ASCENT 019 Development of Aviation Air Quality Tools for Airshed-Specific Impact Assessment: Air Quality Modeling

University of North Carolina at Chapel Hill

Project Lead Investigator

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- PI: Saravanan Arunachalam, Research Associate Professor
- FAA Award Number: 13-C-AJFE-UNC Amendments 1 - 5
- Period of Performance: September 13, 2013 – December 31, 2016
- Task(s):
  1. Develop and Assess Efficacy of Multiple Emissions Scenarios using the APMT-Impacts Air Quality Modeling Platform for year-over-year analysis to achieve Air Quality (and Health) Goals under FAA's Policy Initiatives
  2. Extend current prototype modeling for CMAQ-DDM-3D to compute Airport-specific Sensitivities for the year 2005, and explore possibilities to extrapolate for a future year
  3. Assess PM Size Distribution Impacts of Aircraft Emissions
  4. Assess impacts of coupled models on Aviation-related AQ Impacts
  5. Develop High Fidelity Weather for Global Inventories using AEDT

Project Funding Level

$369,966

Matching funds from

A) Los Angeles World Airport Authority (LAWA)
B) North American Insulation Manufacturers Association (NAIMA).

Investigation Team

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Project Overview

With aviation forecasted to grow steadily in upcoming years,[1] a variety of aviation environmental policies will be required to meet emissions reduction goals in aviation-related air quality and health impacts, and tools will be needed to rapidly assess the implications of alternative policies in the context of an evolving population and atmosphere. In addition, tools are required to understand the implications of global aviation emissions, in the context of the International Civil Aviation Organization (ICAO)'s Committee on Aviation Environmental Protection (CAEP).

The overall objective of this project is to continue to develop and subsequently implement tools to allow for assessment of year-over-year changes in significant health outcomes, both within the US and globally. These tools are intended to be acceptable to FAA (in the context of Destination 2025) or to other decision-makers, while providing outputs quickly enough to allow for a variety of "what if" analyses and other investigations. While the tools for use within and outside the US (for CAEP) need not be identical, a number of attributes would be ideal to include in both:

- Enable the assessment of premature mortality and morbidity risk due to aviation-attributable $PM_{2.5}$, ozone, and any other pollutants determined to contribute to significant health impacts from aviation emissions;
- Capture airport-specific health impacts at a regional and local scale;
- Account for the impact of non-LTO and LTO emissions, including separation of effects;
- Allow for the assessment of a wide range of aircraft emissions scenarios, including differential growth rates and emissions indices;
- Account for changes in non-aviation emissions and allow for assessing sensitivity to meteorology;
- Provide domestic and global results;
- Have quantified uncertainties and quantified differences from EPA practices, which are to be minimized where scientifically appropriate; and
- Be computationally efficient such that tools can be used in time-sensitive rapid turnaround contexts and for uncertainty quantification.

The overall scope of work is being conducted amongst three collaborating universities – Boston University (BU), Massachusetts Institute of Technology (MIT) and the University of North Carolina at Chapel Hill (UNC). However, while the reporting is being done under three separate projects (ASCENT 18, 19 and 20) by each collaborating university, the project is performed as a coordinated effort with extensive interactions among the three institutions. The components led by the University of North Carolina at Chapel Hill's Institute for the Environment (UNC-IE) included detailed modeling of air quality using the Community Multiscale Air Quality (CMAQ) model. UNC-IE is collaborating with BU to develop health risk estimates on a national scale using CMAQ outputs, and with MIT for inter-comparing against nested GEOS-Chem model applications within the US and to further compare/contrast the forward sensitivity versus the inverse sensitivity (such as adjoint) techniques for source attribution. Our efforts for this project build directly on previous efforts within Project 16 of PARTNER, including detailed air quality modeling and analyses using CMAQ at multiple scales for multiple current and future year scenarios, health risk projection work that successfully characterizes the influence of time-varying emissions, background concentrations, and population patterns on the public health impacts of aviation emissions under a notional future emissions scenario for 2025. Under Project 16, we started to develop a new state-of-the-art base year modeling platform for the US using the latest version of models (CMAQ, WRF, SMOKE) and emissions datasets (AEDT, NEI), and tools (MERRA-2-WRF, CAM-2-CMAQ) to downscale from GCMs being used in Aviation Climate Change Research Initiative (ACCRI).

In this project, we are performing research on multiple fronts during the stated period of performance:

1. Develop and assess efficacy of multiple emissions scenarios using the APMT-Impacts Air Quality Modeling Platform for year-over-year modeling to achieve air quality (and health) goals under FAA's Policy Initiatives
2. Extend current prototype modeling for CMAQ-DDM-3D to compute higher order sensitivity coefficients
3. Assess PM size distribution impacts of aircraft emissions on ambient air quality

[1] Boeing Commercial Airplane Market Analysis, 2010.

4. Assess impacts of meteorology-chemistry coupled models and the feedback processes on Aviation-related AQ Impacts
5. Develop High Fidelity Weather for Global Inventories using AEDT

Task 1: Develop and Assess Efficacy of Multiple Emissions Scenarios using the APMT-Impacts Air Quality Modeling Platform for Year-over-year Analysis to Achieve Air Quality (and Health) Goals under FAA's Policy Initiatives

University of North Carolina at Chapel Hill

Objective(s)

The objective of this task is to develop a multi-year WRF-SMOKE-CMAQ modeling platform to assess the past, present and future year US-wide aviation impacts on air quality. This platform helps to address the aspirational goal of FAA to reduce aviation emissions contribution to significant air quality and health impacts in future years.

Research Approach

We reported WRF-SMOKE-CMAQ modeling framework development and model predictions for annual years 2005 and 2010 in last year's annual report. This year, we worked on few additional tasks to improve the future CMAQ modeling framework for air quality and health assessment studies. Figure 1.1 shows the modeling framework that UNC has been developing. While initially the years identified were 2005, 2010 and 2018, recently FAA has recommended that we model 2011 and 2015 moving forward.

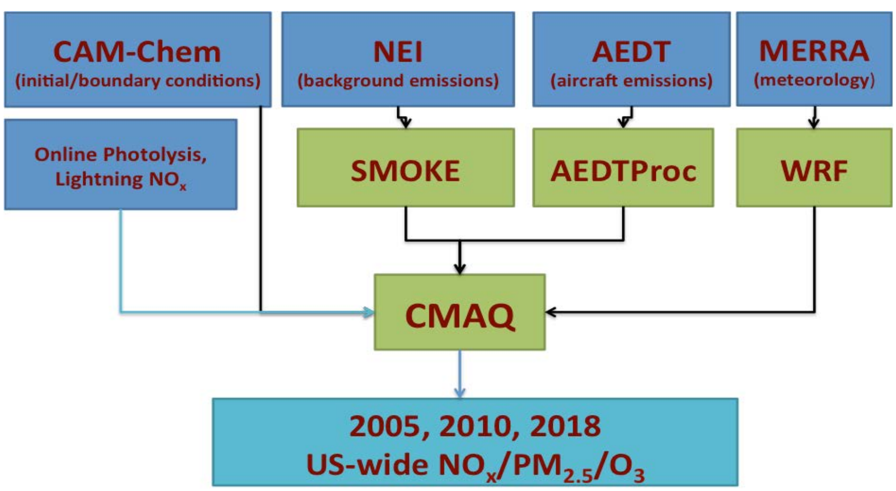

Figure 1.1: Flowchart representing the modeling methodology platform.

