:10-01:00 UTC, prior to reduction in sunlight and the quality of the visible images.

Figure 6. The Oklahoma LMA total and NLDN CG lightning flash data per 1-minute provided for the lifetime of the observed 29-30 May 2012 severe supercell system (21:10-04:19 UTC).
Figure 7. The Oklahoma LMA total and NLDN CG lightning flash data per 10-minutes provided over the lifetime of the observed 29-30 May 2012 severe supercell system (21:10-04:19 UTC).

Figure 8. The IC:CG ratios per 10-minutes provided over the lifetime of the observed 29-30 May 2012 severe supercell system (21:10-04:19 UTC). The ratios are based on the Oklahoma LMA total lightning and NLDN CG flash data in Figure 7.
The WRF-Chem is a cloud-resolving model, which combines the mesoscale forecasting capabilities of the WRF model with chemistry modeling (Grell et al., 2005). The WRF-Chem allows for online simulations, which more accurately characterize the production and transport of trace gases and aerosols than offline simulations and guarantees consistency with the meteorological fields. It can be initialized and constrained by the larger-scale meteorological conditions provided by sources such as the Global Forecasting System (GFS). The model also allows the inclusion of feedback processes of the chemistry and aerosols on the meteorological fields, which is significant when determining the effects of chemistry on climate.

The physical and chemical processes represented in the WRF-Chem include transport, deposition, emission, chemical transformation, aerosol interactions, photolysis, and radiation (Grell et al., 2005). The LNO$_x$ production may be estimated for both cloud-resolved and parameterized convection given the lightning flash rate time series, the horizontal and vertical distribution of lightning flashes, and the NO production per IC and CG flashes. Flash rates can either be predicted from storm parameters (see Section 2.3) or, to reduce uncertainty, prescribed directly from lightning observations (DeCaria et al., 2005; Ott et al., 2010; Cummings et al., 2013). Likewise, the flash type can be predicted (Price and Rind, 1993; Pickering et al., 1998; Fehr et al., 2004) or prescribed from observations (DeCaria et al., 2005; Ott et al., 2007, 2010; Cummings et al., 2013).
5.1 Model set-up

Bela et al. (2016) simulated the 29-30 May supercell system at cloud-resolved resolution using the WRF-Chem model, version 3.6.1. We use the same model conditions as Bela et al. (2016), but with some modifications, which are outlined below, to improve the model-observations agreement. The model domain contains $480 \times 420 \times 89$ grid points in the x, y, and z directions with 1-km horizontal resolution and variable vertical resolution from 50 m near the surface to 250 m at the top of the domain (50 hPa). The southwest corner of the domain is located at 33.8196 °N, -99.7726 °W and the northeast corner is located at 38.1354 °N, -95.0998 °W. The initial 8-hour simulation ran from 18:00 UTC on 29 May to 02:00 UTC on 30 May using 480 processors on the NCAR Yellowstone supercomputer. The simulation does not extend past 02:00 UTC because we are interested in the time period when lightning would be influencing the NO$_x$ mixing ratios sampled by the DC3 aircraft in the anvil outflow (Cummings et al., 2017a). For subsequent simulations a restart file was used at 21:00 UTC to reduce computation time since the observed convection began just after 21:00 UTC. The simulation is integrated with a 3 sec time step, while the lightning parameterization is called every 6 sec.

The initial model configuration and physics and chemistry options are based on Bela et al. (2016) Meteorological initial and boundary conditions were provided by the 6-hour interval North American Mesoscale Analysis (NAM-ANL) at 12 km resolution. The constant initial and boundary chemistry conditions are reset at 21 UTC using a combination of data from the DC8 profile (i.e., for the boundary layer and free troposphere) and the Model for Ozone and Related chemical Tracers version 4 (MOZART; available from NCAR). Table 9 provides the final model physics and
chemistry options selected for this analysis. Detailed descriptions of some of the selected schemes are provided below.

Table 9. WRF model physics and chemistry options selected for 29-30 May 2012 Oklahoma case study.

<table>
<thead>
<tr>
<th>WRF Model Options</th>
<th>Name of Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>Microphysics</td>
<td>Morrison two-moment scheme</td>
</tr>
<tr>
<td>Planetary boundary layer</td>
<td>YSU scheme</td>
</tr>
<tr>
<td>Surface layer</td>
<td>MM5 similarity scheme</td>
</tr>
<tr>
<td>Land surface</td>
<td>Unified Noah LSM</td>
</tr>
<tr>
<td>Radiation (shortwave &amp; longwave)</td>
<td>RRTMG</td>
</tr>
<tr>
<td>Cumulus parameterization</td>
<td>None</td>
</tr>
<tr>
<td>Convective damping</td>
<td>21:00-21:20 UTC (Li et al., 2017)</td>
</tr>
<tr>
<td>Lightning data assimilation</td>
<td>21:30-23:00 UTC (Fierro et al., 2012)</td>
</tr>
<tr>
<td>Lightning flash rate parameterization</td>
<td>• 18 FRPSs (Table 1)</td>
</tr>
<tr>
<td></td>
<td>• IC:CG ratios based on LMA &amp; NLDN observations</td>
</tr>
<tr>
<td>LNO\textsubscript{x} vertical &amp; horizontal distributions</td>
<td>• Observed CG &amp; IC flash channel vertical distributions</td>
</tr>
<tr>
<td></td>
<td>• Radar reflectivity (\geq 20) dBZ</td>
</tr>
<tr>
<td>Temperature of peak of LNO\textsubscript{x} vertical distribution for lightning</td>
<td>• IC peak = -45 °C</td>
</tr>
<tr>
<td></td>
<td>• CG peak = -40 °C</td>
</tr>
<tr>
<td>Moles NO emitted per flash</td>
<td>• IC = 82; CG = 82</td>
</tr>
<tr>
<td>Chemical mechanism</td>
<td>MOZCART (MOZART chemistry &amp; GOCART aerosols)</td>
</tr>
<tr>
<td>Wet scavenging &amp; ice retention</td>
<td>Assume zero retention for trace gases (Bela et al., 2016)</td>
</tr>
</tbody>
</table>

The Morrison two-moment microphysics scheme predicts the mass mixing ratio for cloud droplets, and both mass and number mixing ratios for rain, cloud ice, snow, and graupel/hail (Morrison et al., 2015). The dense precipitating ice options can influence the storm structure, cold pool, and precipitation of deep convection due to differences in their terminal fall speed and bulk density (Morrison and Milbrandt, 2011; Bryan and Morrison, 2012; Adams-Selin et al., 2013; van Weverberg, 2013). For severe continental deep
convection, such as the 29-30 May case study, we set the dense precipitating ice to have hail characteristics.

MOZART is an offline global chemical transport model, which is suited for the troposphere (Emmons et al., 2010). The output from MOZART is used for chemical initial and boundary conditions the WRF-Chem regional model. Several of the WRF-Chem online calculations include photolysis rates, dry deposition, and biogenic emissions. Several gas-phase chemistry mechanisms are available for use in WRF-Chem. I have selected the MOZART mechanism to be consistent with the incoming initial and boundary conditions. This chemical mechanism contains gas-phase species, bulk aerosol compounds, and photolysis and gas-phase reactions, in addition to an updated isoprene oxidation scheme and a separation of volatile organic compounds into three groups (i.e., alkanes, alkenes, and aromatics). The MOZART chemical scheme is connected to WRF-Chem via the Kinetic PreProcessor (KPP) and can be combined with the Georgia Tech/Goddard Chemistry Aerosol Radiation and Transport (GOCART) aerosol scheme (MOZCART). To simulate the observed trace gas mixing ratios in storm outflow, Bela et al. (2016) found an ice retention assumption of zero for all species (i.e., formaldehyde (CH\textsubscript{2}O), hydrogen peroxide (H\textsubscript{2}O\textsubscript{2}), HNO\textsubscript{3}, sulfur dioxide, and methyl hydrogen peroxide) provided the best agreement for CH\textsubscript{2}O and H\textsubscript{2}O\textsubscript{2} observations when used in combination with MOZART’s simple wet scavenging scheme (i.e., Neu and Prather, 2012).

The GOCART model is generally a bulk aerosol scheme, which determines the total mass of each aerosol type, but does not provide particle size information, except for dust and sea salt (Chin et al., 2000). This scheme is considered numerically efficient and
allows for simulations with complex gas-phase and aqueous chemistry. GOCART is connected with the radiation schemes in WRF-Chem, such that the direct effect of aerosols can be considered. However, it is not connected with the cloud microphysics schemes in the WRF-Chem version used for this case study. Therefore, the indirect effects associated with clouds cannot be computed with this aerosol scheme. Additional types of aerosol modules are also available in WRF-Chem (i.e., modal and sectional).

5.2 Convective damping and lightning data assimilation techniques

Methods can be used to guide the model when simulations do not reproduce the observed convection in the correct space or time. I implemented these techniques in this cloud-resolved simulation as a way to try to bring the hydrometeors in the WRF simulated storm closer in the line with the proxy observations (Cummings et al., 2017a).

The convective damping technique clears convection from the model prior to the observed convective initiation by reducing the model-simulated water vapor at each 3D grid point where relative humidity exceeds a specific threshold (Li et al., 2017). In the 29-30 May case study, water vapor was constrained to be less than a relative humidity of 75% from 21:00-21:30 UTC (prior to the beginning of continuous observed lightning flashes at 21:31 UTC) in order to decrease excessive buoyancy.

Fierro et al. (2012) developed a lightning data assimilation (LDA) technique to guide the placement of water vapor, so buoyancy is generated at the proper times and locations for convective development. Their equation is:

\[ Q_v = AQ_{sat} + BQ_{sat} \tan(CX) \left[ 1 - \tanh(DQ_x^2) \right], \]

(2)
where $Q_v$ is the water vapor mixing ratio (g kg$^{-1}$), $Q_{sat}$ is the water vapor saturated mixing ratio (g kg$^{-1}$), $Q_g$ is the graupel mixing ratio (g kg$^{-1}$), $X$ is the flash rate, and constant coefficients are represented by $A$, $B$, $C$, and $D$. For this case study, the coefficient values are 0.93, 0.20, 0.01, and 0.25, respectively. Coefficient $A$ controls the minimum threshold for relative humidity within a grid column to ensure the relative humidity stays above a predefined minimum value (93%). The default value for coefficient $A$ is 0.81, but can be increased for weakly electrified storms (Fierro et al., 2012). While this case study is considered a high flash rate event, coefficient $A$ was varied between 0.81 and 0.95. A value of 0.93 provided a closer representation of the observed storm when used in combination with the convective damping and other LDA variables. Previous studies have added water vapor back into the column within the mixed-phase graupel-rich region (0 °C to −20 °C) (Fierro et al., 2012), the lower troposphere (< 700 mb) (Marchand and Fuelberg, 2014; Fierro et al., 2016), and between the lifting condensation level (LCL) and $w_{max}$ height (Li et al., 2017). Our focus was on improving the mixing ratio and vertical placement of the simulated hydrometeors (e.g., graupel), so water vapor was introduced between the LCL (16 °C) and the lower level of the mixed-phase region (−5 °C). If this lower limit was extended to colder temperatures, it is possible the water vapor may instantly deposit onto ice particles and not provide the desired improvement.

The lightning stroke counts detected by the Earth Network Total Lightning Networks (ENTLN) from 21:30-23:00 UTC (i.e., roughly the beginning of the continuous lightning to the mature stage) were gridded using the same 1 km × 1km horizontal resolution as the WRF and introduced into the model over the same time period. At
model grid points with more than one stroke, graupel mixing ratios < 3.0 g kg\(^{-1}\), and ambient relative humidity < 95%, the LDA modifies the water vapor between -5 °C and 16 °C. The relative humidity is also constrained to be ≤ 103%.

5.3 Lightning flash rate parameterization in WRF-Chem

The \( w_{\text{max}} \) and CTH FRPSs are the only schemes currently available in the publicly accessible version of the WRF. I added the other 16 FRPSs provided in Table 1 for this case study. I also wrote the code for 11 of the 16 schemes (i.e., schemes developed after 2009) and made slight modifications to all 18 schemes (i.e., hydrometeor scaling). The equations for all 18 FRPSs (Table 1), except the ICEFLUX and LTG3 schemes, are calculated for bulk quantities in each computer processor within the model domain. Each processor is roughly 18 km \( \times \) 19 km in area and will likely contain either complete or partial storm cores as the simulated storm moves through the domain. This approach could overestimate total lightning flashes for the linear schemes with positive y-intercepts, as well as non-linear schemes. Flash rates may also be underestimated by linear schemes with negative y-intercepts.

In addition, the linear FRPSs with non-zero y-intercepts are only used when the storm parameter calculated for the processor exceeds a specific minimum value. This prevents negative flash rates, which are not realistic, from occurring in the UV, IWP, and PIM schemes and positive flash rates from occurring when the IMFP value is zero.

The WRF provides several options for controlling the IC:CG ratio. One method uses the coarsely prescribed ratios based on the 1995-1999 NLDN/OTD climatologies from Boccippio et al. (2001). For this case study, this method assigns an IC:CG ratio of 3.55 to the central United States (90-105 °W). This ratio is similar to the climatological
mean IC:CG ratio calculated specifically for the Oklahoma domain (3.90±0.49), which is based on the Boccippio gridded data for May. I replaced the single climatological value for the central United States (3.55) by the actual observed 10-minute time evolving IC:CG ratios (Figure 8) only within the area of the associated 10-minute moving spatial mask that surrounds the storm system.

5.4 Lightning NO\textsubscript{x} parameterization in WRF-Chem

I replaced the default Gaussian vertical distributions for CG and IC lightning, which are appropriate for WRF-Chem thunderstorm simulations at cloud-resolved scales (DeCaria et al., 2000), with the observed vertical profiles constructed using the source data detected by the central Oklahoma LMA network during the 29-30 May convective event. The observed CG and IC vertical distributions at 1-min resolution showed the profile shape and the altitude of the peak in flash channel lengths varied over the lifetime of the convection; however, the mean profiles for both flash types were unimodal Gaussian distributions (Figure 9). The CG vertical profile maximizes at a considerably colder temperature (-40 °C or 9.5 km) than the default vertical distribution (-15 °C or 6 km). The observed and default IC vertical profiles both peak at -45 °C (10.5 km), but the observed profile does not have the lower second peak shown in the default distribution. The horizontal placement of the LNO\textsubscript{x} follows the bulk approach and is injected within the 20 dBZ reflectivity contour (DeCaria et al., 2005; Ott et al., 2010). The radar reflectivity threshold is not modified because the majority of the observed LMA sources are within the 20 dBZ contour (Figure 10).
Figure 9. (Top) The default CG and IC vertical distributions of flash channel lengths by DeCaria et al. (2000). (Bottom) The mean CG and IC vertical distributions of flash channel lengths observed 29-30 May 2012 severe supercell system.
Prior analyses for the 29-30 May convective event suggested an LNO\textsubscript{x} production scenario of 125 moles NO flash\textsuperscript{1} was appropriate (Bela et al., 2016; Cummings et al., 2016) given the default model parameters for the flash channel vertical profiles (DeCaria et al., 2000) and IC:CG ratio (Boccippio et al., 2001). However, I tested additional scenarios with the modified model to determine if a different amount of LNO\textsubscript{x} or unequal LNO\textsubscript{x} production per CG and IC flash provide a closer representation of the aircraft observed NO\textsubscript{x} in the anvil outflow.

Figure 10. Percentage of VHF sources observed by the central Oklahoma LMA from the 29-30 May 2012 severe supercell system (21:10-04:19 UTC) by altitude and reflectivity.
Prior to inclusion of the convective damping and LDA techniques, the WRF represented the observed storm location, dimensions, and vertical motion reasonably well; however, the model-simulated anvil area was ~60-95% smaller than the observations during the first hour and roughly 20-50% smaller after that time. Thirteen of the 18 FRPSs also grossly overestimated (> 100%) the LMA flash rates observed in the 29-30 May severe supercell system. Every hydrometeor-based scheme overpredicted, which prompted an investigation of the model-simulated hydrometeor mixing ratios and their location within the convection.

