How the Chemical Composition of the Pre-storm and Inflow Regions Compare to each other and to the Outflow Region of Deep Convection in the Upper Troposphere

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ABSTRACT

Ozone in the upper troposphere is considered a greenhouse gas, which can contribute to climate change. Convection in thunderstorms can carry ozone precursors upward from the boundary layer into the upper tropospheric region. Production of nitrogen oxides associated with lightning in the storm can also play a role in the transformation of the upper troposphere chemical composition. Data from the Deep Convective Clouds and Chemistry (DC3) Field Campaign were used to compare pre-storm, inflow, and outflow data using four different storm events in diverse regions. Vertical profiles of ozone, its precursors, and other related compounds were used to highlight the inflow and outflow aircraft measurements in relation to pre-storm and near storm concentrations. This comparison allowed us to determine whether the pre-storm data can be used for the analysis of convective transport and scavenging of trace gases in the upper troposphere. It was found that the chemical species’ concentration in the inflow didn’t always match the concentration of other times in the boundary layer. Though some constituents showed similarities, there was variability among the different cases. Despite this variability, it may still be useful to incorporate pre-storm data for future studies. Comparison of the outflow data to the inflow data revealed the degree of scavenging for each constituent trace gas and aerosol for different boundary layer environments and storm types. It was found that while some species consistently either scavenged or didn’t, others showed that they were scavenged in some cases but not all. For the latter situation more detailed analysis of storm location and characteristics would be beneficial.

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1. Introduction

Deep convection contributes to the transport of chemical compounds from near the surface to the upper troposphere (e.g., Chatfield and Crutzen, 1984; Dickerson et al., 1987). These relocated chemical compounds in the upper troposphere typically have a better chance to be carried globally since they tend to live longer. This is due to colder temperatures in the upper troposphere in which chemical reactions typically occur at a slower rate (Brasseur, Orlando & Tyndall, 1999). Therefore, this is not just a region-specific occurrence, but it affects the atmosphere universally. One of the chemical compounds that experiences this event is ozone ($O_3$). Ozone, a greenhouse gas when in the upper troposphere, may be moved wholly from near the surface and brought up by convection or may be formed chemically in the upper troposphere after the transport of its precursors from near the surface (Bertram et al. 2007). A study by Lawrence et al. (2003) found that the chemical production of upper troposphere ozone is greater because of the movement of its precursors than of ozone itself (Tost et al. 2010). Ozone’s precursors NO$_x$ (NO+ NO$_2$), HO$_x$ (OH+HO$_2$), CH$_2$O, H$_2$O$_2$, and CO contribute to the creation of upper troposphere ozone when sunlight causes them to react. Though these chemical compounds may get carried from near the surface due to deep convective transport, a large quantity of NO$_x$ contributes to the upper troposphere by the creation of NO from lightning in thunderstorms (Brasseur, Orlando & Tyndall, 1999). This shows the significance that convective movement of chemical compounds has to our knowledge of climate change, atmospheric chemistry, and air quality (Brasseur, Orlando & Tyndall, 1999).

The importance of this research has been noticed by many scientists who have sought to gain understanding of this subject area. Barth et al. (2007a) simulated the 10 July 1996 Stratosphere-Troposphere Experiment to focus on the convective transport of HO$_x$ and its precursors to the upper troposphere. However they found that CH$_2$O and H$_2$O$_2$ will differ depending on the storm’s characteristics due to aqueous chemistry processes. One important storm characteristic is the temperature of the cloud base and whether it contains ice or water. Since these types of chemical species are soluble in water they can dissolve into liquid cloud droplets and precipitate to the surface (Brasseur, Orlando & Tyndall, 1999). Therefore it was determined that it would be useful to analyze multiple different storms to expand the knowledge of convective transport to the upper troposphere. A follow-up study (Barth et al., 2007b) compared different models’ abilities to move chemicals to the upper troposphere by the process of convection. From this they found that the model predictions agreed with each other and with observations for species—such as CO and O$_3$—expected to only be transported by convection. The models disagreed on transport and scavenging of soluble species—such as HNO$_3$, H$_2$O$_2$, and CH$_2$O—but there were no measurements to evaluate results, and that NO$_x$ predictions varied and some model results agreed with observations. They learned that there was a need for data from both inflow and the outflow regions of the storm of these chemical compounds as well as data for the study of the budget of multiple chemical compounds (Barth et al. 2007b).