CMAQ-DDM v4.7.1 Results: We completed 2005 annual year all-airports CMAQ-DDM (direct decoupled method) model simulations and provided annual and quarterly average results to Boston university (BU) for health studies. Figure 1.2 shows the domain wide $PM_{2.5}$ and O_3 aviation-attributable concentrations from CMAQ-DDM model outputs. Here we compared pseudo two-month average contributions with four annual quarters (P1: JFM, P2: AMJ, P3: JAS, P4: OND months) and annual averages to understand the differences in various temporal averaging. This exercise will also explain if it is necessary to conduct annual simulations or the pseudo two-month simulations are sufficient to estimate the annual aviation-attributable perturbations. The results indicate that in the case of $PM_{2.5}$ the monthly and quarterly averages are comparable to annual average whereas in the case of O_3, due to non-linear chemistry, we observed high seasonal differences (summer contributions were higher than winter), which are averaged with the annual average. Therefore in the case of O_3, it is important to conduct a full annual model simulation to capture the annual seasonal trend.

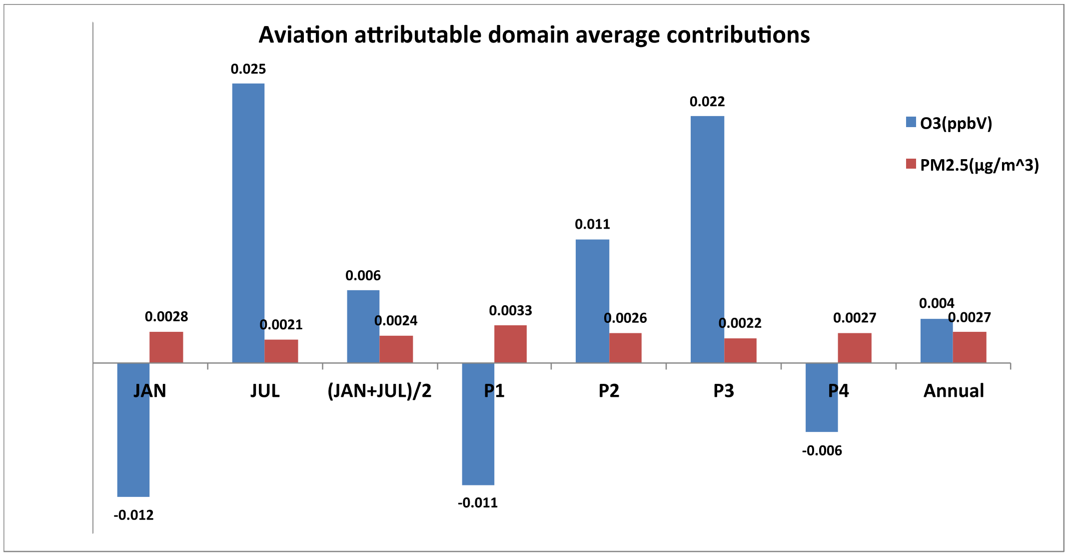

Figure 1.2: Aviation attributable domain average contributions of O_3 (blue) and $PM_{2.5}$ (red) for January, July, pseudo two-month (JAN+JUL/2), quarterly (P1, P2, P3, P4) and annual time periods.

Meteorological Inputs: In support of the High Fidelity Weather task, we migrated to drive WRF with inputs from NASA's Modern-Era Retrospective Analysis for Research and Applications reanalysis data (MERRA) (Rienecker et al., 2011). We completed downscaling MERRA with WRF for the year 2013 and 2015 is in progress.

Boundary conditions for future CMAQ modeling: In this task we generated downscaled dynamical boundary conditions for CMAQ model from global model CAM-Chem modeling scenarios provided by UIUC under ACCRI project. The 2005 and 2050 scenarios are described in Table 1.1 which indicates the emission modifications that went into future year 2050 modeling. We generated 2005, 2050 boundary conditions and compared them for four quarters in the modeling period, as shown in Figure 1.2. In the case of O_3 at the surface (as represented in Figure 1.3), the 2050 boundary concentrations are lower than in 2005, whereas in upper model layers (not shown here) 2050 concentrations are higher than 2005. Therefore, for future modeling, these downscaled boundary conditions can be utilized as inputs to run a regional scale CMAQ model for both present and future year scenarios. In addition, we also explored another option to use a hemispheric CMAQ application to generate boundary conditions for regional CMAQ, which should also be considered for future work.

Table 1.1: 2005 and 2050 ACCRI modeling scenarios for CAM-Chem global model

Scenarios	Emissions Description
2005 sens	2005 all sources + aviation
2050 SC1	2050 all sources + aviation (technology improvement, reduction in NOx emissions)
2050 Alt	2050 all sources + aviation (alternative fuel, zero sulfur emissions and 50% reduction in BC emissions)

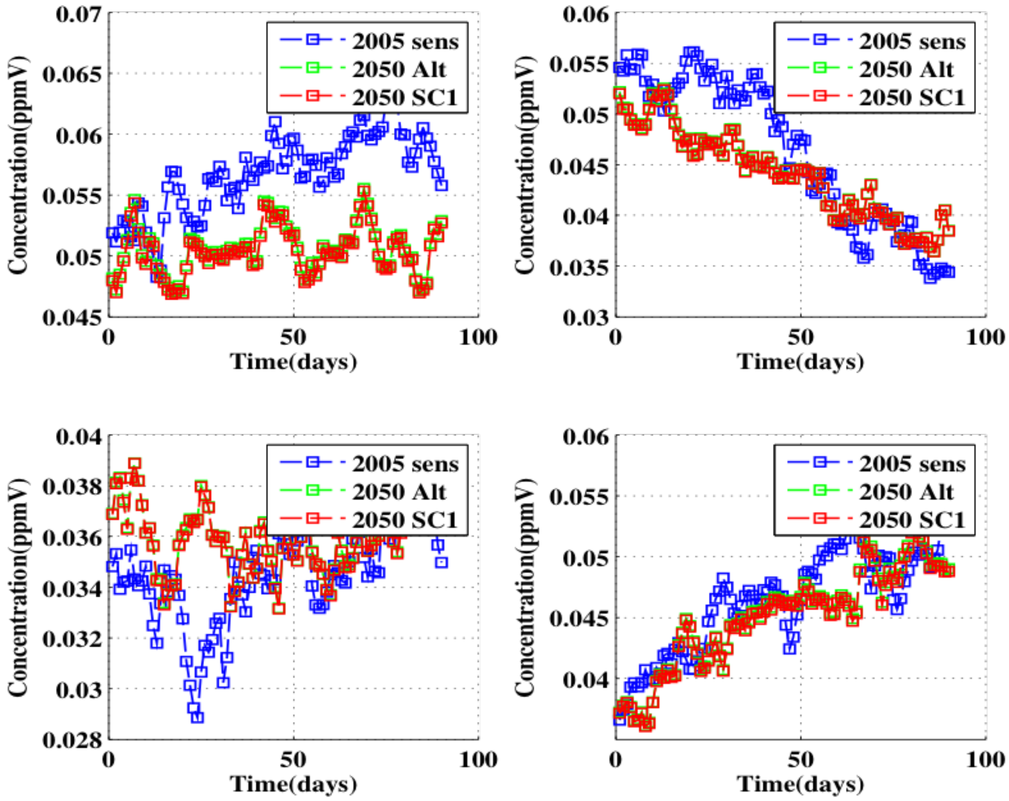

Figure 1.3: Layer 1 (model surface layer) daily average boundary conditions of Ozone for four quarters P1 (JFM, top left), P2 (AMJ, top right), P3 (JAS, bottom left) and P4 (OND, bottom right) in annual year.