The damping and LDA methods were tested with the intent of improving the location and mixing ratio of the hydrometeors in the model. By removing excess moisture from the atmosphere in locations with no observed convection and then guiding water vapor back into the atmosphere with the help of lightning observations, the maximum graupel mixing ratio decreased by ~2 g kg\(^{-1}\) and the height of the maximum appeared to lower by ~1 km. While these methods have provided the best results thus far for modifying the hydrometeors in this case study, the remaining differences between the proxy observations (Section 6.2) and WRF simulation are likely due to microphysics scheme assumptions. The simulation results in Section 6.1 are based on the model’s final configuration, which includes damping and LDA (Table 9).

In addition to incorporating the damping and LDA, several other approaches were used to explore the overprediction. These included assigning thresholds to the frozen hydrometeors and scaling the model hydrometeors to proxy observations. Each approach
is described in Section 6.2. The NSSL two-moment microphysics scheme (Mansell et al., 2010) was also tested using the LDA assumptions of Bela et al. (2016) and the damping and LDA assumptions in this study; however, both simulations yielded a poorer representation of the storm system. The FRPS performance is evaluated in Section 6.3 using the final model configuration, as well as a set of criteria and hydrometeor scalings. A discussion about why the FRPSs succeeded and failed in replicating the observed flash rate trends follows in Section 6.4.

6.1 Meteorological conditions

The observed and model-simulated storms both initiated along the Kansas-Oklahoma border. The model-simulated storm initiated at 22:10 UTC, approximately an hour after the observed convection; however, as the simulated convection matures the offset is 30-50 minutes. Figure 11 shows the location of the observed (left column) and simulated (right column) cells at the observed and model times where the spatial agreement is best. Figures 11a and 11b show the location of the observed and simulated cells 40 minutes after their respective initiations. As the cells form a north-south line, both the observations (Figure 11e) and model (Figure 11f) indicate radar reflectivities of 60-65 dBZ in similar locations. To the east of the line new cells develop beneath the anvil, although the model-simulated cells (Figure 11h) are not as individualized as the observations (Figure 11g). While the observations show an orientation of the line toward the southeast, the WRF tilts the line toward the southwest by the end of the simulation. However, both the NEXRAD (Figure 11i) and WRF (Figure 11j) indicate that the southernmost cell in the main system is most dominant (the “Kingfisher storm”).
Figure 11. Composite radar reflectivity from the 29-30 May 2012 severe supercell system for the observed storm at (11a) 21:50 UTC, (11c) 22:40 UTC, (11e) 23:00 UTC, (11g) 00:20 UTC, and (11i) 01:00 UTC observed time, and the WRF model-simulated storm with damping and LDA techniques at (11b) 22:50 UTC, (11d) 23:10 UTC, (11f) 23:50 UTC, (11h) 00:50 UTC, and (11j) 01:40 UTC model time. Note, there is a 1-hour delay in the model-simulated storm initiation, but this offset is not maintained as the storm matures. The black box in each image highlights the portion of the convection that is the focus of the observed and modeled storm at the selected time. The black dashed line in a plot represents where a vertical cross section is located.
The WRF simulation captures several additional aspects of the severe supercell system: (1) the east-southeast progression of the line and the cells that form to its east and west, (2) the development of the “Kingfisher storm” and its merger with the northern cell, and (3) the initiation and northeast motion of the cell to the south that merges with the convective system. However, the convection to the northwest and southwest of the line of supercells is slightly delayed in the model. A comparison between the observed visible satellite imagery and the model-simulated total hydrometeors (i.e., cloud water, rain, snow, ice and hail) at 10.5 km altitude from 22:10-01:00 UTC model time suggests the model storm underestimates the anvil area by ~60-70% for the initial 30-40 minutes of development and is then within 10% until 01:00 UTC model time (Figure 12). The eastern edge of the anvil begins to move outside the model domain after 01:00 UTC; therefore, no further comparisons were made.
Figure 12. Comparison of the anvil area from the 29-30 May 2012 severe supercell system detected by GOES-13 at (a) 21:30 UTC and (c) 23:40 UTC observed time and by the WRF model-simulated total hydrometeors (g kg\(^{-1}\)) at 10.5 km altitude at (b) 22:30 UTC and (d) 00:40 UTC model time. The dashed black box in each image highlights the portion of the convection that is the focus of the observed and modeled storm at the selected time.
The model-simulated composite radar reflectivity suggested the size of the convective cores was similar to the storm observed by NEXRAD, both in the horizontal and vertical. Generally the convective regions (>30 dBZ) had dimensions of 20-40 km in the east-west and 20-30 km in the north-south directions for both the observed and model-simulated storms. However, the model has difficulty maintaining the individualized areas of higher reflectivity that are noted in the NEXRAD composite reflectivity. While the LDA was being applied, the convective cells in the simulated storm appeared more individualized, as in the observations. After the LDA stopped, it became more difficult to discern individual cells as the areas of simulated higher reflectivity appeared to merge. The maximum radar reflectivity simulated by the model (~69 dBZ) was within the range of the observations (65-70 dBZ). The 0 dBZ contour indicates the model-simulated radar top of the storm (~16 km) was within 10% of the observed radar top height (~17 km). Unlike the observations, radar reflectivities > 50 dBZ tend not to extend above roughly 6 km altitude in the model (Figure 13).

**Figure 13.** Vertical cross-section of composite radar reflectivity from the 29-30 May 2012 severe supercell system for the (a) observed storm at 01:00 UTC observed time and (b) WRF model storm with damping and LDA techniques at 01:40 UTC model time.
Since six FRPSs rely on radar reflectivity to compute storm parameters, the observed and model-simulated radar volumes are compared. During the first hour the observed 18 dBZ, 25 dBZ, and 35 dBZ echo volumes are underestimated by ~16%, overestimated by ~23%, and overestimated by ~500%, respectively. The simulated echo volumes overestimated the observations by ~10-35% over the next 1.5-2 hours and underestimated the observations by ~15-30% the last 1-1.5 hours. This suggests the model storm is initially too intense based on the large overestimation of the 35 dBZ volume, but becomes more similar to the observations as the storm matures.

The model-simulated convection generated a maximum vertical velocity (~62 m s\(^{-1}\)) within ~5% of the mobile radars observations (~65 m s\(^{-1}\)) (DiGangi et al., 2016). The observed and simulated maximum values both occurred in the southernmost cell of the system at the same time relative to storm initiation (23:30 UTC observed time and 00:30 UTC model time), but the maximum was located at 8-9.5 km altitude in the observations (Bela et al., 2016) and at ~10 km altitude in the simulation. The WRF model generates a storm in an environment with a mixed-layer convective available potential energy (MLCAPE) of 2553 J kg\(^{-1}\). This is similar to the 22:55 UTC observed mobile sounding (2759 J kg\(^{-1}\)), although the simulated upper air profile is slightly drier in the boundary layer and more moist in the upper troposphere, particularly at ~240 hPa (Figure 14). Similar to the observed sounding, the simulated profile indicates veering in the lower troposphere with upper level winds with a westerly component, along with a surface-6 km bulk shear (25 m s\(^{-1}\)) that is comparable to the observations (24 m s\(^{-1}\)).
Figure 14. The observed (black) and model-simulated (blue) skew-t diagrams on 29-30 May 2012. The NSSL MGAUS was released from (35.854 °N, 98.066 °W) at 22:55 UTC. The WRF model-simulated upper air profile represents the one-hour offset in convection (23:50 UTC model time) at (35.86 °N, 97.70 °W). Wind speed is in m s⁻¹.

6.2 Hydrometeors

6.2.1 Proxy observations

Hydrometeors play a key role in the FRPSs that are tested in WRF, with 10 of the 18 schemes directly involving relationships between total lightning activity and hydrometeors and three schemes involving calculated radar reflectivity, which is dependent on the hydrometeors. Before the current damping and LDA techniques were applied, the model-simulated flash trends based on hydrometeors were overpredicting the observed total lightning. DiGangi (2014) investigated the hydrometeors in the Kingfisher storm for three specific times over a 40-minute period (00:00-00:40 UTC model time) using a diabatic Lagrangian analysis (DLA) approach. The DLA is constrained by the observed 4-dimensional radar winds and a simple cloud model (Ziegler, 2013a). Since the Kingfisher storm composed the southern portion of the severe convection analyzed in this case study, the DLA hydrometeor output are assumed to be a close approximation of
the actual hydrometeors. These proxy observations are provided at three to five altitude levels ranging from 1.2 to 12.2 km for graupel/hail, 6.2 to 16.2 km for snow/ice, and 4.7 to 7.2 km for rain water and cloud water at each of three times. It is assumed that if WRF closely captures the hydrometeors of the Kingfisher storm, then it is likely that the northern section of the convective system will also be represented to the same degree.

Horizontal and vertical hydrometeor cross-sections through the WRF simulated southern convection, prior to the current damping and LDA assumptions, were compared against the DLA hydrometeor mixing ratios provided by DiGangi (2014). A comparison of the maximum WRF and DLA hydrometeor concentrations averaged over all of the available altitudes during the 40-minute period indicated that WRF overestimated the maximum DLA graupel mixing ratios by roughly 25% and underestimated the snow/ice by roughly 20%. Since WRF underestimates cloud water by less than 10%, it is considered similar to the proxy observations below 7.2 km. Rain water, however, is overestimated by ~70% below 7.2 km. Bela et al. (2016) compared the simulated precipitation (rain and graupel) from their WRF-Chem run against the mean hourly precipitation from the NCEP Stage IV analysis. The comparison suggested that although there were differences in the precipitation distribution, the observed total precipitation received at the surface was overestimated by < 20% in the northern convection from 23:40-00:40 UTC model time.

6.2.2 Ice hydrometeor thresholds

Initially the FRPSs requiring graupel and snow used mixing ratio thresholds of $1.0 \times 10^{-12} \text{ g kg}^{-1}$. This was believed to be too low and a possible cause for the overestimation by the hydrometeor-based FRPSs (not shown), as these thresholds would
potentially include grid cells outside the charging region (e.g., stratiform anvil precipitation region). The minimum graupel and snow mixing ratio thresholds were increased to 0.5 g kg\(^{-1}\) and 0.25 g kg\(^{-1}\), respectively, to better represent the kinematic and microphysical processes related to charging in the convective core. Raising both thresholds helped to reduce the total flashes. For example, for the CSU GEV scheme, the estimated total flashes were reduced by \(\sim 20\%\). However, the LMA observations were still overestimated by the hydrometeor-based schemes.

Based on the results from Section 6.2.1, several attempts were made to reduce the graupel/hail and increase the snow within the convection by modifying the Morrison two-moment microphysics scheme. The threshold for converting snow to graupel/hail by riming was increased, which should decrease the amount of graupel/hail within the cloud (Hugh Morrison, personal communication, February 24, 2016). The results (not shown) indicate that increasing the snow threshold from 0.1 g kg\(^{-1}\) to 0.5 g kg\(^{-1}\) or 1.0 g kg\(^{-1}\) led to a 1-10\% and 2-50\% decrease in the model-simulated graupel/hail and snow/ice concentrations, respectively. Therefore, this modification did not significantly reduce the amount of graupel/hail present in the 29-30 May model-simulated storm and it also decreased the amount of snow when an increase was needed.

6.2.3 Scaling hydrometeor mixing ratios

The vertical cross sections of model hydrometeors from the WRF simulation with damping and LDA (Figure 15) also show the model-simulated graupel, snow, and ice do not extend over the same altitude ranges as indicated by the proxy observations. Rain water was not investigated in more detail because it was assumed to be precipitating and not contributing to the overestimation of the hydrometeor-based FRPSs. Therefore, a
closer inspection was taken of the WRF frozen hydrometeors’ vertical distribution and compared with that from the DLA. The analysis suggests the graupel overestimation is primarily above 9 km altitude and the snow/ice underestimation mainly occurs between 11-13 km altitude. By focusing on these specific altitudes for the three times during the 40-minute period, instead of all altitudes, it was determined that WRF (1) overestimated graupel by roughly 55% above 9 km altitude and (2) overestimated snow/ice by 31% below 11 km altitude and underestimated snow/ice by 42% between 11-13 km altitude. Altitude-specific scaling factors for the hydrometeors were developed based on these percentage biases.

Figure 15 uses vertical cross sections through the approximate location of the Kingfisher storm in the southern portion of the WRF model-simulated convection to compare the graupel and snow/ice mixing ratios before and after the altitude specific scaling factors are applied to the hydrometeors in the WRF output. The results show the altitudes of maximum mixing ratio of the model-simulated graupel and snow/ice are more representative of the proxy observations after scaling is applied. For example, at 23:40 UTC observed time DiGangi (2014) indicated that above the freezing layer the maximum observed graupel/hail mixing ratio is ~9.0 g kg\(^{-1}\) between 8.2-8.7 km. Prior to scaling the WRF-simulated graupel/hail, the largest mixing ratios (9-10.8 g kg\(^{-1}\)) at the corresponding model time (00:20 UTC) are located between ~8.3-14.4 km (Figure 15a). After applying the scaling factors (Figure 15b) the maximum mixing ratios are similar (9-10.2 g kg\(^{-1}\)), but found over a smaller altitude range (~8.5-9 km) that is closer to the observed height. For the proxy observed snow/ice, the maximum mixing ratio (8-10 g kg\(^{-1}\)) is between 11.7-13.2 km (DiGangi, 2014). The maximum WRF-simulated
snow/ice mixing ratio increases from 3.1 g kg$^{-1}$ between 11.3-12.5 km (Figure 15c) to 5.3 g kg$^{-1}$ within a similar altitude range (11-13 km) after scaling (Figure 15d). While the WRF-simulated snow/ice is still underestimating the proxy observations at this time and vertical cross-section location, the horizontal distance covered by the simulated snow/ice mixing ratios (1-5 g kg$^{-1}$) has slightly increased within this altitude layer.

With the application of the current damping and LDA assumptions, the location and maximum mixing ratio of the model-simulated hydrometeors were adjusted closer to the observations. These techniques did not correct the hydrometeors perfectly, so scaling to the DLA proxy observations was required to improve the simulated hydrometeors for our case study. However, some discrepancies still exist after scaling (i.e., graupel is slightly overestimated and snow/ice is slightly underestimated). For use in the WRF simulation, the altitude-specific scaling factors are only applied to the hydrometeors in the FRPS code, not in the microphysics scheme.
Figure 15. The WRF model-simulated graupel (top) and snow/ice (bottom) mixing ratios at 00:20 UTC model time before (a,c) and after (b,d) the altitude-specific scaling factors are applied to the hydrometeors in the FRPS code only. The solid black line represents the outline of the cloud, where total hydrometeors equal 0.01 g kg\(^{-1}\). The dashed black lines indicate the specific altitudes where the scaling factors are applied. In the top figures, a graupel scaling factor is only applied above 9 km. In the bottom figures, a different snow/ice scaling factor is applied below 11 km and between 11-13 km.

6.3 Lightning Prediction

We examine the flash rate time series and total flashes predicted by the 18 FRPSs over the simulation period and compare them with the LMA observations. The lightning included in the analysis occurs within the bounding boxes that envelop and adjust to the simulated and observed convection every 10-minutes as the system matures. An example of the location of these boxes is provided in Figure 11. Figure 16 shows the observed and
model-simulated flash time series for the six schemes analyzed by Barthe et al. (2010). These schemes are evaluated against the observations and each other starting at the moment when reflectivity is first noted in the NEXRAD (21:10 UTC) and the model (22:10 UTC). Since the storm simulation ends at 02:00 UTC model time, the primary peak and downward trend in the flash rate time series cannot be compared with observations for the final two hours of the storm system. As indicated by the reflectivity analysis, the time evolution of the observed and model storms differ, which may affect the flash rate comparisons. The number of total flash counts generated by each FRPS before and after scaling the hydrometeors is provided in Table 10. This shows the overestimation of the flash rates and total flashes persists for the five non-hydrometeor-based schemes and 12 of the 13 hydrometeor-based schemes. The remainder of this section presents the results from the WRF simulations with LDA, damping, and hydrometeor scaling based on the proxy observations.
Figure 16. The total lightning flash rates per 10-minutes from the LMA (black) and the FRPSs based on relationships between total lightning activity and storm parameters from the literature. The top and bottom figures show the same data, except the y-axis on the top plot is expanded. The model-simulated lightning flash rates are based on a WRF run with damping/LDA techniques, and hydrometeor altitude specific scaling factors applied to the FRPS code only. The model-simulated lightning flash time series is adjusted 60 minutes earlier, so the observed (21:10 UTC) and model-simulated (22:10 UTC) storm initiation times coincide. The FRPSs represent the model-simulated trends from 22:10-02:00 UTC model time. The solid black line represents the observed lightning flashes from 21:10-01:00 UTC, which covers the same time period as the simulated flashes. The dashed black line represents the continuation of the observed time series after 01:00 UTC.
Table 10. Number of model-simulated total lightning flashes predicted from 22:10-02:00 UTC model time by the 18 flash rate parameterization schemes before and after the model-simulated hydrometeors are scaled within the schemes. Results are from simulations that include damping and LDA. The LMA observed 15,060 total lightning flashes from 21:10-01:00 UTC.