The Deep Convective Clouds and Chemistry (DC3) experiment was designed to take measurements of the inflow and outflow regions of a variety of different storms in diverse environments and a range of chemical compounds instead of just a select few (Barth et al. 2012).
This inflow data, when analyzed and compared to pre-storm data, the variety of types of storms, and their environments, will help to increase the understanding of the processes of a range of chemical reactions and transport into the upper troposphere and determine the importance of pre-storm data in future analysis. Additionally, when the outflow region’s chemical composition is compared to the inflow region and the pre-storm; it provides information about the convective transport of chemicals from the boundary layer and allows a better understanding of the scavenging of chemicals in convective clouds.

This paper is outlined as follows: Section 2 explains the methods used in selecting the cases and the processes in analyzing the data sets. Section 3 will provide plots describing each case and Section 4 will include the interpretations, discussion of each, and information for future work involving this topic. Section 5 will provide brief summary and final conclusions of this research.

2. Methods

a. Study Locations

The DC3 field campaign sampled storms in northeast Colorado, west Texas to central Oklahoma, and northern Alabama (Barth, Brune, Cantrell & Rutledge, 2012). One of the reasons these regions were selected is that storms in these areas would be close to useful ground facilities. In northeast Colorado the CSU-CHILL and Pawnee radars, 3-D lightning mapping array (LMA), and sondes were some of the ground based facilities used in this region. In west Texas to central Oklahoma two SMART radars, 3 LMAs, and radiosondes were available for use in this region. In northern Alabama the ARMOR and MAX radars, UA-H LMA, and radiosondes were used in this region (Barth, Brune, Cantrell & Rutledge, 2012).

These locations were selected because of the convection possibility and the opportunity to analyze a variety of types of storms depending on the region. Colorado storms typically have high shear, high cloud bases and a lot of ice; central Oklahoma and west Texas storms have both high shear and convective available potential energy (CAPE) and are strong, severe storms; northern Alabama storms usually have low shear with moderate CAPE and are short-lived storms (Barth, Brune, Cantrell & Rutledge, 2012). Sampling different types of storms helps to develop a greater understanding of what influences and processes are behind convective transport.

These three regions provide a good diversity in the boundary layer composition. Northeast Colorado and the central Oklahoma and west Texas regions both contain agriculture, however northern Alabama is more forested (Barth, Brune, Cantrell & Rutledge, 2012). Contrasting environments are important when observing the types of chemicals that get transported. Each region may contain more of one chemical than another due to its environment.

b. Data Collection

It is important to focus on more chemical compounds rather than a select few because these all can play a role in influencing upper troposphere ozone through different types of chemical reactions. This increases the understandings as to which of these chemical species are
the primary ones to focus on when researching climate change. The DC3 Field campaign collected data from May-June 2012 using the NSF/NCAR Gulfstream V (GV) and NASA DC-8. These aircraft were equipped to measure a variety of different types of chemical species. The GV typically flew at a higher altitude and the DC-8 usually measured closer to the boundary layer collecting data near the inflow region of the storm (Barth, Brune, Cantrell & Rutledge, 2012).

c. Case Selection

To compare different environments and chemical species, four specific cases were selected from the DC3 field campaign’s 17 coordinated flights of the GV and DC-8. The cases that were selected for this research consist of 4 of these 17 flights. These cases were May 29th in Oklahoma, June 6th in Colorado, May 21st in Alabama and a Mesoscale Convective System on June 11th near southern Missouri and Arkansas. Each case is unique in the location as well as the storm type. This provides a variety of data to be compared and develop the understanding of convective transport in different environments.