Airport-based emissions: We analyzed airport-based emissions from raw AEDT segment data to understand the contribution from top airports in U.S. This data was performed in support of BU's health assessment study, so we provided airport specific annual, as well as monthly, fuel burn and emissions information. We calculated all U.S. airport total fuel burn and emissions for year 2005 and estimated the total contribution from the top 66, 100, 150, 200 and 300 airports relative to all U.S. airports fuel burn, as shown in Table 1.2. It appears that the top 300 airports cover ~97% of the U.S. aviation fuel burn. The highest fuel burn percentage is shown at the ATL airport, contributing ~5.2% to the total U.S. airport fuel burn, followed by ORD (~ 5.1%), LAX (~4%), DFW (~4%) and JFK (~3.5%). This information can be very helpful in future airport-specific DDM modeling work to make decisions regarding the number of airports that need to be considered for first and second aviation emissions-related sensitivities.

Table 1.2: Airports grouping and their respective Fuel Burn percentage

Airports	Fuel Burn (%)
DDM – 66 airports work	77%
Top 66 airports	84%
Top 100	89%
Top 150	94%
Top 200	95%
Top 300	97%

AEDT testing: This year we received sample recent years of AEDT segment and flight data a few different times (early 2016 and again during end of 2016). We tested our tool each time and reported the issues to FAA. Finally last month, we received recent years' raw AEDT (2010, 2015) annual segment and flight data. The initial single day testing was completed and presently we are processing month-long gridded data with our AEDTProc processing tool (Baek et al., 2012). Once we complete this phase of testing, we are ready to generate annual flight gridded emission inputs for multiple annual years.

Milestone(s)

April 2016 - Completed generating boundary conditions for CMAQ platform using CAM-Chem global model outputs from model ensemble ACCRI project for 2005 and 2050 scenarios.
July 2016 - Generated 2005 airport-by-airport based fuel burn percentages and provided the top airports emissions that contribute to 97% of U.S. fuel burn.
December 2016 - Tested and processed new 2010 and 2015 AEDT raw segment data using our AEDTProc gridding tool to generate CMAQ domain specific gridded emission inputs.

Major Accomplishments

The different study areas conducted in task 1 provide us the information necessary for various NAS-wide modeling future work decisions. The tools tested and the data generated in this task will be used in the remaining all other DDM, coupled WRF-CMAQ and particulate matter size distribution tasks under this project.

Publications

None

Outreach Efforts

None

Awards

None

Student Involvement

Pradeepa Vennam conducted most of the work under this task and graduated this semester with her PhD.

Plans for Next Period

NAS-wide modeling platform possible updates:

For the next phase of modeling, we are planning to update and change several modeling specifications and data inputs. Below are the details for some possible updates to improve the NAS-wide modeling platform to perform year-by-year simulations.

1) MERRA2: New reanalysis of MERRA2 meteorology data (data available from 1978-recent) is released with recent updates to MERRA, which showed improvement in seasonal mean climate, re-evaporation of frozen precipitation and cloud condensate (Molod et al., 2015; Bosilovich et al., 2015).
2) CMAQv5.1: EPA released new CMAQ version 5.1 (Bash et al., 2015) with important updates (ACM2 scheme (vertical velocity calculation) modification, potential vorticity update, SOA updates). We will use this version or CMAQ v5.2 Beta, which is expected to be finalized in spring 2017 for next phase of modeling.
3) Boundary conditions: Generate downscaled boundary conditions from hemispheric CMAQ to drive regional CMAQ. This approach maintains the consistency in chemical and physical processes used between the regional scale model and boundary conditions. Hemispheric model based tools were already developed for some of our other projects that can be utilized and applied here. We strongly recommend the benefits of using hemispheric boundary conditions based on availability instead of different global model boundary conditions.
4) Domain resolution: In recent years, EPA started to use 12-km grid resolution for most of their policy related modeling tasks and CMAQ testing purposes. So upgrading to 12-km model grid resolution from 36-km in our modeling work will better capture the fine-scale impacts near the airports and will be consistent to other regulatory modeling protocols.

5) Background emissions: Update background emissions for all sources to the latest NEI emissions (2014 or 2011) from the EPA.

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Task 2: Develop 2nd Order Sensitivities with CMAQ-DDM

University of North Carolina at Chapel Hill

Objective(s)

The objective of this task is to implement and explore second order Decoupled Direct Method (DDM) sensitivity coefficient calculations with LTO emissions from aircraft across the United States. This will be done with the Community Multiscale Air Quality Model (CMAQ) version 5.0.2.

Research Approach

Introduction

Air quality models are used to estimate concentrations of pollutants in the atmosphere. We aim to use air quality models to estimate concentrations of pollutants from aircraft emissions in order to model the impact of aircraft emissions on human health for populations in the vicinity of airports.

Sensitivity analysis tools are often used within the air quality modeling framework to evaluate impacts due to changing input parameters in the model such as emission rates, initial conditions, or boundary conditions. These become important for utilizing models as a way to guide emission reduction policies. Sensitivity tools have been limited to finite difference and regression-based methods that often become computationally intractable and are often unable to describe *ad hoc* analyses. Furthermore, to calculate pollutant concentration sensitivities to LTO emissions, we use the Decoupled Direct Method (DDM) in CMAQ. DDM methods calculate sensitivity coefficients in a single model run (Russell, 2005; Zhang et al., 2012), allowing for *ad hoc* analyses from changing multiple input parameters at a time. And perhaps most importantly, the use of DDM allows for the inline calculation of both first and higher order sensitivity coefficients, which become important for pollutant species that may not be linearly dependent on certain precursors. First order sensitivity calculations will yield information about the change in species concentrations with respect to varying one input parameter. In our case, these calculations will only describe linear changes of concentrations with respect to increasing or decreasing emissions from aircraft. However, some changes in species, such as secondary organic aerosols, do not linearly change with increasing or decreasing precursor emissions and higher order sensitivity coefficients can capture the non-linear change in species concentrations.

Methodology

Higher order DDM was implemented in CMAQ version 5.0.2. DDM becomes an ideal choice for describing aircraft (airport) emissions since the relatively small quantity of emissions emitted by each source can lead to numerical noise with other sensitivity methods that require multiple model runs for each varied parameter (Napelenok, Cohan, Hu, & Russell, 2006). CMAQ-DDM first and second order runs were performed for all airports (~2100 airports) in the continental United States (CONUS) in January and July of 2005. Ten day spin-up simulations were performed prior to the start of each month (December and June, respectively). Six precursor species groups (NO_x, SO_2, VOCs, PSO_4, PEC and POC) were designated as sensitivity input parameters. First and second order sensitivities of O_3 and $PM_{2.5}$ to the emissions of these six precursors were calculated.

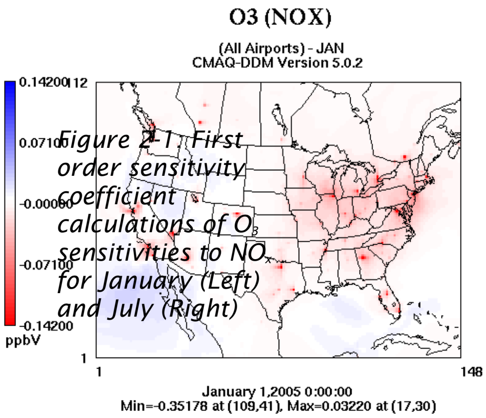
Flight segment data from AEDT (Roof & Fleming, 2007; Wilkerson et al., 2010) were processed into gridded emission rate files using AEDTProc (Baek, B.H., Arunachalam, S., Woody, M., Vennam, L.P., Omary, M., Binkowski, F., Fleming, 2012). Landing and takeoff operations were considered by capping full-flight aircraft emissions at 3,000 feet. Our domain covered the continental United States with 36x36 km horizontal grid resolution and thirty-four time-varying pressure-based vertical layers (LTO constrained to the first 17 layers around 3,000 feet or 914 meters).