<table>
<thead>
<tr>
<th>Flash Rate Parameterization Scheme</th>
<th>Model-Simulated Lightning Flashes</th>
<th>No Scaling</th>
<th>Scaling</th>
<th>Percent Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>w_{max}</td>
<td></td>
<td>134,870</td>
<td>134,791</td>
<td>-0.1%</td>
</tr>
<tr>
<td>CTH</td>
<td></td>
<td>31,264</td>
<td>31,547</td>
<td>+0.9%</td>
</tr>
<tr>
<td>UV</td>
<td></td>
<td>29,147</td>
<td>29,151</td>
<td>+0.0%</td>
</tr>
<tr>
<td>IWP</td>
<td></td>
<td>175,589</td>
<td>157,787</td>
<td>-10.1%</td>
</tr>
<tr>
<td>PIM</td>
<td></td>
<td>143,918</td>
<td>116,949</td>
<td>-18.7%</td>
</tr>
<tr>
<td>IMFP</td>
<td></td>
<td>1,087,677</td>
<td>971,504</td>
<td>-10.7%</td>
</tr>
<tr>
<td>CSU GEV</td>
<td></td>
<td>108,250</td>
<td>99,455</td>
<td>-8.1%</td>
</tr>
<tr>
<td>CSU 35EV</td>
<td></td>
<td>156,896</td>
<td>110,818</td>
<td>-29.4%</td>
</tr>
<tr>
<td>CSU PIM</td>
<td></td>
<td>192,513</td>
<td>116,908</td>
<td>-39.3%</td>
</tr>
<tr>
<td>UAH GEV10</td>
<td></td>
<td>102,534</td>
<td>99,853</td>
<td>-2.6%</td>
</tr>
<tr>
<td>UAH GEV5</td>
<td></td>
<td>95,302</td>
<td>93,138</td>
<td>-2.3%</td>
</tr>
<tr>
<td>UAH UV</td>
<td></td>
<td>16,096</td>
<td>16,089</td>
<td>-0.0%</td>
</tr>
<tr>
<td>UAH GEV10S</td>
<td></td>
<td>129,417</td>
<td>126,030</td>
<td>-2.6%</td>
</tr>
<tr>
<td>UAH GEV5S</td>
<td></td>
<td>126,109</td>
<td>123,246</td>
<td>-2.3%</td>
</tr>
<tr>
<td>UAH UVS</td>
<td></td>
<td>19,249</td>
<td>19,240</td>
<td>-0.0%</td>
</tr>
<tr>
<td>ICEFLUX</td>
<td></td>
<td>13,698</td>
<td>9,938</td>
<td>-27.5%</td>
</tr>
<tr>
<td>OK 35EV</td>
<td></td>
<td>24,783</td>
<td>23,488</td>
<td>-5.2%</td>
</tr>
<tr>
<td>LGT3</td>
<td></td>
<td>57,376</td>
<td>57,350</td>
<td>-0.1%</td>
</tr>
</tbody>
</table>

* When IWP is evaluated at 25 dBZ, the number of total lightning flashes is 143,743 (-18.1%).

* When ICEFLUX is evaluated at 390 hPa, the number of total lightning flashes is 14,419 (+5.3%).

Literature indicates that several FRPSs are sensitive to their application criteria. IWP involves a radar reflectivity threshold of 18 dBZ; however, if the model-simulated reflectivity produces higher values than observed, the threshold should be increased to better represent the IWP (Barthe et al., 2010). In a study by Mecikalski and Carey (2017) over northern Alabama for a supercellular system that produced 72,068 flashes, it was found that the peak of the LMA sources occurred between 7-9 km altitude and between
20-25 dBZ, although the majority of the sources from this system occurred between 4-13 km and between 15-55 dBZ. The LMA sources in our case study are generally located between 6.5-11.5 km within the 20-55 dBZ reflectivity contours and maximize at 9.5 km between 25-30 dBZ (Figure 10). Therefore, the threshold used in the scheme is increased to 25 dBZ to better represent the electrified portion of the storm and reduce the overestimation. While this helps decrease the total flashes by 9% for this scheme (i.e., 157,787 to 143,743 flashes), the overprediction is still a factor of 9.5, as indicated in Table 10 and Figure 16.

Figures 17 through 19 show results from the 12 other FRPSs. Figure 17 focuses on the three CSU-developed schemes (Basarab et al., 2015), the ICEFLUX scheme (Finney et al., 2014), the LTG3 scheme (McCaul et al., 2009), and the scheme developed with the 29-30 May data. Figure 18 displays results from the FRPSs developed by UAH (Carey et al., 2015) and Figure 19 shows the flash rate time series for the six schemes that provided the closest prediction of the number of flashes observed between 21:00-01:00 UTC observed time.
Figure 17. Same as Figure 16, except the FRPSs are based on relationships between total lightning activity and storm parameters developed by CSU (Basarab et al., 2015), Finney et al. (2014), and McCaul et al. (2009).

Figure 18. Same as Figure 16, except the FRPSs are based on relationships between total lightning activity and storm parameters developed by UAH (Carey et al., 2015).
Figure 19. Same as Figure 16, except the FRPSs are based on relationships between total lightning activity and storm parameters with an overall total lightning flash count most similar to the central Oklahoma LMA observations.

ICEFLUX is sensitive to the pressure level the scheme is evaluated at (Finney et al., 2014), as well as which hydrometeors are classified as suspended ice crystals. Finney et al. (2014) developed this scheme using the specific cloud ice water content variable from the ERA-Interim reanalysis, which includes graupel, snow, and ice. To mimic this variable with WRF, the mixing ratios of the three hydrometeors were summed and only included graupel and snow if their fall speeds were less than the updraft velocity. Upon initial evaluation the results showed ICEFLUX overestimates the LMA total lightning flashes by roughly a factor of 4. However, if graupel is considered to be precipitating (i.e., not suspended), then ICEFLUX underestimates (9,938) the observations (15,060) (Table 10).
The 440 hPa pressure level used by ICEFLUX is the ISCCP cloud top pressure threshold for deep convective clouds (Rossow et al., 1996). However, 440 hPa is found at the very lowest location of cloud ice in our model-simulated storm. If we evaluate the scheme at 340 hPa, as tested by Finney et al. (2014), the underestimation becomes an overestimation (19,216). Therefore, a 100 hPa decrease in pressure (i.e., 440 hPa to 340 hPa) resulted in a 10,000 total flash increase. If the ICEFLUX pressure level is adjusted by 50 hPa (390 hPa) instead, then the total number of model-simulated flashes (14,419) is within ~4.5% of the observations (15,060), as shown in Figures 17 and 19.

On average the non-hydrometeor-based FRPSs overestimated the number of LMA total flashes by a factor of 3, while the hydrometeor-based schemes overpredicted by a factor of 10.7. IMFP has the largest difference between the model-simulated and observed total flashes (a factor of > 60). If the IMFP scheme is excluded, the observations are overestimated by a factor of 6.7 by the remaining hydrometeor-based schemes.

The total flash counts predicted by every FRPS increase earlier in the model-simulated storm than in the observed storm. The initial peak in the observed flashes (~100 flashes 10-min\(^{-1}\); Figure 19) occurs 50 minutes after convective initiation, while seven of the 18 schemes (CTH, ICEFLUX, IMFP, IWP, CSU PIM, LTG3, and \(w_{\text{max}}\)) predict peaks of varying magnitudes (~50-1400 flashes 10-min\(^{-1}\)) roughly 20 minutes after the model storm develops.

An interesting feature that appears in most of the FRPS trends is a change in the steepness of the flash rate slope just after 22:00 UTC observed time (23:00 UTC model time). While the trends are generally steeper than the observations within the first few
hours of storm initiation, the model trend becomes slightly smaller after the first hour. In both UAH UV schemes, this change results in a slightly flatter slope than the other schemes that also exhibit this feature. The timing of this feature coincides with the end of the LDA and its modification of the water vapor in the atmosphere. For the $w_{\text{max}}$, IMFP, PIM, LTG3, and ICEFLUX schemes, this transition is not apparent in the trends. This suggests that the storm parameters used in these five FRPSs use variables and criteria thresholds that are not influenced by the LDA to the same degree as the other schemes.

The model-simulated flash rate time series for the IWP and PIM schemes have peaks that coincide with the observed peaks at 23:50 UTC and 01:00 UTC observed time (Figure 16). The four UAH GEV (Figure 18) and three CSU (GEV, 35EV, PIM) (Figure 17) schemes show multiple peaks between 23:00-00:00 UTC, instead of one like the observations and the IWP and PIM schemes; however, these schemes are similar because there is no prolonged increase in the flash rates during this time. The UV scheme hints at the presence of the peaks at 22:50 UTC and 23:50 UTC, although the trend is fluctuating at these times. The total lightning flashes per 10-min predicted by the CTH and UV schemes at 02:00 UTC model time is similar to the number of observed total flashes per 10-min at 01:00 UTC observed time. The LTG3 scheme is the only FRPS that clearly shows the presence of the observed peak at 01:00 UTC, although the UV scheme also hints at this feature. The two schemes that appear to replicate the timing and general shape of the observed peaks fairly well from 21:30-00:30 UTC, but not the magnitude, are those based on IMFP and $w_{\text{max}}$. ICEFLUX behaves similarly, but the peak at 22:50 UTC is not as distinct as it is in the observed, IMFP, and $w_{\text{max}}$ flash rate trends, plus it
occurs ~30 minutes earlier. Generally, when the flash rate peaked in a scheme, the time offset from the observations was consistent with the storm evolution noted in the radar reflectivity.

Prior to this study a FRPS had not been developed for Oklahoma convection. Since 35EV was considered a robust storm parameter based on its performance in regions outside of Colorado, the FRPS was tailored for Oklahoma using observations from our 29-30 May case study. However, when the scheme was employed in WRF, the total number of observed lightning flashes was still overestimated (~56%; Table 10). Figures 17 and 19 also show the detailed features of the observed flash rate trend are missing, which is likely due to the high-bias in storm intensity during convective initiation. This is noticed by the large overestimation of the 35 dBZ echo volume (~500%) in the initial cells that develop at the start of the simulations both with and without LDA. After roughly 1-hr, the overprediction by the 35 dBZ echo volume becomes smaller (~30%) before turning into a slight underestimation (~15%). The increased intensity during the developing stage of the storm system may help explain why the predicted flash rates for this scheme, and others, lack some of the details seen in the observed flash rate trend (i.e., the observed peak at 22:50 UTC).

An additional technique used the mean bias between the observed and model-simulated flash data per 10-min to evaluate the performance of the FRPSs. The schemes were ranked based on their root mean square error after the mean bias between the observed and simulated flashes was removed (i.e., centered root mean square error) and based on their mean bias (Table 11). For this case study, both calculations identified the same six FRPSs (i.e., ICEFLUX, OK 35EV, UV schemes and CTH) in Table 11 as being
the best at predicting flash rate fluctuations and total flashes over the life of the convection, and selected the same lowest ranked scheme (i.e., IMFP).

In terms of biases and the total flashes predicted over the simulation, the best performing FRPSs (Figure 19) include ICEFLUX (which very slightly underestimates the LMA total lightning flashes), the three UV schemes developed by Deierling et al. (2008) and UAH (Carey et al., 2015) (i.e., all convection types and supercell-only in northern Alabama), the OK 35EV scheme, and the CTH scheme. Of all the schemes not involving hydrometeors, the UAH UV scheme performed the best. Overall, ICEFLUX is the FRPS that best represents the total number of lightning flashes and their fluctuations. The individual 10-min flash rates from this scheme were also the closest to the observed rates for almost the entire simulation. Figure 20 displays the location of each model-simulated total lightning flash generated by the ICEFLUX scheme as the system tracked southeast. This track is similar to the observed flashes in Figure 5 and both the observed and simulated flashes appear to cover a similar area from 21:10-01:00 UTC. While the observed convection shows a higher density of flashes along its southwest side, the simulated storm system shows more flashes located on its northeast side. Three distinct paths are also visible in Figure 20, which is likely due to the larger areas of higher reflectivity that are present later in the simulated storm’s lifecycle.
Table 11. Centered root mean square error of the model-simulated total lightning flashes per 10-min (left) and mean bias in the model-simulated total lightning flashes per 10-min (right) predicted from 22:10-02:00 UTC model time. The LMA flashes used in the calculation are from 21:10-01:00 UTC observed time.

<table>
<thead>
<tr>
<th>Flash Rate Parameterization Scheme</th>
<th>Centered Root Mean Square Error (flashes)</th>
<th>Flash Rate Parameterization Scheme</th>
<th>Mean Bias (flashes)</th>
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Figure 20. Location of the model-simulated total lightning flashes (≥ 0.5 total flash) predicted by the ICEFLUX FRPS. For comparison with the LMA total lightning, the convective initiation of the model-simulated storm (22:10 UTC) is adjusted 60 minutes earlier to coincide with the start of the NEXRAD observed storm (21:10 UTC). The time scale is color coded from 21:10 UTC on 29 May to 04:10 UTC on 30 May 2012.

However, when the model-simulated flash rates are not adjusted an hour earlier to coincide with the start time of the observed storm, then the initial trend in the model flash rate time series appears to better represent the increasing trend and variation in the LMA observations. This suggests the rapid intensification of the model storm may offset the delay in convective initiation. Figure 21 shows how the top six FRPSs, previously discussed, compare against the LMA observations with the modification to timing. The FRPS performance was also evaluated in terms of bias using the observed and model flashes from 22:10-01:00 UTC observed time. Table 12 indicates the same six FRPS, as previously suggested by the 1-hour offset, as being the best at predicting flash rate fluctuations and total flashes over the ~3-hour interval. However, the order of schemes is
slightly different, with the OK 35EV scheme having the smallest mean bias with respect to the number of flashes observed during the ~3-hour period. This scheme, which was developed using data from the 29-30 May convective event, appears to represent the observed flashes from 22:10-01:00 UTC slightly better than when the model flashes were adjusted an hour earlier (Figure 19). Very little difference was noted in the centered root mean square error among the top four schemes (OK 35EV, CTH, ICEFLUX, and UV).

From a LNOx chemistry perspective, it is important to properly simulate the total number of flashes, in addition to their variation. For this reason, the ICEFLUX scheme was selected as the most appropriate scheme given the delay in the model storm’s initiation and the fact that it best predicted the total number of flashes from 21:10-01:00 UTC when the aircraft were sampling the convective outflow (i.e., trace gas measurements).

Figure 21. Same as Figure 19, except the model-simulated flashes are not adjusted 60 minutes earlier to coincide with the observed storm initiation at 21:10 UTC. The FRPSs represent the model-simulated trends from 22:10-02:00 UTC model time.
Table 12. Centered root mean square error of the model-simulated total lightning flashes per 10-min (left) and mean bias in the model-simulated total lightning flashes per 10-min (right) predicted from 22:10-01:00 UTC model time. The LMA flashes used in the calculation are from 22:10-01:00 UTC observed time.