d. Data Analysis

The goal of this research is to identify and compare pre-storm, inflow, and outflow data to gain a better understanding of which chemical species get ingested into storms and convectively transported. To do this, first, data were used from the general region only and then it was averaged from one second to one minute. Then inflow and outflow times were identified using Catalog Earth (found at http://catalog.eol.ucar.edu/dc3_catalog_earth) and flight notes from the field campaign. Also cloud variables were used to help determine when the aircraft were in outflow except for the Alabama case in which the DC-8 outflow used only outflow times. The inflow and outflow measurements were marked on vertical profiles and on time series plots of altitude and chemical concentration. It was found that the vertical profiles were sufficient for the analysis so those were the only plots shown. To compare the pre-storm, inflow, and outflow regions of the storm, it was done mainly visually using the vertical profile plots.

3. Results of Vertical Profiles

These plots show the vertical profiles, with inflow and outflow times highlighted in blue and red, of each chemical species for each of the four cases. In the MCS case, the GV aircraft sampled the outflow region in two separate intervals—one early in the storm and one later. The orange represents the earlier interval. The “x” represents data taken from the GV aircraft and the dots represent data taken from the DC8.
a. Transported Species

**Figure 1.** The vertical profile of Carbon Monoxide for each of the four cases. This shows the similarity of CO’s concentration in the inflow region and during the pre-storm and other times in the boundary layer. It also shows how the species is transported to the upper troposphere.
O$_3$: Figure 2. The vertical profile of Ozone for each of the four cases. This shows the same as in Figure 1.
**Toluene**: Figure 3. The vertical profile of Toluene for each of the four cases. This shows the variability of Toluene’s concentration in the inflow region and during the pre-storm and other times in the boundary layer. It also shows how the species varies among the cases in its transportation to the upper troposphere and how the profile in each case of Toluene has somewhat differing shapes.
Benzene: Figure 4. The vertical profile of Benzene for each of the four cases. This shows the same as in Figure 3.
Isoprene: Figure 5. The vertical profile of Isoprene for each of the four cases. This shows the same as in Figure 1. This plot is plotted logarithmically, unlike the others, in order to get a closer look at the data.
**Figure 6.** The vertical profile of OH for each of the four cases. This shows the same as in Figure 3.
**Black Carbon: Figure 7.** The vertical profile of Black Carbon for each of the four cases. This shows the same as in Figure 1.
b. Lightning-Production

\textbf{NO}_x: Figure 8. The vertical profile of Nitrogen Oxides for each of the four cases. This shows the same as in figure 3 except the vertical profiles have similar shapes in all four cases.
c. Soluble Species

**H₂O₂: Figure 9.** The vertical profile of Hydrogen Peroxide for each of the four cases. This shows the same as figure 3, however the species is scavenged in the upper troposphere and the profiles in each case of H₂O₂ have similar shapes.
SO₂: Figure 10. The vertical profile of Sulfur Dioxide for each of the four cases. This shows the same as figure 9 with the exception of the Oklahoma case in which the shape and scavenging differ from the other cases.
**HNO$_3$: Figure 11.** The vertical profile of Nitric Acid for each of the four cases. This shows the same as figure 9. It is also shown how the species is scavenged in the upper troposphere; however in the Alabama and MCS cases the scavenging is not as clear. The profiles in each case of HNO$_3$ have similar shapes with the exception of the Alabama case.
**CH$_3$OOH:** Figure 12. The vertical profile of CH$_3$OOH for each of the four cases. This shows the same as figure 9. However the Oklahoma and Colorado cases show inflow and pre-storm data to be similar.
**CH$_2$O: Figure 13.** The vertical profile of Formaldehyde for each of the four cases. This shows the same as figure 9. However the Alabama and Colorado cases show inflow and pre-storm data to be dissimilar. CH$_2$O appears to be transported more than scavenged. The profiles in each case of CH$_2$O have similar shapes in the Colorado and Alabama data but differ in the Oklahoma and MCS cases.
4. Discussion