Other background anthropogenic emission sources were obtained from EPA's National Emissions Inventories (NEI-2005) and 2005 boundary conditions were derived from global CAM-chem simulations (Lamarque et al., 2012). Meteorology conditions for 2005 were obtained from the Weather Research and Forecasting model (WRF) (Skamarock et al., 2008), with outputs downscaled from NASA's Modern-Era Retrospective Analysis for Research and Applications data (MERRA) (Rienecker et al., 2011).

Results

A key milestone of the overall work of this project has been the successful implementation of HDDM with CMAQ version 5.0.2. Prior studies (Boone, n.d.) only looked at first order DDM sensitivity coefficient calculations with CMAQ version 4.7.1. By utilizing a more up to date version of the model, we hope to utilize more accurate chemical mechanisms and science modules. Model evaluation will be performed by comparing CMAQ HDDM sensitivity coefficient output with CMAQ Brute Force sensitivity calculations. We will also compare CMAQ HDDM concentration outputs to observed data using the Atmospheric Model Evaluation Tool (AMET). Preliminary model runs have been performed, calculating the sensitivity of O_3 to first order changes in NO_x emissions, first order changes in VOC emissions, and second order changes to NO_x and VOC emissions ($\frac{dC_{O_3}}{dE_{NO_x}dE_{VOC}}$). We also calculated the sensitivity of Nitrate aerosols, Sulfate aerosols, and total $PM_{2.5}$ to first order changes in NO_x emissions, first order changes in SO_2 emissions, and second order changes to NO_x and SO_2 emissions.

Figures 2-1 through 2-3 show spatial plots of the calculated sensitivity coefficients in our domain for the months of January (left figures) and July (right figures) for first order changes to O_3 concentrations with respect to NO_x emissions (Fig. 2-1) and VOC emissions (Fig. 2-2), and second order changes to O_3 concentrations with respect to NO_x emissions and VOC emissions (Fig. 2-3). Figures 2-4 through 2-6 show spatial plots of the calculated sensitivity coefficients in our domain for the months of January (left figures) and July (right figures) for first order changes to $PM_{2.5}$ concentrations with respect to NO_x emissions (Fig. 2-4) and SO_2 emissions (Fig. 2-5), and second order changes to $PM_{2.5}$ concentrations with respect to NO_x emissions and SO_2 emissions (Fig. 2-6). Figure 2-7 shows linear regression plots comparing DDM-generated sensitivities and brute force deltas.



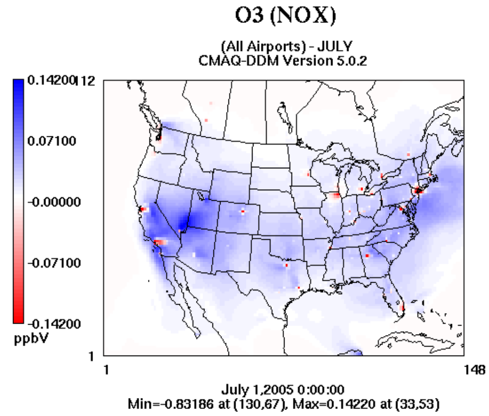
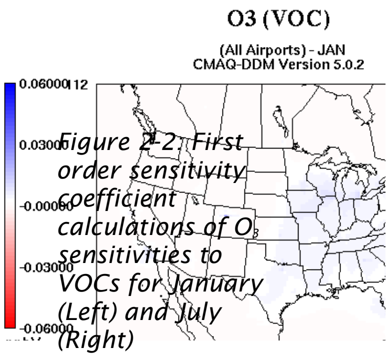


Figure 2-1: First order sensitivity coefficient calculations of O_3 sensitivities to NO_x for January (Left) and July (Right)



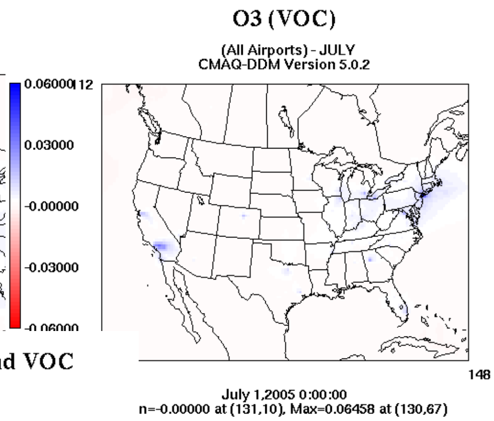
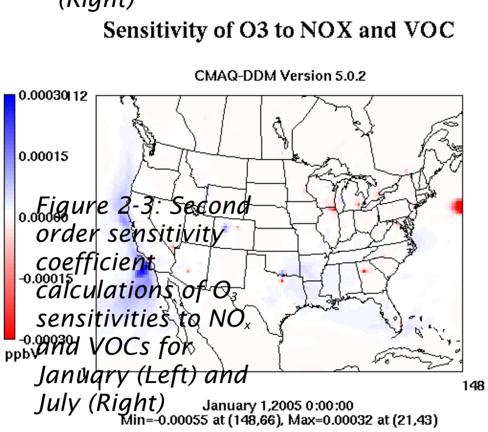


Figure 2-2: First order sensitivity coefficient calculations of O_3 sensitivities to VOCs for January (Left) and July (Right)



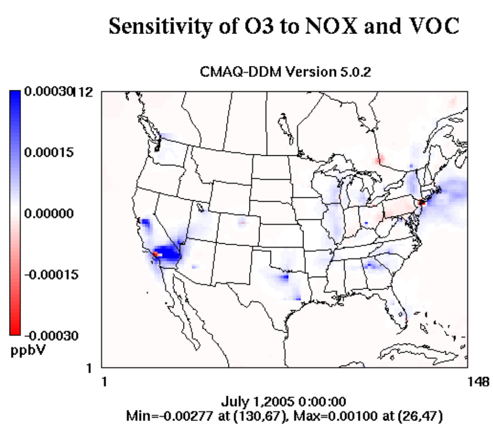


Figure 2-3: Second order sensitivity coefficient calculations of O_3 sensitivities to NO_x and VOCs for January (Left) and July (Right)

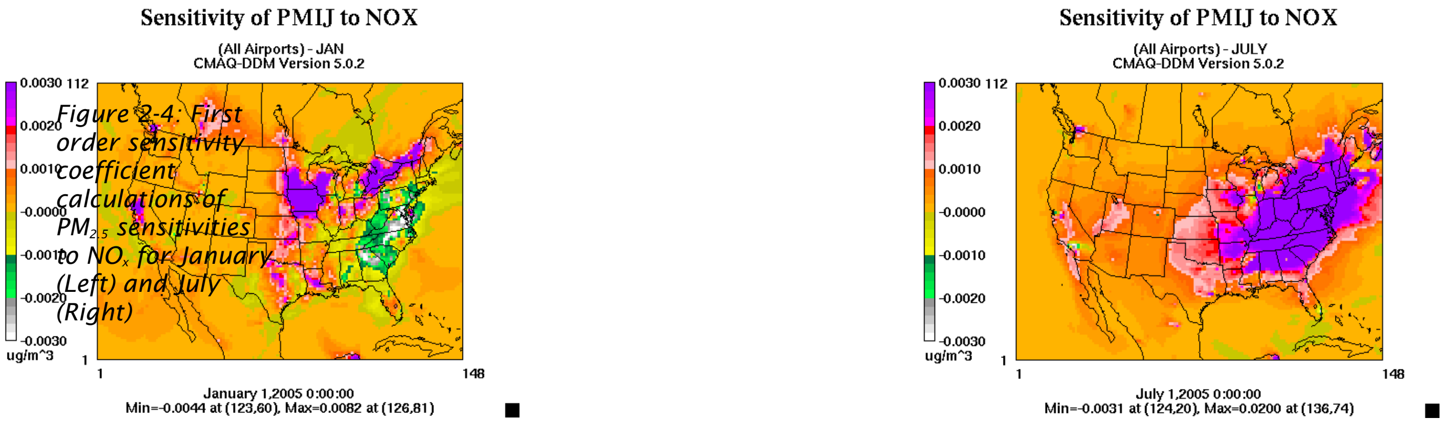


Figure 2-4: First order sensitivity coefficient calculations of $PM_{2.5}$ sensitivities to NO_x for January (Left) and July (Right)