<table>
<thead>
<tr>
<th>Flash Rate Parameterization Scheme</th>
<th>Centered Root Mean Square Error (flashes)</th>
<th>Flash Rate Parameterization Scheme</th>
<th>Mean Bias (flashes)</th>
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6.4 Flash rate parameterization scheme discussion

The 29-30 May 2012 severe supercell system was reproduced fairly well by WRF regarding its area, height, and vertical motion, as well as the instability of the storm environment. However, the majority of the FRPSs overpredicted the total flashes even after adjusting the model-simulated hydrometeors to bring them closer to the proxy observations. Here we explore why the FRPSs succeeded and failed in reproducing features in the observed flash rate trends, as well as how the results compare against the performance of FRPSs in other cloud-resolved simulations.
6.4.1 Ice-phase hydrometeors

Hydrometeors from observed radar data are determined by a very different method than those derived from model output. Thirteen of the 18 FRPSs involve relationships between total lightning activity and hydrometeors themselves or via radar reflectivity. Fuzzy logic algorithms were used to derive hydrometeor types from polarimetric radar for eight of these 13 (i.e., PIM, IMFP, CSU PIM and GEV, and four UAH GEV). The fuzzy logic algorithms developed by Dolan et al. (2013) and Vivekanandan et al. (1999) contain 10 and 14 hydrometeor categories, respectively, while the microphysics schemes available in WRF have about half that number available. Both bulk and bin microphysics parameterization scheme options are provided in WRF. The bulk schemes, in addition to many of the bin schemes, separate ice particles into predefined categories (e.g., cloud ice, snow, graupel, and hail) and the particle size distributions vary slightly between schemes. The disadvantage of having multiple ice categories is that this distinct separation is not natural. Instead there should be a gradual transition between the different ice types (Morrison and Grabowski, 2008; Morrison et al., 2015).

The differences between how observed and model-simulated hydrometeors are defined and determined could explain why the observed lightning is overestimated. For our case study we defined dense precipitating ice as hail in the Morrison two-moment microphysics scheme as this is more appropriate for continental deep convection. This means hail was used when a FRPS indicated the use of graupel. The CSU GEV schemes (Basarab et al., 2015) include both low- and high-density graupel categories, while the UAH GEV (Carey et al., 2015) calculations only used grid boxes where the graupel/small hail category dominated. The difference in the number of hydrometeor categories and
how specific hydrometeors are applied highlights a potential issue when calculating hydrometeor-based storm parameters.

The PIM and IMFP FRPSs (Deierling, 2006; Deierling et al., 2008) were developed using thunderstorms in Colorado, Kansas, and northern Alabama. The observed 1-min LMA data from our 29-30 May case study were used to back calculate the PIM and IMFP parameters from their respective FRPS equations. The calculation indicated that we should expect the PIM and IMFP values to be within the range with which these schemes were developed based on the High Plains and Alabama convection. However, when the flash rates are calculated online in WRF, the IMFP and PIM greatly overestimate the observed total lightning flashes. While IMFP produced the greatest overprediction of the 18 FRPSs, as indicated by the large bias in total flashes and fluctuations (Table 11), this scheme does reproduce flash rate trends similar to the 29-30 May observations. Barthe et al. (2010) also found that IMFP was able to recreate the trends of the observed total lightning flash rate time series, especially for a severe versus airmass thunderstorm, but was unable to reproduce the magnitude and produced the largest overestimation of the schemes tested. The severe storm simulated by Barthe et al. (2010) also produced similar features in the flash rate time series predicted by PIM and overestimated their magnitudes, which is similar to our severe system. The uncertainty with IMFP and PIM may also be related to assumptions made within a microphysics scheme, which may generate errors when calculating ice mass (Barthe et al., 2010). IMFP and PIM are plausible schemes because they are based on storm characteristics involved with cloud electrification; however, they appear to be very dependent on the proper prediction of variables within model-simulated storms.
FRPSs may instead benefit from total lightning activity and storm parameter relationships that avoid using specific ice hydrometeors (e.g., graupel). The transition between ice types is not gradual in microphysics schemes that offer multiple ice-phase categories, such as the Morrison two-moment. This characteristic may not be appropriate when trying to generate lightning with a FRPS that involves specific ice categories. A solution may be to use a scheme based on a single ice-phase category, such as the predicted particle properties (P3) scheme (Morrison et al., 2015). This scheme predicts mass and number mixing ratios of rain and cloud water, as well as four ice mixing ratio variables (i.e., total ice mass, rime ice mass, rime volume, and total number). One of the advantages of the P3 scheme is its ability to allow for smooth transitions as ice particles grow. A final version of this scheme was not available to test at the time of this analysis.

6.4.2 Development and application environments for FRPSs

The three FRPSs (CSU PIM, 35EV, and GEV) developed using isolated Colorado thunderstorms (Basarab et al., 2015) overestimated the total number of LMA flashes in the 29-30 May simulated storms. Generally, Colorado storms have higher flash rates than Oklahoma thunderstorms, which is likely due to the shallower warm cloud depths of Colorado convection (Fuchs et al., 2015). The CSU 35EV scheme was considered the most robust of the three schemes because it performed well in other areas (i.e., Oklahoma, northern Alabama, and Washington, D.C.), but the 29-30 May Oklahoma storms had deep warm cloud depth (2.5 km) and developed in an environment with extreme NCAPE (0.37 m s\(^{-2}\)) and high vertical wind shear (24 m s\(^{-1}\)). According to Basarab et al. (2015), this convective environment does not lend itself to a successful application of the CSU 35EV scheme because the observed storm developed in an
environment that did not maximize the performance of the FRPS. In addition, the cell-tracking algorithm used by CSU identified a cell as convective if the areas covered by two reflectivity thresholds (i.e., 35 dBZ and 45 dBZ) each exceeded a specified threshold (Basarab et al., 2015; Fuchs et al., 2015). In our cloud-resolved application of the CSU FRPSs, it was assumed the 35 dBZ criteria with no area threshold would be sufficient to differentiate between convective and stratiform regions in the model-simulated storms. However, it is possible the simulated storm region > 35 dBZ included non-convective areas, especially since the model cells were not as individualized as the observations.

The four UAH GEV schemes that are based on northern Alabama thunderstorms (Carey et al., 2015) all overestimated the observed 29-30 May Oklahoma total flash rates. However, the UAH UV scheme, which is applied between -10 °C and -40 °C where \( w > 5 \text{ m s}^{-1} \), only overestimated the observed flashes by 6.7%. This was the best performing non-hydrometeor scheme. This suggests that using a FRPS based on the criteria relevant to cloud electrification (i.e., temperature and vertical velocity) may be most appropriate for predicting flash rates if the model has difficulty simulating the hydrometeors. When supercell-only versions of the schemes are used, the overprediction is roughly 30% larger than when the versions using all convection types are considered, even though the May 29-30 system consisted of supercells.

The three CSU schemes and the four UAH GEV schemes represent linear relationships with total lightning activity. However, the flash rates observed over the lifetime of our 29-30 May Oklahoma case study (max=312 flashes min\(^{-1}\); mean=75.5 flashes min\(^{-1}\)) are higher than the flash rates observed in the northern Alabama (max=102 flashes min\(^{-1}\); mean=12.5 flashes min\(^{-1}\)) and Colorado
(max=287.8 flashes min⁻¹; mean=53.9 flashes min⁻¹) thunderstorm datasets, which were used to develop their respective FRPSs. This suggests the coefficients associated with these schemes may not be appropriate for the Oklahoma region or our 29-30 May event. For example, Basarab (2015) evaluated the same Alabama thunderstorm (18 May 2012) as Carey et al. (2014) using similar FRPSs (e.g., GEV). The schemes developed using Colorado storms had different coefficients than those based on Alabama convection and therefore did not predict the observed flash rates and trends as well. This suggests that FRPSs may not be applicable for use on storms outside of the region used to develop the scheme.

The LTG3 scheme developed by McCaul et al. (2009) has only been implemented in models with horizontal resolutions of 2-4 km and with microphysics and PBL schemes other than the combination that our case study employed. While the flash rates do not increase as quickly after convective initiation as some of the other FRPSs predict, the trend does become steeper after roughly 40 minutes and overestimates the observations by a factor of 3.8. It is possible that using the LTG3 scheme at a 1 km horizontal resolution with 89 vertical levels is too fine and is resolving additional storm features as the system matures. The production of stronger vertical velocities than would occur at 2-4 km resolution is one possibility, which would lead to an overestimation of flashes; however, the maximum updraft speed generated during the simulation is within 5% of the observations, although located at a slightly higher altitude. It is also possible our combination of the Morrison two-moment microphysics and YSU PBL schemes, which has not been previously used to evaluate LTG3, requires this FRPS to be recalibrated. Initial tests of the Morrison two-moment microphysics and MYJ PBL schemes have
indicated that graupel production is overly strong (Eugene McCaul, personal communication, January 13, 2017).

6.4.3 Non-linear FRPSs

The majority of the FRPSs are built using data from individual storms. This includes CTH and $w_{\text{max}}$, which were designed to represent a storm with one maximum value; however, these non-linear FRPS equations are applied per model processor in WRF. While the non-linear schemes (i.e., CTH and $w_{\text{max}}$) are generally applied in the manner they were intended (i.e., storm height is similar to the width of the processor), CTH roughly doubles the LMA observations and $w_{\text{max}}$ overpredicts by a factor of 4 larger than CTH. For our case study, each processor covering the model domain is roughly $18 \text{ km} \times 19 \text{ km}$ in area, which is slightly smaller than the horizontal dimension of the 29-30 May observed and simulated supercells. The width of the processors is only ~13-19% larger than the maximum model-simulated storm height (~16 km). Even if a storm were smaller than a processor, the cell would eventually span multiple tiles unless it remained stationary and near the processor’s center. This means additional total lightning flashes are generated by the non-linear schemes when the cell spans more than one processor.

The $w_{\text{max}}$ FRPS was built using two non-linear schemes (Price and Rind, 1992), where the slightly non-linear relation between $w_{\text{max}}$ and CTH is incorporated into the fifth-power relationship between CTH and flash rate. While the non-linearity of $w_{\text{max}}$ may not pose a problem when it is applied to a single area that envelops the convection of interest, any errors may be exacerbated when the non-linear scheme is applied to a cell spanning multiple processors. Barthe et al. (2010) suggested $w_{\text{max}}$ works better for severe
than for weak thunderstorms; however, they point out that $w_{\text{max}}$ is dependent on the simulation’s horizontal resolution.

Barthe et al. (2010) simulated lightning flash rates for a severe storm and an airmass thunderstorm using WRF output. The results suggested that when an adjustment factor was applied to the storm parameter, CTH performed better for the airmass thunderstorm, while $w_{\text{max}}$ predicted the flash rate well for the severe storm. Wong et al. (2013) also discussed the need for a “calibration factor” due to the resolution dependency of the Price and Rind (1992) CTH scheme. Allen and Pickering (2002) did not favor the CTH scheme because the fifth-power in the FRPS equation causes the scheme to be very sensitive to any biases in the CTH of model-simulated continental convection. Giannaros et al. (2016) also suggest CTH is a poor proxy for the intensity of convection and lightning activity and that tuning is almost always necessary when implementing parameterizations similar to Price and Rind (1992). In a study by Giannaros et al. (2015), when a masking filter was used in conjunction with CTH and a convective parameterization in WRF, more realistic lightning predictions were possible for 10 different convective events observed in Greece. The masking filter only applied the CTH scheme when specific total ice content, $w_{\text{max}}$, and CAPE thresholds were met.

Further investigation of the sensitivity of the non-linear, and linear, schemes to the number of model processors and resolution would require additional model runs at coarser resolutions. Initial analysis with the instantaneous model output every 10 min indicates a negligible change in the flash counts generated by the linear FRPSs without a y-intercept as resolution is increased to 2 km and 4 km; however, the UV FRPS, which is a linear scheme with a negative y-intercept, indicates a factor of 5 and factor of 60
decrease in the simulated flash counts as the resolution is modified. Barthe et al. (2010) found the flash rates predicted by a FRPS (i.e., $w_{\text{max}}$, CTH, UV, IWP PIM, and IMFP) were similar for a severe storm at model resolutions of 500 m, 1 km, and 2 km, and for an airmass thunderstorm at 1 km and 3 km resolution.

6.4.4 Vertical velocity

The four FRPSs that produced flash counts within a factor of 2 of the observations were based on UV (Deierling, 2006; Deierling et al., 2008; Carey et al., 2015) and ICEFLUX (Finney et al., 2014). Unlike the other FRPSs, the UV schemes have a specific vertical velocity criterion applied within the mixed-phased region. Other schemes are more complex, since they require additional criteria within the mixed-phase region, such as reflectivity and/or hydrometeors (see Table 2). Using a vertical motion threshold may help the model focus on the charged portion of the convective cloud, since updrafts play an important role in supplying water vapor for particle growth, ice particle collisions, and charge separation. In the model simulations prior to and with the current damping and LDA methods, all of the UV schemes were considered to be among the best performing schemes. Of the non-hydrometeor-based schemes, the UAH UV scheme represented the number of total flashes and almost the entire flash rate time series fairly well.

While the ICEFLUX scheme is more complex because it involves several frozen hydrometeors and their fall speeds, it is only evaluating these criteria at a specific pressure level. This scheme is related to the IMFP because it focuses on the intensity of the flux of nonprecipitation ice particles, not just the mass. The ICEFLUX scheme does the best at reproducing the total number of lightning flashes for our 29-30 May case. It also generates a similar trend as the observations; however, the increase of the flash rate
is steeper than the initial observations, which causes the more detailed shape of the observed peaks to not be well replicated. This scheme is also similar to the upward convective mass flux scheme, which Allen and Pickering (2002) determined was able to generate flash rates fairly well at most locations. Based on its performance in our case study and its inclusion of both vertical motion and ice particles, which are equally important for cloud electrification, we suggest the ICEFLUX scheme has promise for future use at cloud-resolved scales.
CHAPTER 7: LIGHTNING-GENERATED NITROGEN OXIDES PRODUCTION

One of the objectives of this work is to estimate the mean LNO$_x$ production per flash in an observed DC3 storm using a combination of a cloud-resolved WRF-Chem simulation and observations. Ten WRF-Chem simulations were evaluated using the FRPS based on ICEFLUX. The simulations included one run with no lightning chemistry and nine runs with different LNO$_x$ production scenarios. Prior WRF-Chem cloud-resolved simulations of the 29-30 May case study used the default model parameters for the fractional CG and IC flash channel vertical profiles (DeCaria et al., 2000) and the IC:CG ratio (Boccippio et al., 2001) with the $w_{\text{max}}$ FRPS with a 0.106 adjustment factor (Bela et al., 2016) and the UAH UVS scheme with no adjustment factor (Cummings et al., 2016). Both analyses tentatively suggested an LNO$_x$ production scenario of 125 moles flash$^{-1}$. However, observations of the vertical distributions of CG and IC flash channels and of the IC:CG ratio are available for the 29-30 May storm. I modified the model to allow use of these data. Therefore, the current analysis first tests the performance of the use of these observations through four different combinations of the default and observed vertical distributions of lightning flash channel lengths and IC:CG ratios.

The five subsequent simulations were used to determine if the LNO$_x$ production needed adjustment based on comparisons with the DC3 aircraft observations. These WRF-Chem runs only used the observed flash channel length vertical distributions and time evolving observed IC:CG ratios. The previously suggested 500 moles per CG and IC flash (Ott et al., 2010) scenario was tested, along with the 604 moles per CG flash and 38 moles per IC flash from the Koshak (2014) LNOM scenario. The LNOM scenario
yields a mean 151 moles flash\textsuperscript{-1} using the 29-30 May observed mean IC:CG ratio of about four. Pollack et al. (2016) concluded 107 moles flash\textsuperscript{-1} was appropriate for the 29-30 May case using a volume-based method to analyze DC3 aircraft measurements, and this scenario was tested in the model. A comparison of the model with 107 moles flash\textsuperscript{-1} and aircraft NO\textsubscript{x} mixing ratios suggested the LNO\textsubscript{x} production scenario should be adjusted to 82 moles flash\textsuperscript{-1} to achieve a best match with observations. When the LNOM scenario (Koshak, 2014) is adjusted to use 82 moles flash\textsuperscript{-1} as its mean value, but maintain the same ratio of NO production per CG flash and per IC flash, it suggests CG=328 moles flash\textsuperscript{-1} and IC=21 moles flash\textsuperscript{-1}.