These vertical profiles display information about how certain chemical species behaved when either being transported or scavenged. In Figures 1, 2, 5, 12, and 13 it is shown that there is some similarity of the CO, O₃, isoprene, CH₃OOH, and CH₂O chemical concentrations in the inflow times with that of the pre-storm times in the boundary layer. There were, however, other species in the remaining figures that showed variability among the concentrations of species in the boundary layer in different cases. This could be due to local sources of emissions like wildfires, nearby power plants, etc.

There were also similarities in the profile shapes of some of these species however for others there were some differing shapes. Some of the species that differed were OH (figure 6) and SO₂ (figure 10) in at least one of the cases. It is recommended to look closer at these flight tracks and storm characteristics to determine what may be causing this difference in the profiles.

In most of the plots of the Alabama case it appears that there is a deeper outflow causing some variability in the profile shapes, this could be due to a lower tropopause and low wind shear environment allowing slower updraft speeds and detrainment at lower altitudes, so this could be useful information to look into in future studies. Lastly, when looking at the profiles of the scavenged species, it appears that HNO₃ (in figure 11) differs in the way that it is scavenged in the Alabama case, this could be due to mixing of the troposphere before the storm and it would be helpful moving forward to carefully examine the pre-storm environment using the aircraft and sonde data. Model simulations could also be used to provide information about surrounding storms that could have been affecting the upper troposphere composition. CH₂O (in figure 13) also varies from case to case. CH₂O profiles show very little scavenging in most of the cases. It would be helpful moving forward with this analysis, since the majority of this study’s analysis was done visually, to quantify the transport and scavenging efficiencies to get a better idea of how these species behave and to decrease the variability in parameterizations to better predict scavenging of these species. It may also be useful to compare different species in the same environments instead of looking at how the same species behaves in different environments.

Originally, as stated above, timeseries plots were also created, however it was found that these plots didn’t express anything different than these vertical profile plots so it was decided that the vertical profiles were sufficient enough in helping with this analysis. In the future, it may be helpful to incorporate these timeseries plots in a spatial way and look at maps to help determine where some of these emissions are originating. Additionally, it would be beneficial to look into the other cases of the DC3 field campaign and the other chemical concentrations measured to compare with these results.

This study sought to improve understanding of chemical processes that occur in convective environments that may influence upper troposphere ozone. With this research we got a better understanding of whether the pre-storm boundary layer composition is similar to the inflow air composition. We can then use this information to determine if we have to exclude pre-storm data from our analysis when examining convective transport and scavenging of trace gases.
5. Conclusions

This study used measurements of 15 different chemical constituent concentrations taken from four cases of the Deep Convective Clouds and Chemistry (DC3) Field campaign to compare concentrations of the pre-storm, inflow, and outflow regions of the storms. These data were organized into vertical profile plots to observe the behavior of the transported and scavenged species in each case. When comparing the chemical composition of the inflow and other times in the boundary layer, it was found that some species’ concentrations were similar in the boundary layer: CO, O₃, isoprene, CH₃OOH, and CH₂O. The other species’ concentrations in the boundary layer didn’t always match among cases. Regardless of this variability, it was determined that it still may be helpful to include pre-storm data in future studies.

The outflow data helped to increase the understanding of which species were scavenged and how they compared in different boundary layer environments and storm types. It was found that some species were consistently scavenged — like H₂O₂ and CH₃OOH — while others were scavenged in some cases but not all — like SO₂, HNO₃, and CH₂O. These variations among cases would benefit from more detailed examination of flight tracks and storm characteristics. This study aided in developing knowledge for future studies of the different regions of the storms including how pre-storm environments compare to inflow regions and also the likelihood of scavenging and transport of certain species through the use of outflow region data compared to the inflow region.

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