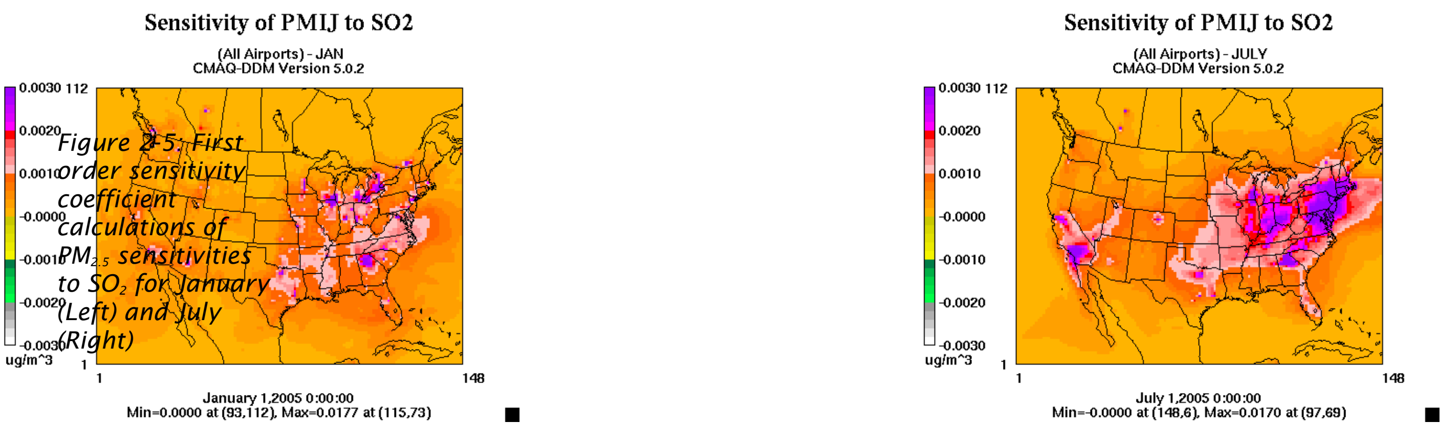
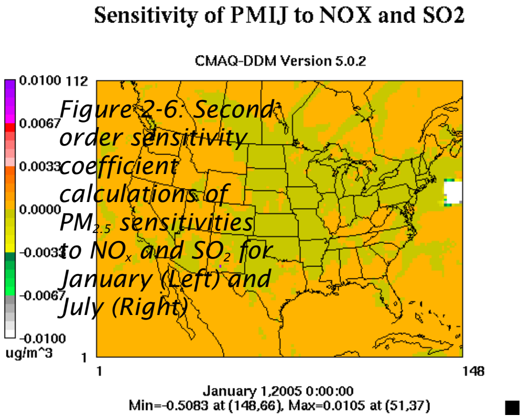


Figure 2-5: First order sensitivity coefficient calculations of $PM_{2.5}$ sensitivities to SO_2 for January (Left) and July (Right)



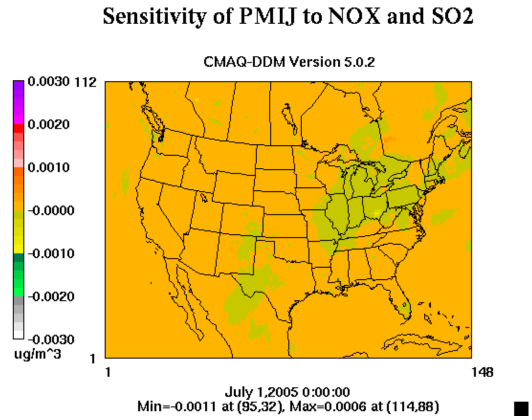


Figure 2-6: Second order sensitivity coefficient calculations of $PM_{2.5}$ sensitivities to NO_x and SO_2 for January (Left) and July (Right)

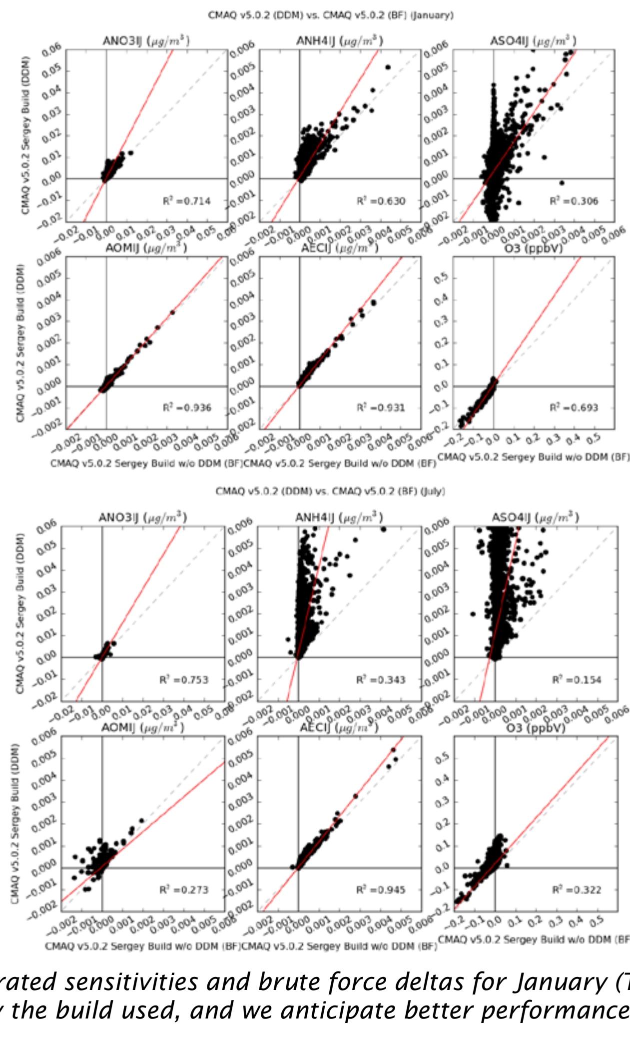


Figure 2-7: Comparison of DDM-generated sensitivities and brute force deltas for January (Top) and July (Bottom). Model setups between the two runs differ by the build used, and we anticipate better performance with consistent builds across setups.

Milestone(s)
December 2016 – First implementation of CMAQ-HDDM for aircraft emissions for test simulation period

Major Accomplishments
We have successfully implemented and tested higher order sensitivity in CMAQ v5.0.2 for aircraft emissions. With continued testing and evaluation, we will be able to assess the potential non-linearities in second order sensitivities that were not captured with first order sensitivities that have been the focus of this project to date. We will thus be able to better inform emission reduction policies with regards to mitigating air quality (and health) impacts around key airsheds of the nation.