Section 7.1 discusses the differences in the mixing ratios of the tracer species in the anvil outflow for the various simulations. Section 7.2 examines the variation in the anvil outflow NO\textsubscript{x} mixing ratios among the nine different LNO\textsubscript{x} production scenarios, with a focus on the scenario that best represents the aircraft observations. The relationships between lightning characteristics and LNO\textsubscript{x} production is discussed in Section 7.3 and the variation in simulated flash rate time series among the LNO\textsubscript{x} production scenarios is investigated in Section 7.4.

**7.1 Tracer species**

The anvil outflow was sampled by the DC8 between 10.72-11.21 km from 23:48:30-23:58:30 UTC and by the GV between 11.71-12.20 km from 23:59:30-00:23:30 UTC. Each altitude interval corresponds to two model layers. The GV and DC8 anvil outflow sampling periods, defined by Fried et al. (2016), were divided into 10-min intervals to correspond with the 10-min model output. Data points must be within anvil cloud outflow (total hydrometeors > 0.01 g kg\textsuperscript{-1}) and within tropospheric air (O\textsubscript{3}:CO ratio
< 1.25; Hudman et al., 2007) to be included. Since the observed and simulated anvil clouds were of similar area, outflow sampling boxes of comparable size were identified in the model-simulated convection. The box locations were adjusted in the horizontal plane to represent a similar distance from the center of the observed high composite reflectivity, as well as a region with similar features as the observed convection. The only exception was the DC8 outflow box from 23:50-00:00 UTC. The southwest portion of the flight track was located between 10.97-11.21 km and the northern half was between 10.72-10.97 km. In this lower layer the model-simulated wind speed was slightly weaker and the LNO$x$ plume was thicker than observed; therefore, this layer was shifted farther east in the model than the observations. Increasing the distance of the lower layer from the model-simulated convective core during this time interval placed the northern portion of the outflow box in a region of the anvil that is more representative of the observed anvil environment.

A direct comparison of the aircraft observed and model-simulated CO and O$_3$ mixing ratios within the same layers indicate the convective transport from the boundary layer is slightly underestimated in the model (Figure 22a and 22b). One model layer (i.e., 0.25 km) beneath each layer the aircraft flew at (i.e., 10.48-10.72 km, 10.72-10.97 km, 11.46-11.71 km, and 11.71-11.95 km) provides a better match to the observations (Figure 22c and 22d). Using these layers as a correction for the underestimated vertical transport, the overall mean model-simulated mixing ratios from these four model layers are within 1% and 3% of the aircraft observed CO (118.7 ppbv) and O$_3$ (86.1 ppbv), respectively (Table 13). This is true for each of the WRF-Chem simulations run with and without lightning chemistry.
Figure 22. Aircraft observed and model-simulated mean (a) CO and (b) O$_3$ mixing ratios within the same layers. Model-simulated mean (c) CO and (d) O$_3$ mixing ratios moved up 0.25 km. The ±1 standard deviation is represented by solid black lines for the observations and dotted color lines for the model.

Horizontal cross-sections of the model-simulated convection suggest that lower CO and higher O$_3$ mixing ratios are transported downward around the rear anvil (Figures 23 and 24). During DC3 research aircraft encountered O$_3$-rich stratospheric air wrapped around the cloud edge of the MCS observed on 30 May 2012 (Pan et al., 2014; Huntrieser et al., 2016). Pan et al. (2014) also simulated this “ram’s horn” shape using the WRF model at cloud-resolved resolution. In addition, Li et al. (2017, in review) simulated the vertical flux divergence in three additional DC3 convective events using WRF-Chem at different spatial scales, including our 29-30 May case study, and captured a similar O$_3$ enhancement 2-3 km below the tropopause.

Vertical cross-sections show model-simulated boundary layer CO (> 130 ppbv) and O$_3$ (< 65 ppbv) are present in the convective updrafts (Figures 23 and 24). A layer of
higher CO mixing ratios (> 120 ppbv) also exists at ~10.5 km, as well as within the anvils. Minima in O\(_3\) mixing ratios are visible in the anvil for over several hours in the 5-hour simulation. Above 10.8 km within the convective system, the mean O\(_3\) mixing ratio decreased by greater than 40 ppbv where the initial O\(_3\) mixing ratios exceeded 100 ppbv. A comparison of the decrease in O\(_3\) with and without lightning chemistry indicates that titration by lightning NO\(_x\) only accounts for roughly a 2 ppbv decrease at most. This suggests the upward transport of lower O\(_3\) mixing ratio boundary layer air into the cloud is responsible for almost all of the decrease in O\(_3\) at anvil levels.

Table 13. The mean trace gas mixing ratios over the four model layers the aircraft flew within (10.72-10.97 km, 10.97-11.21 km, 11.71-11.95 km, and 11.95-12.20 km). CO and O\(_3\) model values taken over (10.48-10.72 km, 10.72-10.97 km, 11.46-11.71 km, and 11.71-11.95 km). The asterisk indicates the observed LNO\(_x\) is an estimation based on mean aircraft observed total NO\(_x\) and the mean model-simulated background NO\(_x\) based on 82 moles fl\(^{-1}\). Unless noted otherwise, each LNO\(_x\) production scenario used the observed flash channel vertical distribution and IC:CG ratio.

<table>
<thead>
<tr>
<th>Aircraft Observed Mean Mixing Ratios</th>
<th>(\text{CO (ppbv)})</th>
<th>(\text{O}_3 \text{ (ppbv)})</th>
<th>(\text{NO}_x \text{ (ppbv)})</th>
<th>(\text{LNO}_x \text{ (ppbv)})</th>
</tr>
</thead>
<tbody>
<tr>
<td>118.7±4.7</td>
<td>86.1±6.6</td>
<td>1.4±0.6</td>
<td>1.2 *</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LNO(_x) Production Scenario</th>
<th>Model-Simulated Mean Mixing Ratios</th>
<th>(\text{CO (ppbv)})</th>
<th>(\text{O}_3 \text{ (ppbv)})</th>
<th>(\text{NO}_x \text{ (ppbv)})</th>
<th>(\text{LNO}_x \text{ (ppbv)})</th>
</tr>
</thead>
<tbody>
<tr>
<td>IC=CG=0</td>
<td>118.3±5.5</td>
<td>85.8±8.7</td>
<td>0.6±0.0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>IC=CG=125; DeCaria vertical; Boccippio IC:CG</td>
<td>118.5±4.9</td>
<td>86.8±7.8</td>
<td>1.2±0.4</td>
<td>1.1±0.4</td>
<td></td>
</tr>
<tr>
<td>IC=CG=125; DeCaria vertical; Observed IC:CG</td>
<td>118.7±4.6</td>
<td>86.4±7.4</td>
<td>1.2±0.4</td>
<td>1.1±0.4</td>
<td></td>
</tr>
<tr>
<td>IC=CG=125; Observed vertical; Boccippio IC:CG</td>
<td>117.8±4.9</td>
<td>87.8±8.1</td>
<td>2.0±0.7</td>
<td>1.9±1.3</td>
<td></td>
</tr>
<tr>
<td>IC=CG=125</td>
<td>118.4±5.1</td>
<td>86.6±8.5</td>
<td>1.9±0.6</td>
<td>1.8±0.6</td>
<td></td>
</tr>
<tr>
<td>IC=CG=500</td>
<td>117.9±4.6</td>
<td>85.0±8.0</td>
<td>7.3±2.4</td>
<td>7.1±2.4</td>
<td></td>
</tr>
<tr>
<td>IC=CG=107</td>
<td>118.1±5.0</td>
<td>86.4±7.9</td>
<td>1.7±0.5</td>
<td>1.5±0.5</td>
<td></td>
</tr>
<tr>
<td>IC=CG=82</td>
<td>117.6±5.0</td>
<td>88.3±8.1</td>
<td>1.3±0.4</td>
<td>1.2±0.4</td>
<td></td>
</tr>
<tr>
<td>IC=38; CG=604</td>
<td>118.1±5.4</td>
<td>87.1±8.3</td>
<td>2.6±0.7</td>
<td>2.4±0.7</td>
<td></td>
</tr>
<tr>
<td>IC=21; CG=328</td>
<td>118.5±4.7</td>
<td>86.4±7.7</td>
<td>1.5±0.4</td>
<td>1.4±0.5</td>
<td></td>
</tr>
</tbody>
</table>
Figure 23. Horizontal and vertical cross sections of model-simulated CO at (left) 23:50 UTC model time and (right) 01:40 UTC model time. Units in ppbv.
Figure 24. Horizontal and vertical cross sections of model-simulated O\textsubscript{3} at (left) 23:50 UTC model time and (right) 01:40 UTC model time. Units in ppbv.

7.2 Nitrogen oxides

7.2.1 NO\textsubscript{x} and LNO\textsubscript{x} mixing ratios

Since NOx is being injected into middle to upper troposphere, it is not influenced by convective transport to the same degree as CO and O\textsubscript{3}. For the 29-30 May event the peak in CG and IC flash channel lengths and LNO\textsubscript{x} occurs at 9.5 km and 10.5 km, respectively. In addition, LNO\textsubscript{x} is inserted into the model following a bulk approach (not
a filament approach), so it is not realistic to expect the model to capture the proper mixing ratios at specific locations. Therefore, the NO\textsubscript{x} and LNO\textsubscript{x} mixing ratios were only compared within the model layers where the aircraft flew (Figure 25) on the basis of means and standard deviations.

**Figure 25.** Aircraft observed and model-simulated mean (top) NO\textsubscript{x} and (bottom) LNO\textsubscript{x} mixing ratios within the same layers. The ±1 standard deviation is represented by solid black lines for the observed NO\textsubscript{x} and dotted color lines for the model NO\textsubscript{x} and LNO\textsubscript{x}.
With lightning chemistry turned off, the overall mean NO\textsubscript{x} from the four model layers (0.6 ppbv) underestimates the aircraft observed NO\textsubscript{x} (1.4 ppbv) by ~55% over the same altitude intervals (Table 13). Depending on which LNO\textsubscript{x} production scenario is assumed, the mean model-simulated NO\textsubscript{x} mixing ratio bias varies anywhere from roughly -11% to +438%. An LNO\textsubscript{x} production scenario of 82 moles per CG and IC flashes best represents the aircraft observations in the anvil outflow for the 29-30 May supercell storm system. Based on the overall mean from the four model layers, the model-simulated NO\textsubscript{x} mixing ratio (1.3 ppbv) is within 5% of the aircraft observation. This scenario is much smaller than the mean value suggested by Ott et al. (2010) for midlatitude and subtropical storms (500 moles ft\textsuperscript{-1}). It is within the range of the LNO\textsubscript{x} volume-based estimate Pollack et al. (2016) determined for this case study (107±24 moles ft\textsuperscript{-1}); however, Pollack et al. (2016) believe this estimate may be biased low. The storm volume associated with thunderstorms outside of the aircraft’s sampling region was not accounted for in the calculation, while the additional LNO\textsubscript{x} they produced was likely transported downwind and observed by the aircraft. Schumann and Huntrieser (2007) suggest the best estimate of the LNO\textsubscript{x} production is a mean 250 moles ft\textsuperscript{-1} (33-660 mole ft\textsuperscript{-1}) based on their review of theories, laboratory studies, field data, cloud-resolved modeling, and reviews from 1976-2007.

Both scenarios that incorporate the default model parameters for the fractional CG and IC flash channel vertical profiles (DeCaria et al., 2000) underestimate the aircraft observed NO\textsubscript{x} by < 20%; however, these profiles emit LNO\textsubscript{x} lower in the troposphere and are not representative of the observations. The default CG LNO\textsubscript{x} peaks 3.5 km below the
observed peak for this storm system, while the default IC LNO$_x$ has a secondary peak that maximizes at 6 km (Figure 9).

The two LNOM-based scenarios where the LNO$_x$ production per CG flash was substantially greater than that for an IC flash both overestimated the observed NO$_x$. The scenario based on the LNOM estimate by Koshak et al. (2014) overestimated by ~88%, which is likely due to the mean 151 moles fl$^{-1}$ being too large. The LNOM scenario that was adjusted to use a mean of 82 moles fl$^{-1}$ was within 12% of the aircraft observed NO$_x$ averaged over all four layers; however, the largest overestimate is within the 10.72-10.97 km layer (~80%), while the mean model-simulated NO$_x$ within the other three model layers ranged from -20% to +11%. This results in a poorer simulation than the scenario that uses 82 moles per CG and IC flash in which each of the four layers are within ~20% of the observations and the model NO$_x$ averaged over these layers underestimates the observations by ~4%. This suggests the partitioning of CG and IC LNO$_x$ based on the LNOM scenario may not be as appropriate as equal LNO$_x$ between CG and IC flashes, or the original LNOM estimate (Koshak et al., 2014), which is based on northern Alabama convection, may not be scaled for application in thunderstorms in other regions.

All further analyses and discussions will be based on the LNO$_x$ production scenario of 82 moles NO per CG and IC flashes, unless otherwise noted. Since the aircraft cannot directly measure LNO$_x$ in the anvil outflow, the observed LNO$_x$ is estimated by taking the difference between the total NO$_x$ observed by the aircraft and the model-simulated background NO$_x$. Table 13 shows that for this scenario the overall mean model-simulated LNO$_x$ within the four model layers is within 5% of the estimation
of the mean observed LNO\textsubscript{x} (1.2 ppbv). The results in Table 13 also suggest that there is loss of NO\textsubscript{x} due to chemistry (i.e., formation of HNO\textsubscript{3} and organic nitrates). The summation of the mean total NO\textsubscript{x} from the WRF-Chem simulation with no lightning chemistry (0.6 ppbv) and the average model-simulated LNO\textsubscript{x} (1.2 ppbv) within the anvil outflow is greater than the mean total NO\textsubscript{x} from the run with lightning chemistry (1.3 ppbv).

In the model simulation, NO\textsubscript{x} and LNO\textsubscript{x} maxima were collocated with the O\textsubscript{3} minimum in the upper portion of the convective core (> ~7 km), as well as the anvil. Here the mixing ratios for NO\textsubscript{x} and LNO\textsubscript{x} exceeded 2 ppbv. While the vertical cross-sections suggest boundary layer NO\textsubscript{x} is transported into the upper region of the convective cells, the model-simulated LNO\textsubscript{x} appears to make up ~88% of the NO\textsubscript{x} within the anvil. A comparison of the mean O\textsubscript{3} mixing ratios between the background profile and the in-cloud profiles with and without LNO\textsubscript{x} indicated O\textsubscript{3} decreased by at least 40 ppbv above 10.8 km altitude by the end of the simulation at 02:00 UTC model time. The difference between the two in-cloud mean O\textsubscript{3} profiles showed the O\textsubscript{3} mixing ratios were 1-2 ppbv lower in the WRF-Chem simulation with lightning chemistry. This suggests almost all decreases in O\textsubscript{3} were due to the upward transport of boundary layer air into the storm system and only a 1-2 ppbv O\textsubscript{3} loss was due to titration by NO.

7.2.2 LNO\textsubscript{x} columns

The NO contribution from lightning is also analyzed from a remote sensing perspective by determining the partial lightning NO\textsubscript{2} columns from the tropopause to 400 hPa, which would be analogous to what a UV-Vis satellite spectrometer (such as the Ozone Monitoring Instrument; OMI) would observe. In addition, the column amounts of LNO
and LNO\textsubscript{x} are also computed. During this convective event, the tropopause was observed near 200 hPa by sounding and aircraft. Using the area of OMI’s nadir footprint (13×24 km\textsuperscript{2}), the model-simulated partial LNO\textsubscript{x} columns were calculated using the model NO\textsubscript{x} output without and with (82 moles NO per flash) lightning chemistry. The model-simulated partial lightning NO, NO\textsubscript{2}, and NO\textsubscript{x} columns are shown in Figure 26. The maximum partial LNO\textsubscript{x} column between 22:10-02:00 UTC model time was 8.2×10\textsuperscript{15} molecules cm\textsuperscript{-2} at 00:50 UTC while the free troposphere away from the convection provided a mean background of 0.031×10\textsuperscript{15} molecules cm\textsuperscript{-2}. Prior to 02:00 UTC, the peak partial lightning NO column was 5.3×10\textsuperscript{15} molecules cm\textsuperscript{-2} at 01:00 UTC and the peak partial NO\textsubscript{2} column due to lightning was 7.3×10\textsuperscript{15} molecules cm\textsuperscript{-2} at 01:50 UTC. The partial NO\textsubscript{2} column is slightly less than, but similar in magnitude to the peak determined by Ott et al. (2010) for their cloud-resolved simulation of the 21 July 1998 thunderstorm (9.0×10\textsuperscript{15} molecules cm\textsuperscript{-2}) observed during the European Lightning Nitrogen Oxides Project (EULINOX). The mean NO\textsubscript{2} background for the 29-30 May Oklahoma storm ranges from 0.022×10\textsuperscript{15} to 0.047×10\textsuperscript{15} molecules cm\textsuperscript{-2} from 00:00-02:00 UTC model time, which is an order of magnitude less than the mean backgrounds of the five subtropical and midlatitude thunderstorms simulated by Ott et al. (2010).

Figure 27 shows a time series of the summation of the moles within the partial columns over the convective core and anvil from 00:00-02:00 UTC. The simulated anvil begins to exit the model domain at 01:00 UTC model time. The downward trend in moles NO due to lightning is likely related to sunset, which occurred at 01:38 UTC observed time on 29 May. This means the NO\textsubscript{2} photolysis shuts off and the NO\textsubscript{2} component of NO\textsubscript{x} increases, since NO is no longer being produced via this reaction.
Figure 26. Model-simulated partial lightning NO, NO$_2$, and NO$_x$ columns from tropopause (200 mb) to 400 mb at 00:50 UTC (top row), 01:00 UTC (middle row), and 01:50 UTC (bottom row). Each grid cell represents a 13 km $\times$ 24 km area.
7.3 Relationships between flash rate, flash extent, flash energy and LNO$_x$ production

One of the objectives of this work is to determine if the LNO$_x$ production per flash can be related to characteristics of the lightning itself or to other storm features such as the wind profile. The 29-30 May severe supercell system, which includes the Kingfisher storm (DiGangi et al., 2016), is considered a high flash rate event. High flash rate storms have shorter lengths per flash (Bruning and MacGorman, 2013; Bruning and Thomas, 2015; Mecikalski et al., 2015), which may result in a smaller amount of NO$_x$ produced per flash. While this hypothesis regarding LNO$_x$ production variability focuses on cloud electrification characteristics, an alternative hypothesis concerning LNO$_x$ production considers vertical wind shear, which is defined as the difference in the wind vectors between the anvil outflow and steering level (~700 hPa). This hypothesis suggests NO$_x$ production increases as lightning flashes are elongated with increasing vertical wind
shear (Huntrieser et al., 2008, 2009, 2011). The vertical wind shears observed between
the anvil outflow and the steering level (~700 hPa) during the Tropical Convection,
Cirrus and Nitrogen Oxides Experiment (TROCCINOX; Huntrieser et al., 2008),
SCOUT-O3/ACTIVE (Huntrieser et al., 2009), and African Monsoon Multidisciplinary
Analysis (AMMA; Huntrieser et al., 2011) campaigns ranged from 2.8-20.0 m s\(^{-1}\) with a
mean of 10.4 m s\(^{-1}\). The estimated LNO\(_x\) production per flash in these tropical and
subtropical regions ranged from 67-391 moles flash\(^{-1}\) with a mean of 161 moles flash\(^{-1}\).
During DC3 the mean wind speed was 35.8 m s\(^{-1}\) in the anvil outflow while the GV and
DC3 were making anvil transects between 10.9-12.2 km from 23:48-00:23 UTC. The
00:00 UTC observed sounding showed steering flow was 17.4 m s\(^{-1}\) from the west-
southwest (~250°). The observed mean vertical wind shear on 30 May was 23.8 m s\(^{-1}\) at
west-northwest (~285°), which is roughly two times stronger than the convection
observed in the tropics and subtropics. This suggests the wind shear hypothesis is not
ture for the 29-30 May convection given the stronger vertical wind shear and small LNO\(_x\) production per flash (82 moles flash\(^{-1}\)).

Total lightning flashes associated with the convection are within the 2D detection
capability of the central OK LMA (200 km) for the majority of the system’s life cycle
(21:10-04:20 UTC). However, the 3D features of the system are detectable from ~23:40-
03:00 UTC, when the convection is within ~100 km of the network (Figure 5). The LMA
data, averaged in 10-min intervals, was used to calculate the Pearson correlation
coefficient and assess the relationship between total flash rate and specific lightning
characteristics within the 3D coverage. During this time period the mean flash extent and
mean energy per flash were ~6.5 km and ~76 J s\(^{2}\) kg\(^{-1}\), respectively, with a mean flash
rate of 133 total flashes per 10-min. There was a moderate negative correlation between mean flash rate and mean flash extent \((r = -0.69, n = 21, p = 0.01; \text{Figure 28})\) and between mean flash rate and mean energy per flash \((r = -0.70, n = 21, p = 0.01; \text{Figure 29})\). This means there is a 1% chance that either relationship would exist if the variables were not related and implies the correlations were not due to chance. This also suggests that while the convection was within the 3D coverage that 48% of the variability in mean flash extent and 49% of the variability in mean energy per flash are explained by mean flash rate.

While the relationships appear to continue as very weakly negative \((r = -0.20 \text{ to } -0.30)\) after 03:00 UTC, the data suggests that within the first 2.5 hours after convective initiation \((21:10 \text{ to } 23:40 \text{ UTC})\) both relationships are instead moderate positive \((\text{roughly } r = +0.70);\) however, during these two periods there is much uncertainty with these results, since the lightning is mainly outside of the 3D region. A more accurate determination of the flash detection efficiency and location errors on this day could be made using a closer inspection of the active LMA stations along with the open-source simulation tools by Chmielewski and Bruning (2016). However, the moderate negative correlations during the period of 3D data suggest an estimate of flash rate can yield rough approximation of extent and energy per flash.
Figure 28. Correlation between the observed 10-min mean flash rate and mean flash extent within the 3D coverage of the central OK LMA network (23:40-03:00 UTC). The red plus represents the data points within the 3D coverage. The purple asterisk represents the data points prior to the 3D coverage (21:30-23:30 UTC). The blue cross represents the data points after the 3D coverage (03:10-04:20 UTC).

Figure 29. Same as Figure 28, except the correlation is between the observed 10-min mean flash rate and mean energy per flash.
Using data provided by Pollack et al. (2016) from six DC3 events, I further investigated the relationship between flash extent and LNO\textsubscript{x} production. Figure 10 in Pollack et al. (2016) indicated a weak to moderate positive correlation exists between cumulative flash area and LNO\textsubscript{x} production per flash over these events. I investigated whether a more relevant relationship exists between the mean flash areas for each event and their respective mean moles NO flash\textsuperscript{-1}. The mean flash area was calculated for each event using the sum of the flash energy during the convection, which is proportional to total flash area (Bruning and Thomas, 2015), given the time periods specified in Table 3 of Pollack et al. (2016) and dividing by the total number of flashes in that time interval. Since the LMA data is based on the slightly larger 3-hour moving spatial masks I initially defined (Bruning, 2014a, 2014b), I included a second data point for the 29-30 May case, which is based on 10-min masks that cover the more specific portion of the convection considered in the simulation. The mean flash area for this data point uses the same method as described above, except only the flash data within the LMA 3D coverage is used (23:40-03:00 UTC). Figure 30 shows a weak to moderate positive correlation (r = +0.42, n = 13, p = 0.01) also exists when the mean flash area is considered instead of total flash area. Although this relationship is moderate at best, it suggests the correlation is not due to chance and that mean flash area explains 18\% of the variability in mean LNO\textsubscript{x} production. Therefore, the relationship is worth further exploration since it indicates the potential development of a parameterization scheme for LNO\textsubscript{x} production per flash based on flash rate.
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Figure 30. Correlation between the mean flash area and LNO$_x$ production per flash for six convective events observed during DC3. The squares and triangles represent Oklahoma and Colorado convection, respectively. LNO$_x$ production using the flux-based approach is represented by orange and blue, while the volume-based approach is represented by red and purple. The green asterisk represents the 29-30 May event based on data within the 10-min moving spatial masks and 3D coverage of the central OK LMA network (23:40-03:00 UTC).

7.4 Flash rate variation between LNO$_x$ production scenarios

After the WRF simulations without chemistry, with chemistry and no LNO$_x$, and different LNO$_x$ production scenarios were run, variations in the model-simulated flash rates were noticed. The number of total flashes simulated from 22:10-02:00 UTC model time varies by less than 100 flashes between the run with no chemistry (14,419 flashes) and the run with chemistry but no LNO$_x$ production (14,344 flashes). Figure 31 shows slight variation in the flash rate time series occurs around 23:10 UTC, 00:00 UTC, and 02:00 UTC. I decided to investigate the cause of these differences in flash rate. Since
the GOCART aerosols have a direct effect on the radiation in the model, I hypothesize that the resulting heating/cooling changes can affect the calculation of the ICEFLUX storm parameter used in this case study to predict lightning activity. With the chemistry turned on variations in the aerosol concentrations may result, affecting the radiation and, in turn the kinematics of the storm.

**Figure 31.** Model-simulated flash rate time series based on the meteorology only run (No Chem), chemistry run with no lightning chemistry (No LNOₓ), and nine chemistry runs with varying LNOₓ production scenarios, vertical flash channel length distributions, and IC:CG ratios. Each LNOₓ production scenario used the observed flash channel vertical distribution and IC:CG ratio, unless the scenario in the legend contains a D for the DeCaria vertical distribution or a B for the Boccippio IC:CG ratio.
As each of the nine LNO$_x$ production scenarios were tested, their individual flash rate time series showed additional variation from the runs with and without chemistry, as well as between each scenario. Also, the total number of flashes predicted by the nine scenarios from 22:10-02:00 UTC varies by roughly 1,200 flashes. The initial assumption of 125 moles NO flash$^{-1}$ tested four different combinations of flash channel length vertical distributions (default and observed) and IC:CG ratios (default and observed). The two runs that apply the observed IC:CG ratios show similar changes in flash rates, just like the two runs that use the Boccippio IC:CG ratios. A comparison of the total number of flashes showed the two scenarios using the DeCaria flash channel length vertical distributions (DeCaria et al., 2000) produced roughly 195-460 more flashes than the two scenarios using the observed vertical profile. This suggests the CG and IC LNO$_x$ emitted at lower altitudes (6.5 km) in the DeCaria scheme may cause the lightning activity to increase. Also included are two runs that both use 82 moles NO flash$^{-1}$. While the variation in their flash rates is similar, the simulation that assumed equal LNO$_x$ production between the CG and IC flashes shows higher flash rates and predicts more flashes (15,076 flashes) than the run that presumed the CG LNO$_x$ production was larger (14,631 flashes). When 107 moles NO flash$^{-1}$ is assumed, the fluctuation in flash rates is similar to the run with no lightning chemistry.

Among the six scenarios using the observed vertical distributions and IC:CG ratios, the total number of flashes simulated between 22:10-02:00 UTC does not increase or decrease as the moles NO flash$^{-1}$ increases. While the magnitude of the flash rate peaks differ between the six runs, they generally occur at the same time (i.e., 00:10 UTC, 00:50 UTC, 01:10 UTC, and 01:50 UTC) and show a maximum peak between 01:00-
01:10 UTC. However, the simulations that assumed 107 and 125 moles NO flash$^{-1}$ each show two flash rate peaks after 01:10 UTC instead of one. The run using 107 moles also indicates there is one peak at 01:00 UTC instead of at $\pm 10$ minutes like the other five scenarios.

Since these differences are most noticeable after 00:00 UTC, a closer look was taken at the potential variables driving these changes. The ICEFLUX storm parameter considers the nonprecipitation ice and snow that are present at the 390 hPa pressure level. Figure 32 shows the total ICEFLUX time series for each of the 10 scenarios evolves similarly to the simulated flash rates over the 2-hour period; however, based on the time series it is the nonprecipitation snow (Figure 33) that drives the ICEFLUX and not the nonprecipitation ice (Figure 34). The total snow mixing ratios (Figure 35) and the mean upward vertical velocities (Figure 36) both appear to affect the fluctuations in the nonprecipitation snow. While the snow mixing ratio causes the general shape of the nonprecipitation snow time series to increase, the vertical velocity provides the variation in the time series. This helps provide some explanation for what variables have a greater influence on ICEFLUX, but since each simulation is initiated with different chemistry assumptions (i.e., no chemistry and chemistry with and without LNO$_x$), there are likely additional factors responsible for creating the differences in the storm parameter and flash rate time series. However, with the use of the GOCART aerosol scheme, there is no connection of the aerosol with the microphysics. Therefore, changes in aerosol will not directly affect the hydrometeor mixing ratios. But, changes in vertical velocity can affect the amount of ice and snow production in the cloud.
Each of the six simulations with differing LNO$_x$ production scenarios show a general decrease in the mean concentration of dust (Figure 37) and aged (hydrophilic) black carbon (Figure 38) and organic carbon (Figure 39) within the convective system at 390 hPa between 00:00-02:00 UTC model time. There is little variation among these three aerosols in the six simulations except for the assumption of 107 moles NO flash$^{-1}$, which has a slightly lower mean concentration. The general lack of variation suggests these do not contribute to the variation in flash count.

The mean NO$_x$, NO$_2$, and NO time series (Figures 40-42) do not directly contribute to the variation in flash rates, as there is no similarity in the patterns to that of ICEFLUX. However, when using the observed vertical distributions and IC:CG ratios, the time series of these gases, as expected, show that as the production of NO flash$^{-1}$ increases, so do the mixing ratios. (i.e., 82 moles NO flash$^{-1}$ has the lowest mean mixing ratios, while 500 moles NO flash$^{-1}$ has the highest mean mixing ratios). The two scenarios that use the DeCaria et al. (2000) vertical distribution have the highest mixing ratios, which is likely due to how close the 390 hPa pressure level is to the peak in CG and IC lightning flash channel lengths at 6.5 km. The increasing and decreasing trends in NO$_2$ and NO, respectively, are due to photolysis shutting off at the end of the day. Although the mean HO$_2$ and OH time series (Figures 43 and 44) decrease over the 2-hour interval due to the loss of sunlight, these chemical species may play a role in the flash rate variation due to the chemical interaction with NO. The sulfate aerosol time series showed little variation in the model output from the WRF-Chem simulations with no lightning chemistry and with 107 moles NO flash$^{-1}$ (not shown); therefore, additional LNO$_x$ production scenarios were not analyzed. The GOCART aerosol scheme does not
include nitrate, so a different aerosol scheme will need to be used to examine the potential influence of nitrate on the variation in model flash count due to changes in NO$_x$.

It is not clear what is causing the ICEFLUX and flash rates to vary among the nine different LNO$_x$ production scenarios and WRF-Chem run without LNO$_x$ chemistry. However, a combination of aerosol formation reactions and feedback processes to the storm kinematics and microphysics in the presence of varying amounts of LNO$_x$ is likely cause for the variation in ICEFLUX and flash rates.

![VARIABLES IN ICEFLUX FRPS (at 390 mb)](image)

**Figure 32.** Total model-simulated ICEFLUX (kg m$^{-2}$ s$^{-1}$) time series from 00:00 UTC to 02:00 UTC model time based on the meteorology only run (No Chem), chemistry run with no lightning chemistry (No LNO$_x$), and nine chemistry runs with varying LNO$_x$ production scenarios, vertical flash channel length distributions, and IC:CG ratios. Each LNO$_x$ production scenario used the observed flash channel vertical distribution and IC:CG ratio, unless the scenario in the legend contains a D for the DeCaria vertical distribution or a B for the Boccippio IC:CG ratio.
**Figure 33.** Same as Figure 32, except for the total model-simulated nonprecipitation snow (kg m\(^{-2}\) s\(^{-1}\)).