Publications
None

Outreach Efforts
None

Awards
None

Student Involvement
Calvin Arter is a 1st year Ph.D. student who started work on this project in summer 2016.

Plans for Next Period
Next steps will include detailed analyses of the results with regards to constructing an emissions reductions policy. FAA has provided us with a draft set of policy options to use as illustration of applying the DDM-based sensitivity outputs. We plan to utilize these results to answer for e.g., how many airports would be needed in a clean air region to bring that area from attainment to nonattainment for NAAQS of O_3 and $PM_{2.5}$. We can also look to analyze how air pollutant concentrations may change if ultra-low sulfur jet fuel was used across the United States. We also hope to expand our sensitivity matrix to include additional sensitivities to precursors and utilize the second order DDM sensitivity coefficient calculations to accurately observe nonlinear dependence of secondarily formed inorganic aerosols on their precursors. This work will eventually be performed with an updated modeling framework for the year 2011, with all inputs (meteorology, background and aircraft emissions) and modeling framework updated.

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Task 3: Assess PM Size Distribution Impacts of Aircraft Emissions

University of North Carolina at Chapel Hill

Objective(s)

To enhance representation of particle size distribution of aircraft emissions in the Community Multiscale Air Quality (CMAQ) Model.

To understand impacts on CMAQ chemical and physical processes due to changes in particle size distribution of aircraft emissions.

To investigate ultrafine particle (UFP, < 0.1 µm) number concentrations contributed from commercial aircraft landing and take-off (LTO) operations in the U.S.

Research Approach

Introduction

The CMAQ model has been used to understand ground-level air quality impacted by aircraft emissions since 2011 with various model configurations (Woody et al., 2011; Rissman et al., 2013; Woody and Arunachalam, 2013). These studies stated that fine particulate matter ($PM_{2.5}$) mass concentrations impacted by LTO in the contiguous United States (CONUS) domain were relatively minor (up to 0.232 µg m^{-3} near Atlanta airport using plume in grid model) compared to ambient $PM_{2.5}$ level. However, recent field measurements found significant UFP number concentrations increases due to LTO near several U.S. and European airports (Hudda et al., 2016; Hudda and Fruin, 2016; Keuken et al., 2015; Stafoggia et al., 2016). Therefore, the main goal of Task 3 is to understand the impact on UFP number concentrations near airports from LTO using CMAQ.

Default CMAQ considers that all PM are emitted mostly in accumulation mode (size: 0.1-2.5 µm) for all anthropogenic emission sectors (Nolte et al., 2015). However, previous studies based on aircraft measurement campaigns reported PM emitted from aircrafts should be in UFP size range (0.02-0.05 µm) (Kinsey et al., 2010; Petzold et al., 1999). Our first goal in this task was to add a new module which can read aircraft emissions and assign PM size distribution separately from all non-aircraft emissions. The second goal of this task was to apply this new configuration of CMAQ to understand impacts on ground-level $PM_{2.5}$ mass and UFP number concentrations from LTO emissions.

Our hypothesis is that, using the new approach, particle size distribution from aircraft emissions can be better represented than in a traditional CMAQ configuration, and that this will impact PM number concentrations due to aircraft emissions.

Methodology

CMAQ v5.0.2 was used in this study to simulate ground-level PM mass and number concentrations impacted by aircraft emissions. Particles emitted from all emission sources are lumped together and assigned as 0.1 and 99.9% in Aitken (similar to UFP) and accumulation modes, respectively, in default CMAQ v5.0.2. In this study, aircraft and non-aircraft emissions files were generated, separately. A new module was developed to read emissions from aircraft and non-aircraft separately, and assign a reasonable particle size distribution to aircraft emissions based on species (black carbon, organic carbon, and sulfate). We investigated six different configurations for PM emissions from aircraft during two months (January and July 2005) to understand the influences from various particle size distributions for aircrafts. One of these configurations was selected for annual simulation (Table 3.1, New Method), since large amounts of small particle (< 0.005 µm) would skew particle size distribution in ambient air. Three scenarios were simulated to estimate contribution of aircrafts with different particle size configurations to PM mass and number (Table 3.1) for 2005. In this study, only LTO emissions in North America were considered, which were generated from AEDT (Wilkerson et al., 2010). Background emissions were generated based on the National Emission Inventory 2005 (EPA, 2007). The Weather Research and Forecasting model was used to create 2005 meteorological data for CMAQ (Skamarock et al., 2008). Boundary and initial conditions of CAMQ were downscaled from CAM-Chem global model (Lamarque et al., 2012).

Results

Number concentrations of UFP at major airports in North America were simulated by CMAQ with the new module increased 1.2 to 5.1 times (Table 3.2) due to LTO emissions. These numbers are in the range of those reported by recent field studies (Hudda et al., 2016; Hudda and Fruin, 2016). Hudda et al. (2016) and Hudda and Fruin (2016) reported significant increases of UFP number concentrations due to LTO at LAX and BOS at 10km and 6km, respectively. However, CMAQ UFP number concentrations were calculated based on a 36x36 km^2 grid size; therefore, the following equation was used to adjust the spatial effects:

$$C_{adj} = C_{measured} \times \frac{d^2}{36^2}$$

Here, d is the distance from sampling sites to airports. After spatial adjustment of these measurements, UFP number concentrations contributed by LTO at both airports were similar to the numbers reported by new CMAQ simulations.

In downwind areas, aircraft-attributable nitrate was enhanced by high surface areas of aerosols. Because of large amount emissions of NO_x from LTO in the downwind areas of airports, when free ammonia was available ammonium nitrate could be formed. This has been discussed in detail in Woody et al. (2011). New CMAQ simulations even increased surface areas of PM, and nitrate is a semi-volatile species which can partition on PM surfaces, depending on temperature. High surface areas of PM enhanced nitrate concentrations in the new method compared to the traditional approach for treating size distribution in CMAQ. Overall, at the top three airports in North America, number concentration increased dramatically, and its peak shifted to smaller particle diameter. However, only minor changes were observed in surface and volume concentrations (Figure 3.1).

Milestone(s)

Apr, 2016 - Completed developing and testing of new module to treat aircraft emissions with different size distribution
Aug, 2016 - Completed CMAQ model simulations using new module for annual 2005 period

Major Accomplishments

1. Quantified the effect of using new aircraft emissions size distribution information on modeled number concentration
2. Compared model results with recent field measurement campaigns, and seeing comparable results, determined the need to look at UFP from aircraft in increased detail

Publications

Huang, J., L.P. Vennam, F.S. Binkowski, B. Murphy and S. Arunachalam (2016). Impacts on Ambient Particulate Matter by Changing Particle Size Distribution from Emissions Using the Community Air Quality Model (CMAQ): A Case Study of Commercial Aircraft emissions from Landing and Take-off, CMAS, 2016, Chapel Hill, NC.

Outreach Efforts

Research findings were presented in a podium presentation at the 15th Annual CMAS conference held on October 24-26, 2016, at Chapel Hill, NC.

In addition, the UNC PI explored aspects of this work with international researchers at the *FORUM-AE Air Quality workshop* held in Amsterdam, the Netherlands in April 2016, and at the *Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes* (HARMO) in Budapest in May 2016.

Awards

None

Student Involvement

Pradeepa Vennam, Ph. D. student, helped generating the emissions files and initial/boundary conditions for CMAQ simulations and reviewed the data.