**Figure 34.** Same as Figure 32, except for the total model-simulated nonprecipitation ice (kg m\(^{-2}\) s\(^{-1}\)).
Figure 35. Same as Figure 32, except for the total model-simulated snow mixing ratio ($\times 10^3$ g kg$^{-1}$).

Figure 36. Same as Figure 32, except for the mean model-simulated upward vertical velocity (m s$^{-1}$).
Figure 37. Same as Figure 32, except for the mean model-simulated dust ($\mu g\, kg^{-1}$).

Figure 38. Same as Figure 32, except for the mean model-simulated aged (hydrophilic) black carbon ($\mu g\, kg^{-1}$).
Figure 39. Same as Figure 32, except for the mean model-simulated aged (hydrophilic) organic carbon (µg kg⁻¹).

Figure 40. Same as Figure 32, except for the mean model-simulated NOₓ in parts per trillion volume (pptv).
Figure 41. Same as Figure 32, except for the mean model-simulated NO₂ (pptv).

Figure 42. Same as Figure 32, except for the mean model-simulated NO (pptv).
**Figure 43.** Same as Figure 32, except for the mean model-simulated HO$_2$ (pptv).

**Figure 44.** Same as Figure 32, except for the mean model-simulated OH (pptv).
Convective outflow undergoes chemical reactions as it is transported downwind through the upper troposphere. These reactions include oxidation of NO and NO\textsubscript{2} photolysis, which result in O\textsubscript{3} production. NO\textsubscript{2} can be oxidized to HNO\textsubscript{3} and peroxyacetyl nitrate (PAN). Changes to the plume can be tracked and analyzed through the use of aircraft and satellite observations, as well as model simulations. DC3 offered a unique opportunity for aircraft to sample anvil outflow from an active thunderstorm and to locate the same air mass the following day.

8.1 Identifying and classifying areas of enhanced partial lightning NO\textsubscript{2} columns

Remote sensing by satellites help provide information about trace gas concentrations, such as NO\textsubscript{2}, in the earth’s atmosphere. The OMI, which is found onboard NASA’s Earth Observing System (EOS)-Aura satellite, is one example of the instruments that have been used to provide NO\textsubscript{2} retrievals of vertical column content. OMI is a UV-Vis spectrometer and can sense sunlight that is backscattered between 270-500 nm (Boersma et al., 2011). NO dominates over NO\textsubscript{2} in the daytime in upper tropospheric convective outflow. However, NO\textsubscript{2} is easier to detect than NO through remote sensing (Schumann and Huntrieser, 2007). A near-real-time lightning NO\textsubscript{2} algorithm was developed by Pickering et al. (2014) for use in processing OMI data in relatively clear-sky regions to help identify areas of enhanced NO\textsubscript{2} due to upwind lightning. During DC3, the resulting images generated by the algorithm provided an additional real-time operational product that could be used to help justify the location of the sampling region for the downwind research flights.
As part of the DC3 lightning chemistry team in the field, I analyzed the OMI images generated daily in combination with the forward FLEXPART dispersion model and backward HYSPLIT model trajectories of the upper level air to help direct the DC3 aircraft to the general location of the convective outflow plume that was sampled the previous afternoon/evening. Post-campaign I analyzed every OMI image from May-June 2012 in detail to identify whether each area of enhanced NO$_2$ across the continental United States was related to lightning, as the algorithm indicated, or if these regions were related to some other feature or event, such as wildfires or anthropogenic sources. If the contributions from the non-lightning sources were above the NO$_2$ climatological background value, then the algorithm would incorrectly classify the source as lightning.

For example, Figure 45 shows the tropospheric lightning NO$_2$ columns observed by OMI at ~18:30 UTC on 30 May 2012. On this day the enhanced NO$_2$ over the southern Appalachian region is likely associated with the severe supercell system that was sampled by the DC3 research aircraft as the convection moved through Oklahoma the prior evening. Backward trajectories from the NOAA HYSPLIT model indicated that at 18 UTC on 30 May the air masses at 8 km, 10 km, and 12 km altitude within the region of enhanced LNO$_2$ passed through lightning activity over the previous 12 to 42 hours. Figure 46a shows the 8 km trajectory intercepted lightning at 00 UTC 29 May (Figure 47a), which was not part of the previous day’s research flight, and the 12 km trajectory passed through the convection sampled by the DC3 aircraft between 18 UTC 29 May and 00 UTC 30 May (Figures 47b and 47c). Figure 46b also indicates that the 10 km and 12 km trajectories passed near the supercell system between 00-06 UTC 30 May. The
The vast majority of the downwind impact on NO$_2$ was from the storm system sampled by the aircraft.

**Figure 45.** The OMI tropospheric lightning NO$_2$ columns at ~18:30 UTC on 30 May 2012. The color scale ranges from -3.0 (blue) to +3.0 (red) $\times 10^{15}$ molecules cm$^{-2}$.
Figure 46. Backward trajectories initiating at (a) 35 °N, 81 °W and (b) 35 °N, 84 °W within the region of enhanced LNO$_2$ at 18 UTC 30 May 2012. The trajectories start at 8 km (red), 10 km (blue), and 12 km (green) above mean sea level. (The NOAA HYSPLIT model is available at http://ready.arl.noaa.gov/HYSPLIT.php.)

Figure 47. Location of NLDN 5-min lightning strikes at (a) 00 UTC 29 May 2012, (b) 00 UTC 30 May 2012, and 05 UTC 30 May 2012 over Oklahoma and Texas. (Available in the EOL DC3 field catalog http://catalog.eol.ucar.edu/dc3_2012/.)

Non-lightning sources were also visible in Figure 45. These included the Four Corners Power Plant near Farmington, New Mexico, the Whitewater-Baldy fire in southwestern New Mexico (Voiland, 2012), and agricultural burns in the Mississippi River Valley. FLEXPART indicates elevated levels of the biomass burning tracer in the lower troposphere in the area of the wildfire and agricultural burning (Figure 48).
8.2 Aircraft observations of the convective outflow plume

Based on the satellite information and trajectories, the GV and DC8 were directed toward the southern Appalachian region on 30 May 2012 to locate and sample the convective outflow plume associated with the severe supercell system that developed along the Oklahoma/Kansas border at 21:10 UTC 29 May and moved east-southeast through Oklahoma. The aircraft set up a triangular shaped flight path from Lynchburg, Virginia, to Athens, Georgia, to Snowbird (a waypoint on the Tennessee/North Carolina border).

For the trace gas analyses, the 1-sec DC8 and GV aircraft data was averaged over 5 sec and 4 sec time intervals, respectively, to represent a 1 km × 1 km horizontal resolution based on the aircraft ground speeds. In addition, only observations within tropospheric air were included (O₃:CO ratio < 1.25; Hudman et al., 2007). Plots of the trace gas mixing ratios along the aircraft flight tracks suggest the aircraft encountered the outflow plume along the southwest-to-northeast tracks between Athens and Lynchburg.
Figures 49 and 50 show the aircraft detected NO$_x$ mixing ratios between 1-2 ppbv at 10-12 km altitude along the southern track and the northeast corner of the triangle near Lynchburg. The CO measurements are generally above 110 ppbv within the sampling region (Figures 51 and 52); however, the portion of the track where NO$_x$ is elevated coincides with slightly higher CO mixing ratios (120 ppbv). The DC8 observed enhanced O$_3$ (110-130 ppbv) between roughly 10.5-12.0 km altitude in several locations in the western half of the triangle and as it approached and exited the area (Figure 53). The GV also noticed O$_3$ mixing ratios between 110-130 ppbv; however, these measurements were observed between about 11.0-12.5 km altitude along the northern portion of the sampling region (Figure 54). The flight tracks appear to show that the areas with higher O$_3$ mixing ratios (110-130 ppbv) occurred where the NO$_x$ < 1 ppbv, while elevated NO$_x$ (> 1 ppbv) occurred in locations where O$_3$ mixing ratios slightly lower (90-110 ppbv).

The relationship between the net O$_3$ production rate and NO$_x$ is a nonlinear process. Net O$_3$ destruction occurs at low NO$_x$ values. As NO$_x$ increases, the O$_3$ production rate also increases until the NO$_x$ mixing ratio with peak O$_3$ production efficiency is reached, above which the O$_3$ production decreases (Monks, 2005; Schumann and Huntrieser, 2007). The aircraft observations from the downwind flight are too large to help identify what the critical NO$_x$ threshold was on 30 May for O$_3$ production versus destruction; however, the observations suggest that O$_3$ production was more efficient when NO$_x$ concentrations were below 1 ppbv.
Figure 49. Tropospheric NO\textsubscript{x} mixing ratios observed along the DC8 flight track on 30 May 2012. Observations are color coded in increments of 0.5 ppbv from 0.0-2.0 ppbv, as shown in the middle panel plot.

Figure 50. Tropospheric NO\textsubscript{x} mixing ratios observed along the GV flight track on 30 May 2012. Observations are color coded in increments of 0.5 ppbv from 0.0-2.0 ppbv, as shown in the middle panel plot.
Figure 51. Tropospheric CO mixing ratios observed along the DC8 flight track on 30 May 2012. Observations are color coded in increments of 10 ppbv from 60-140 ppbv, as shown in the middle panel plot.

Figure 52. Tropospheric CO mixing ratios observed along the GV flight track on 30 May 2012. Observations are color coded in increments of 10 ppbv from 60-140 ppbv, as shown in the middle panel plot.
Figure 53. Tropospheric O$_3$ mixing ratios observed along the DC8 flight track on 30 May 2012. Observations are color coded in increments of 10 ppbv from 60-140 ppbv, as shown in the middle panel plot.

Figure 54. Tropospheric O$_3$ mixing ratios observed along the GV flight track on 30 May 2012. Observations are color coded in increments of 10 ppbv from 60-140 ppbv, as shown in the middle panel plot.
Figure 55 provides an example of model-derived O₃ production rates as a function of NOₓ mixing ratio for the clean free troposphere. The O₃ production rate increases with increasing NOₓ from roughly 0.07-0.8 ppbv and decreases with NOₓ concentrations above 0.8 ppbv. According to Monks (2005), the O₃ production rate maximizes at 0.8 ppbv NOₓ in the clean free troposphere (Figure 55); however, on 30 May it appears that this peak occurred at a slightly higher NOₓ value (~1 ppbv) and in an upper tropospheric region influenced by convective outflow that contains enhanced HOₓ and HOₓ precursors (e.g., CH₂O and H₂O₂), which lead to larger O₃ production rates than for the clean free troposphere.

Figure 55. Schematic of the variation in net ozone production with increasing NOₓ mixing ratios in the clean free troposphere (from Monks, 2005).

Figure 56 shows the mean mixing ratio profiles within tropospheric air for five trace gases measured by the aircraft over the southern Appalachian region. The CO and NOₓ profiles suggest the outflow plume may extend from roughly 8-12 km; however, the mean NOₓ profile appears to show the core of the plume is located between 10-12 km.
The aircraft observations suggest that the aircraft did encounter the outflow plume from the previous afternoon/evening, as indicated by the collocation of the highest NO\textsubscript{x} and CO mixing ratios. The anti-correlation between the location of enhanced NO\textsubscript{x} and O\textsubscript{3} mixing ratios suggest that may be associated with efficient O\textsubscript{3} production in the upper troposphere when NO\textsubscript{x} is diluted. The aircraft observations also validate the success of the near-real-time lightning NO\textsubscript{2} algorithm (Pickering et al., 2014). The HYSPLIT backward trajectories also confirm the air mass within the 10-12 km layer over southern Appalachian did pass through or near the active convection.

When the aircraft sampled the anvil outflow of the active convection the previous evening, the average O\textsubscript{3} mixing ratio between 10.7-12.2 km altitude was 86.1 ppbv. Based on the mean O\textsubscript{3} profile from the downwind region in Figure 56, the average O\textsubscript{3} mixing ratio within this same altitude range is 105 ppbv, indicating photochemical O\textsubscript{3} production of 19 ppbv. The convective outflow plume experienced 12 hours of sunlight between the last time it was sampled in the anvil and the first time it was sampled in the downwind region the next day. This suggests the photochemical production rate is roughly an average of 1.6 ppbv per hour. Prior model simulations have shown O\textsubscript{3} enhancements of similar magnitude downwind of convection. DeCaria et al. (2005) found O\textsubscript{3} increased on average by 10 ppbv day\textsuperscript{-1} for a cloud-resolved simulation of the 12 July 1996 storm observed in Colorado during the STERAO-A campaign. More recently, analyses by Apel et al. (2015) showed O\textsubscript{3} increased downwind of two thunderstorms observed on 22 June 2012 in Colorado during DC3 by 11-14 ppbv over a two-day period. The O\textsubscript{3} enhancement observed on 30 May is likely greater than in the clean free troposphere shown by Monks (2005) because of increased HO\textsubscript{x} and HO\textsubscript{x} precursors in the
outflow plume over the southern Appalachians. Updrafts from the active convection the
previous afternoon/evening transported boundary layer air, which may have contained
HO$_x$ precursors, into the upper convective region of the thunderstorms. Based on an
analysis of DC3 aircraft observations, Schroeder et al. (2014) suggest the mixing of
polluted convective outflow and stratospheric air rapidly produces OH. Three of the
stratospherically influenced samples in the Schroeder et al. (2014) analysis were from the
29-30 May convective event. The presence of these additional trace gases would have
aided in producing more O$_3$ in the downwind plume on 30 May than would be present in
the background air.

Figure 56. Mean trace gas mixing ratios based on DC8 and GV observations taken over
the southern Appalachian region within tropospheric air on 30 May 2012. Each
horizontal line represents ±1 standard deviation.
8.3 LNO\textsubscript{x} column and storm flux comparison

The mean partial NO\textsubscript{2} column (400-150 hPa) calculated for the southern Appalachian region based on the aircraft observations is $1.59 \times 10^{15}$ molecules cm\textsuperscript{-2} (Pickering et al., 2014). To determine the total moles of NO\textsubscript{x} within this area, the pressure-weighted mean NO\textsubscript{x}:NO\textsubscript{2} ratio (1.9) is calculated from the mean profiles in Figure 56 and used to find the partial NO\textsubscript{x} column ($3.05 \times 10^{15}$ molecules cm\textsuperscript{-2}). By accounting for the area of the triangular flight track region (34,000 km\textsuperscript{2}), the column content is converted to a total NO\textsubscript{x} content of $1.72 \times 10^6$ moles. A similar calculation is performed using the mean partial OMI LNO\textsubscript{2} column estimate (Pickering et al., 2014), which suggests the partial LNO\textsubscript{x} column is $2.26 \times 10^{15}$ molecules cm\textsuperscript{-2}. Given the area of the sampling region, the total LNO\textsubscript{x} estimate based on OMI data is $1.27 \times 10^6$ moles. OMI LNO\textsubscript{2} estimates have significant uncertainty. However, comparison of OMI LNO\textsubscript{x} with the aircraft total NO\textsubscript{x} suggests that roughly 75\% of the NO\textsubscript{x} in the downwind region is due to lightning.

Over the lifetime of the 29-30 May severe supercell system, approximately 31,633 total lightning flashes were observed. Using the NO\textsubscript{x} production per flash determined by the cloud-resolved WRF-Chem simulation (82 moles), this would imply $2.59 \times 10^6$ moles were produced by this event. If it is assumed all of the LNO\textsubscript{x} in the downwind region ($1.27 \times 10^6$ moles) came from the observed supercell system, then this suggests roughly half of the LNO\textsubscript{x} generated by the convection was lost chemically during transport. However, it is likely that not all of the LNO\textsubscript{x} produced in the storm exited the anvil. A slightly lower percentage of LNO\textsubscript{x} loss due to chemistry during transport (34\%) was found when the average anvil outflow LNO\textsubscript{x} fluxes estimated by Pollack et al. (2016) for each anvil transect were considered. Using the average LNO\textsubscript{x}
fluxes, the moles LNO$_x$ exiting in the anvil outflow were calculated over the length of each aircraft transect. Between the times when visible satellite first showed the anvil becoming elongated (~22:00 UTC) and the first anvil transect (23:13 UTC), only half of the LNO$_x$ flux observed during the first aircraft transect was used. For the time period between the last anvil transect and the end of the convective event (00:41-04:20 UTC), only half of the LNO$_x$ flux observed during the last transect was considered. This approach suggests 74% or $1.91 \times 10^6$ moles LNO$_x$ were advected out of the anvil during the lifetime of the 29-30 May convective event and 66% of this amount was observed in the downwind region. If true, this indicates the severe supercell system had a major impact on the upper tropospheric chemistry in the downwind environment.