Plans for Next Period

Understand negative sulfate mass concentrations at major airports due to change of particle size distribution of aircraft emissions in CMAQ.
Compare CMAQ simulated UFP number concentrations at more airports (not LAX and BOS), if field data are available.
Finalize and submit manuscript.

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Table 3.1: Configurations of CMAQ particle size distribution from emission in annual simulations, nvPM: black carbon, vPM: organic carbon and sulfate

	Emission split factor	GMD (nm)	GSD	Emission data
Background (bkgd)	EC/OC/NCOM Aitken: 0.1 Accumulation: 99.9 OTHER Aitken: 0 Accumulation: 1	EC/OC/NCOM Aitken: 30 Accumulation: 300 OTHER Accumulation: 300	EC/OC/NCOM Aitken: 1.7 Accumulation: 2.0 OTHER Accumulation: 2.0	All emissions without aircraft emissions
Traditional method	nvPM Aitken: 0.1 Accumulation: 99.9 vPM Aitken: 0.1 Accumulation: 99.9	nvPM Aitken: 30 Accumulation: 300 vPM Aitken: 30 Accumulation: 300	nvPM Aitken: 1.7 Accumulation: 2.0 vPM Aitken: 1.7 Accumulation: 2.0	All emissions and aircraft emissions in separate files
New method	nvPM Aitken: 91.8 Accumulation: 8.2 vPM Aitken: 91.8 Accumulation: 8.2	nvPM Aitken: 40 Accumulation: 150 vPM Aitken: 20 Accumulation: 150	nvPM Aitken: 1.6 Accumulation: 1.87 vPM Aitken: 1.5 Accumulation: 1.87	All emissions and aircraft emissions in separate files

Table 3.2: Ultrafine particle concentrations (10^9 number/m^3) at top 10 airports (by fuel burn, 2005 AEDT) in North America, and Boston airport.

	Traditional method	New method	Background	New - background	Measured LTO impact without spatial correction[1]	Measured LTO impact with spatial correction[2]	Ratio (new/bkgd)
ATL	1.8	3.0	1.8	1.2			1.7
ORD	2.2	3.0	2.2	0.8			1.4
LAX	0.4	2.0	0.4	1.6	28-100	2.2-7.7	5.1
DFW	0.6	1.3	0.6	0.7			2.2
JFK	2.4	3.6	2.4	1.2			1.5
EWR	3.0	3.5	3.0	0.5			1.2
IAH	0.6	1.1	0.6	0.5			1.9
DTW	2.8	3.5	2.8	0.6			1.3
MSP	2.1	2.5	2.1	0.4			1.2
MIA	0.4	0.8	0.4	0.4			2.0
BOS	1.9	2.2	1.9	0.3	10-20	0.28-0.56	1.2

1: data directly from Hudda et al., 2016 and Hudda and Fruin, 2016
2: correct the spatial effects from 10 and 6 km to 36 km grid size, respectively.

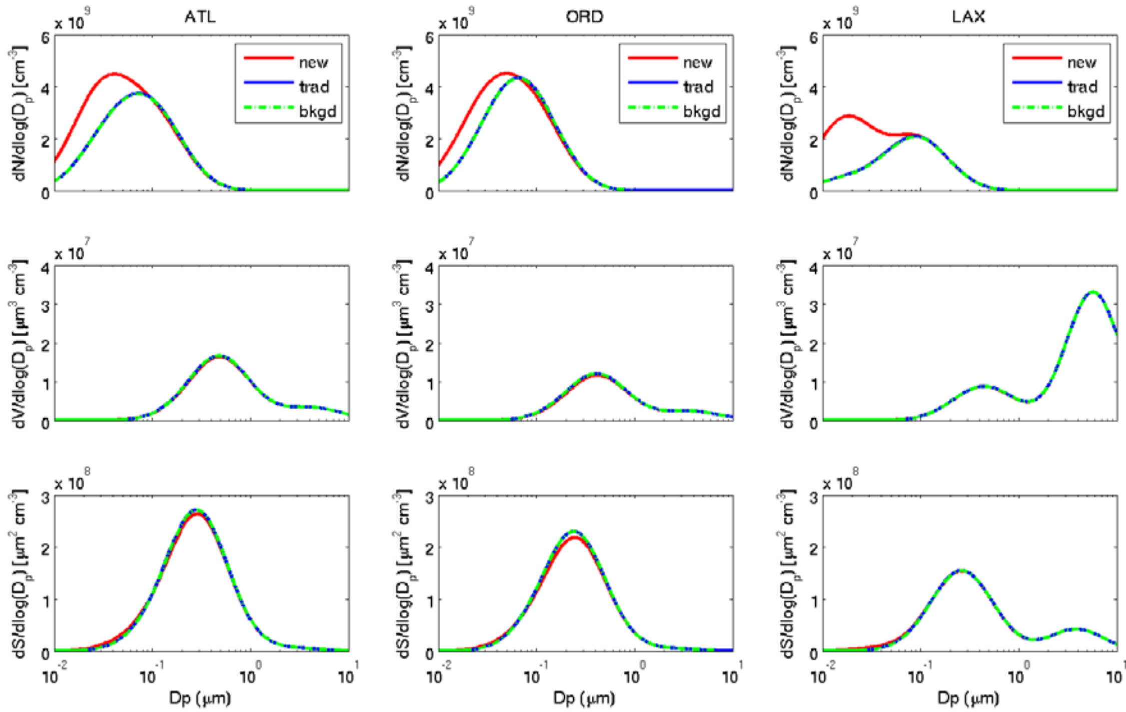

Figure 3.1 – Particle size distribution of ambient particles (annual average) at ATL (left), ORD (middle), and LAX(right), new and trad represent new and traditional CMAQ approaches, respectively. Bkgd is the background scenario.

Task 4: Assess impacts of coupled models on Aviation-related AQ Impacts

University of North Carolina at Chapel Hill

Objective(s)

The objective of task-4 was to study the effect of particulate matter's (PM's) radiative feedback effects on estimating the aircraft's landing and take-off (LTO) emission attributable change in surface ozone (O_3) and PM having a size less than 2.5 micron ($PM_{2.5}$) concentrations and to quantify the aircraft's LTO emission attributable change in some meteorological variables by the WRF-CMAQ coupled meteorology-chemistry transport model.

Research Approach

Introduction

Aircraft LTO emissions contribute to 75 (Levy et al., 2012) to 210 (Brunelle-Yeung et al., 2014) premature deaths in the US. Aircraft LTO emissions cause mortality even as far as 300 km away from a major airport through increases in secondary ammonium nitrate and sulfate (Arunachalam et al., 2011). Aviation emissions also affect global radiative forcing (RF) (global warming or cooling) through greenhouse gases such as CO_2, H_2O, primary and secondary PM and cloud particle interaction (Jacobson et al. 2013, Brasseur et al. 2016). Although all these RF effects are mainly caused by the aircraft emissions during cruise mode, it is also important to know how much RF is affected by the aircraft LTO emitted PM at the surface layers.

Aircraft-emitted PM scatters and absorbs radiation from the sun, which changes temperature, wind speed, relative humidity and planetary boundary layer (PBL) height in the atmosphere. The changes also affect atmospheric pollutant formation chemistry, which causes PM concentration change. This change in PM concentration in the atmosphere then effects meteorology. The process is called aerosol feedback. The aerosol feedback effects are neglected in traditional air quality models (where meteorology is used as input and not affected by chemistry) which cannot simulate real atmospheric pollutant concentration. An online coupled meteorology-chemistry model such as WRF-CMAQ (Wong et al., 2012) can simulate this aerosol feedback effects in estimating aircraft LTO emission attributable change in surface layer O_3 and $PM_{2.5}$ concentrations and also quantifying how much RF is attributed at the surface by the aircraft's LTO-emitted PM. Note that prior to this study, all aviation-attributable air quality impacts research for local-to-regional scale air quality under PARTNER and ASCENT only used CMAQ without this key atmospheric process (feedback of chemistry on meteorology).