However, regions of enhanced LNO$_x$ may not be formed by one convective event or be entirely composed of LNO$_x$. Active convection in Alabama occurred early on 30 May, which influenced the area of enhanced LNO$_x$ (Pickering et al., 2014). In addition, boundary layer NO$_x$ can be carried into a storm by convective updrafts and carried away with the outflow, or NO$_x$ from the free troposphere can be entrained into the convective plume by turbulent mixing.
CHAPTER 9: SUMMARY AND CONCLUSIONS

Lightning is dependent on updraft intensity and the hydrometeors in the mixed-phase region of a convective cloud. Therefore, it is necessary that the inputs to FRPSs from a simulation accurately represent the kinematic and microphysical characteristics of the observed storm. Eighteen FRPSs were evaluated based on their performance in a cloud-resolved simulation of the 29-30 May 2012 severe supercell system that was observed in Oklahoma by ground-based and airborne measurements during DC3. The observed storm location, dimensions, and vertical motion are represented reasonably well by the WRF model prior to and with the convective damping and LDA assumptions. However, the damping and LDA improve the microphysics by providing a better representation of the anvil area and slightly reducing the maximum altitude and value of the graupel mixing ratio. The model storm initiation is delayed 1-hr compared with observations; however, the simulated radar reflectivity and flash rates indicate this offset is not maintained and ranges from 30-50 minutes as the storm evolves. To further improve the model-simulated hydrometeors’ mixing ratio and vertical extent, altitude-specific scaling factors derived by comparison of the model output with DLA proxy observations are applied during the simulation to the hydrometeors in the FRPS code (i.e., the hydrometeors were not adjusted in the microphysics scheme), thereby adjusting the hydrometeors closer to the observations. These steps highlight the dependency FRPSs have on the proper representation of storm parameters in models.

The damping and LDA, along with scaling hydrometeors to proxy observations, provided the best results for modifying the hydrometeors. This allowed for the most
representative FRPS to be selected for this model set up. The scheme most similar to the observed flash rate trends and total number of flashes during the storm is based on ICEFLUX (Finney et al., 2014). The UAH UV scheme (Carey et al., 2015) provided the best comparison to the observations of any non-hydrometeor scheme. These results are described in Cummings et al. (2017a).

Using the ICEFLUX scheme, ten WRF-Chem simulations are run to investigate the mean LNO\textsubscript{x} production per flash and the transport and distribution of other trace gases for the 29-30 May 2012 convective event (Cummings et al., 2017b). The simulations included one run with no lightning chemistry and nine runs with different LNO\textsubscript{x} production scenarios. A comparison of the aircraft and model-simulated CO and O\textsubscript{3} mixing ratios indicates the convective transport is slightly underestimated in the model. To compensate for the transport underestimate, one model layer below each layer the aircraft flew within was analyzed. This adjustment showed the model-simulated CO and O\textsubscript{3} mixing ratios are within 1% and 3% of the aircraft observations, respectively.

With lightning chemistry turned off in the model, the overall mean NO\textsubscript{x} from the four model layers the aircraft flew in is underestimated by ~55%. A comparison of the aircraft and model-simulated NO\textsubscript{x} mixing ratios from the nine different LNO\textsubscript{x} production scenarios suggested 82 moles flash\textsuperscript{-1} achieved a best match within 5% of the observations. This estimate is roughly three times smaller than the mean 250 moles NO flash\textsuperscript{-1} calculated by Schumann and Huntrieser (2007) from a survey of the literature which included theoretical estimates, and values derived from laboratory studies, field data, and cloud-resolved model simulations from 1976-2007; however, the value I derived for the May 29-30 DC3 storm is within the lower end of the range of estimates.
(33-660 moles m⁻³) reported by Schumann and Huntrieser. My estimate for the observed storm is also six times smaller than the mean value suggested by Ott et al. (2010) for midlatitude and subtropical storms (500 moles m⁻³). The observed vertical wind shear between the anvil outflow and steering level (~700 hPa) for the 29-30 May severe supercell system (24 m s⁻¹) suggests longer flashes and larger LNOₓ production than tropical and subtropical convection (67-391 moles flash⁻¹); however, despite the strong shear, this is a high flash rate event with small flash extents (~6.5 km), which suggests the vertical wind shear is not the dominant influence on the LNOₓ production for this case.

Four of the LNOₓ production scenarios investigated the use of default model parameters for the fractional CG and IC flash channel vertical profiles (DeCaria et al., 2000) and IC:CG ratios (Boccippio et al., 2001) versus the use of observed data based on my model modifications. The model parameter that had a greater influence on the mean NOₓ mixing ratio in the anvil outflow for this convective event was the vertical distributions. With the default profiles the CG LNOₓ peaks below the altitude at which it maximizes in the observed storm and the lower IC LNOₓ peak does not exist. This causes the LNOₓ to be emitted lower in the troposphere and not be as close to the altitude of the anvil outflow as is the case with the observed profiles. The default vertical profiles caused the model to underestimate the observed NOₓ in the anvil outflow by < 20%, despite using a higher LNOₓ production scenario (125 moles NO flash⁻¹) than the final scenario that was selected (i.e., 82 moles flash⁻¹ and the observed model parameters).

A weak positive correlation was found between LNOₓ production and the total flash area over several DC3 storms (Pollack et al., 2016). My analysis of a more
meaningful relationship between LNO$_x$ production and mean flash area over the several storms (including the May 29-30 case) yielded a somewhat more moderate correlation. When combined with the moderate negative correlation found between the total flash rate in the observed 29-30 May severe supercell system and flash extent ($r = -0.69$) or energy per flash ($r = -0.70$), it is possible that a new parameterization scheme may be developed to estimate LNO$_x$ production as a function of time from the flash rate in models.

One of the goals in DC3 was to be able to measure changes in the composition and chemistry of the upper troposphere by taking measurements of the same convective outflow while the storm is active and 12-48 hours downwind. Based on aircraft observations, roughly 19 ppbv of O$_3$ was produced by photochemical reactions during the outflow plume’s transit to the southern Appalachian region. While this photochemical production is higher than prior estimates (DeCaria et al., 2005; Apel et al., 2015), the influence of LNO$_x$ from nearby convection in Alabama may have played a role in the O$_3$ production in this downwind region.

DC3 provided a unique opportunity to use observations from ground-based, upper air, and remote sensing instrumentation to further investigate the role lightning and lightning chemistry have on the composition of the upper troposphere both during and following convection. It is also providing greater detail on lightning characteristics (e.g., flash extent and energy), which can be used to better understand LNO$_x$ production, better parameterize it in models of all scales, and reduce the uncertainty in the global LNO$_x$ budget.
CHAPTER 10: FUTURE WORK

Upon completion of my PhD I intend to apply the knowledge I gained from my graduate school research experience toward bridging the gap between research and operational forecasting and to continue furthering the atmospheric chemistry community’s interest in LNO₅, climate, and air quality. Sections 10.1 and 10.2 provide a brief overview of this continued work. However, there are several areas where additional research related to the application of FRPSs and the relationship between lightning and LNO₅ production should be explored. Section 10.3 discusses these topics.

10.1 The DC3 6-7 June 2012 Colorado convective event

The 6-7 June 2012 Colorado convective event is a highly desired case to analyze because of the excellent coverage provided by ground-based (i.e., LMA and radar), upper air, and aircraft observations. The synoptic situation indicated the development of afternoon convection over northeast Colorado with an approaching cold front from the northwest and a shortwave trough moving along a ridge of high pressure over the Central Plains. An important meteorological feature that developed that afternoon was an area of low-level convergence, known as the “Denver Cyclone” (Wilczak and Glendening, 1988; Wilczak and Christian, 1990; Vu et al., 2016).

A significant amount of time was spent trying to select the best model domain set-up, initialization conditions, and physics schemes to simulate the observed convection. Each combination that was evaluated is provided in Table 14. Overall, the size and features of the convection were not satisfactory. The NEXRAD indicated a convective line oriented from the southwest to northeast, which became more north-to-south oriented
with time. The model simulations predicted a convective line that was either tilted more toward the southwest or oriented from north-to-south. Several set-ups also produced multiple lines of convection (i.e., NARR) or the convection was delayed and had more emphasis on the southern portion of the line (i.e., ECMWF). However, in each simulation the stratiform and anvil areas became larger than the observations soon after the convection began to develop, with cells that were not as individualized and radar reflectivities > 30 dBZ that covered a larger area. The maximum radar reflectivities were also lower than the observed. Convective damping (Li et al., 2017) and LDA (Fierro et al., 2012) methods were evaluated, but the model-simulated reflectivity was fairly similar to the previous WRF runs that did not employ these techniques.

A closer analysis of the meteorological source data showed the GFS and NARR lacked the surface mesoscale circulation pattern of the “Denver Cyclone” and the NAM-ANL and ECMWF were lacking the north-northwesterly winds of the low-level circulation between Denver and the Front Range. This difference in the low-level wind pattern may explain part of the variation between the simulated and observed convection.

The real-time 12 UTC NCAR WRF 3 km forecast used during the DC3 field campaign provided a good representation of the convection observed over the Colorado domain on 6-7 June, as well as its timing. While the forecast was run with the Morrison two-moment microphysics and YSU PBL schemes, it was also initialized using the 15 km Data Assimilation Research Testbed (DART) ensemble run. Based on the results from the WRF simulations evaluated in Table 14, further testing is suggested, especially using the real-time output from the DC3 forecasts.
Table 14. WRF model physics options evaluated for 6-7 June 2012 Colorado convective event.

<table>
<thead>
<tr>
<th>WRF Model Physics Options</th>
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<tr>
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<tr>
<td>Parent (3 km horizontal resolution, 500 \times 464 grids); Nested (1 km horizontal resolution, 813 \times 771 grids)</td>
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10.2 Flash rate parameterization schemes for the Florida Space Coast

Florida is the lightning capital of the United States. Its irregular coastlines, inland bodies of water, and land-water thermal contrasts help support the development of mesoscale boundaries involved in convective initiation (Hodanish et al., 1997; Lericos et al., 2002). KSC/CCAFS are located on the eastern edge of “lightning alley,” which stretches across central Florida (Roeder et al., 2014). At these facilities, lightning safety is of the utmost importance because employees and vehicles are exposed daily to rapidly changing weather. Therefore, forecasting the onset and termination of lightning is critical from an operational and safety standpoint. However, the difficulty and uncertainty in forecasting lightning cessation is costly to KSC/CCAFS, both financially and in delaying outdoor work required for readying space vehicles and payloads for launch (Roeder and Glover, 2005). Previous research has generally concentrated on lightning initiation forecasts (e.g., Gremillion and Orville, 1999; Wolf, 2006; Roeder and McNamara, 2011; Woodard et al., 2012). A few studies have investigated lightning cessation, but they only focused on observational data (e.g., Stano et al., 2010; Preston and Fuelberg, 2015; Davey and Fuelberg, 2017). I plan to build on this work and help improve the current guidelines used in terminating a lightning advisory by using a cloud-resolved model with FRPSs.

In April-June 2017, aircraft flights will be conducted to validate instrument performance onboard the GOES-R satellite (now NOAA’s GOES-16 satellite), including the GLM, which was launched in November 2016 (Padula and Goodman, 2016). The NASA ER-2 aircraft will be used to conduct these flights over regions equipped with LMAs. One of these areas is KSC/CCAFS, which has a dense network of ground-based meteorological instrumentation, including several lightning detection networks. Onboard
the aircraft is instrumentation used to optically detect lightning and remotely sense trace gases (e.g., NO₂).

Assuming a convective event occurs over or within range of the KSC/CCAFS ground-based instrumentation (e.g., local lightning detection networks and radar) during the GOES-R validation mission, a cloud-resolved thunderstorm simulation will be performed and the results will be compared with surface, upper air, and aircraft observations. NASA’s Applied Meteorology Unit (AMU) has tuned the NCAR Advanced Research WRF (WRF-ARW) to develop a local mesoscale model that is representative of the meteorological environment in and around KSC/CCAFS (Watson, 2013). This local model will be used to incorporate and evaluate FRPSs for the Florida Space Coast and will help identify the best FRPS(s) for the case study.

The cloud-resolved thunderstorm analysis will also be expanded to include all types of convection (e.g., single cell and multicell), as well as storms with low and high flash counts. If different schemes are more appropriate for certain flow regimes, thunderstorm types, seasons, etc., this information will be critical when implementing the FRPSs into the local mesoscale model and also for forecasting lightning cessation. This research would also benefit local operational forecasters (e.g., United States Air Force’s 45th Weather Squadron) and allow for the testing of FRPSs in an environment (i.e., subtropics) other than the midlatitude (Barthe and Barth, 2008; Barthe et al., 2010; Cummings et al., 2017a) and tropical (Cummings et al., 2013) regions where FRPSs have previously been evaluated in cloud-resolved simulations.
10.3 Additional investigations stemming from the dissertation research

Based on the performance of the 18 FRPSs in the 29-30 May case study, there are several aspects of the FRPS application in cloud-resolved models that need to be explored further. First, as new FRPSs are developed or evolve, the schemes should be assessed using the same set of convective events and same model configuration for evaluation. These events should represent thunderstorms of varying type, severity, location, and flash rates. A complex set of cases will help validate a FRPS’s performance by ensuring the scheme is performing as intended when applied in a model set-up and by testing the limits of its application. Similar intercomparison studies have been performed in the past using specific weather phenomena (e.g., 10 July 1996 STERAO-A storm) to investigate the performance of LNO₃ parameterization schemes (Barth et al., 2007), FRPSs (Barthe et al., 2010), and microphysics schemes (Morrison et al., 2015). This evaluation process will allow for a better understanding of the performance of each FRPS, especially when the schemes are tested on a new convective event.

Second, the FRPS equations are applied to each model processor within the model domain for this case study. Sensitivity studies should be performed to explore how the number of model processors used may modify the model-simulated flash counts, especially when the equations are nonlinear or linear with non-zero y-intercepts, and if there is a better way to apply the FRPSs in online simulations versus using model output to perform the calculations offline. Also, identification of limitations for the horizontal and vertical resolutions at which FRPSs can be applied would also be beneficial. For example, are flash rates significantly overestimated when a 1 km x 1 km horizontal
resolution is used because that resolution resolves storm features (e.g., vertical velocity and hydrometeors) more finely than was the case when the scheme was developed?

Another topic that requires additional investigation is the potential aerosol effects on flash rates. As the nine different LNO\textsubscript{x} production scenarios were evaluated in WRF-Chem, the simulated flash rate time series varied. While the GOCART aerosol scheme used in the model simulation of the 29-30 May case study is connected to the radiation schemes in WRF-Chem, it is not connected with the cloud microphysics schemes and does not contain the nitrate aerosol. Therefore, a different aerosol scheme, which offers these features (e.g., the Model for Simulating Aerosol Interactions and Chemistry (MOSAIC)), should be used to further examine the potential influence the changes in NO\textsubscript{x} due to lightning have on aerosol concentrations (e.g., nitrates and sulfates) and storm microphysics and kinematics. Any potential relationships will be especially important for chemistry-climate simulations and will further strengthen the need to reduce uncertainty in the global LNO\textsubscript{x} budget.

Finally, my results suggest the development of a parameterization scheme that determines LNO\textsubscript{x} production per flash based on flash rate may be possible; however, this is based on a small sample size, which showed a weak to moderate positive correlation between mean flash area and LNO\textsubscript{x} production per flash. A larger dataset needs to be constructed and also focus on data within the LMA network’s 3D coverage where the detection efficiency is highest. This is important for accurately capturing the flash extent and area, since flash size may become distorted as the distance from the network increases.
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