Method

The change in O_3, $PM_{2.5}$ and some important meteorological variables such as temperature at 2 m (T2), short-wave radiation (SWR) at surface and PBL height by the commercial aviation's LTO emission in the continental US are determined by coupled WRF-CMAQ model (Wong et al., 2012) runs for with- and-without LTO emissions for both with- and-without aerosol feedback (the four sensitivity simulation cases are shown in Table 4-1). Deduction of the values of output variables of case 1 from case 3 gives the aviation's LTO emission-attributable change when aerosol feedback was not considered. Deduction of values of output variables of case 2 from case 4 gives the aviation's LTO emission-attributable change when aerosol feedback is considered.

Table 4-1. Four sensitivity simulation cases.

Case number	Case description
1	Without LTO emissions (non-aviation emission only) without aerosol feedback
2	Without LTO emissions (non-aviation emission only) with aerosol feedback
3	With LTO emissions (non-aviation emission +LTO emission) without aerosol feedback
4	With LTO emissions (non-aviation emission +LTO emission) with aerosol feedback

The present study is focused on a 1-year simulation period in 2005 in the continental US, with a 36-km horizontal grid with 34 vertical sigma layers with top of the layer at 50 hPa. WRF model configurations include ACM2 PBL scheme (Pleim 2007), Morrison cloud microphysics scheme (Morrison et al., 2009), Pleim-Xiu land surface model (Pleim and Xiu 1995; Xiu and Pleim 2001), KF2 cumulus cloud parameterization (Kain 2004), USGS 24 land use and RRTMG radiation model (Iacono et al. 2008). The CMAQ configuration includes Carbon Bond 05 gas chemistry (Whitten et al. 2010; Yarwood and Rao 2005) and AER06 aerosol chemistry (Appel et al. 2013).

Input meteorological data for WRF were processed and downscaled from the NASA MERRA data (MERRA 2016; Rienecker et al. 2011). The CMAQ boundary conditions data were taken from CAM-Chem global model outputs. Aircraft LTO emission data were produced by the Federal Aviation Administration, Environmental Design Tool (AEDT) (FAA-AEDT, 2016). Non aircraft emission data were processed by the Sparse Matrix Operator Kernel Emissions (SMOKE) model (SMOKE 2016) using the U.S. EPA, National Emission Inventory for 2005 (EPA 2016).

Results

Aerosol feedback effects in aircraft LTO emission-attributable change in O_3 are shown in Figure 4-1. With feedback, both positive and negative O_3 perturbation were found in almost all of the 48 states in January 2005 (Fig. 4-1d), in July 2005 (Fig. 4-1e), and in the 2005 annual average (Fig 4-1f) caused by the T2 change (shown in Fig. 4-3a,b,c) and PBL changes (shown in Fig. 4-3g,h,i), but without feedback, in most states, it was positive in the west and negative in east in January (Fig. 4-1a), positive almost everywhere in July (Fig. 4-1b) and positive near the airport and negative or zero far away from airports in the annual average (Fig. 4-1c). Perturbation of domain average values for with-feedback for all 12 months and for annual average were found to be different than that without feedback which is not presented in this report, but will be presented in the manuscript (under development).

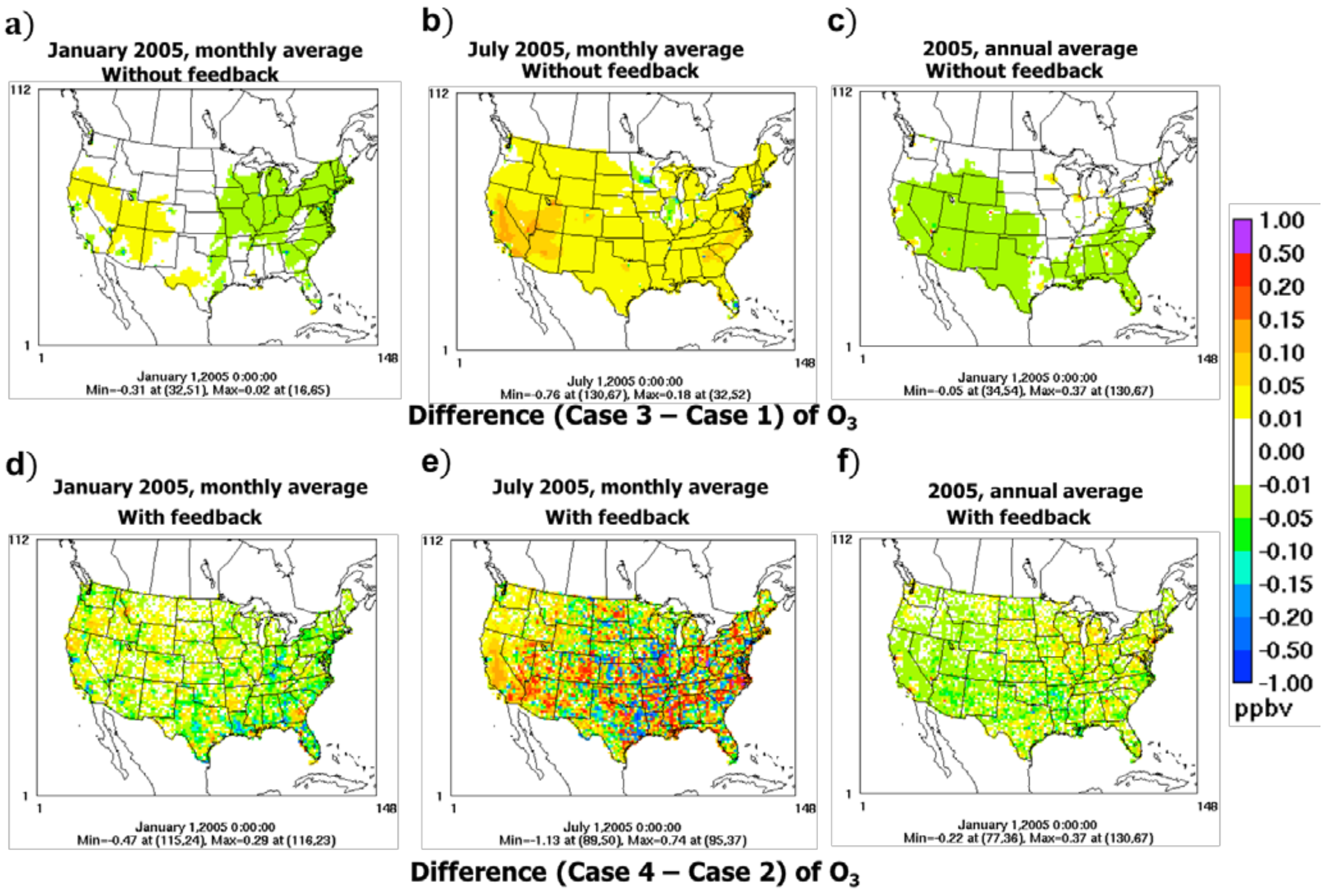

Figure 4-1: Effects of aircraft's LTO emission on surface layer O_3 without feedback (top row): a) monthly average, January 2005, b) monthly average, July 2005 and c) annual average, 2005 and with feedback (bottom row): d) monthly average, January 2005, e) monthly average, July 2005 and f) annual average, 2005 predicted by the coupled WRF-CMAQ model.

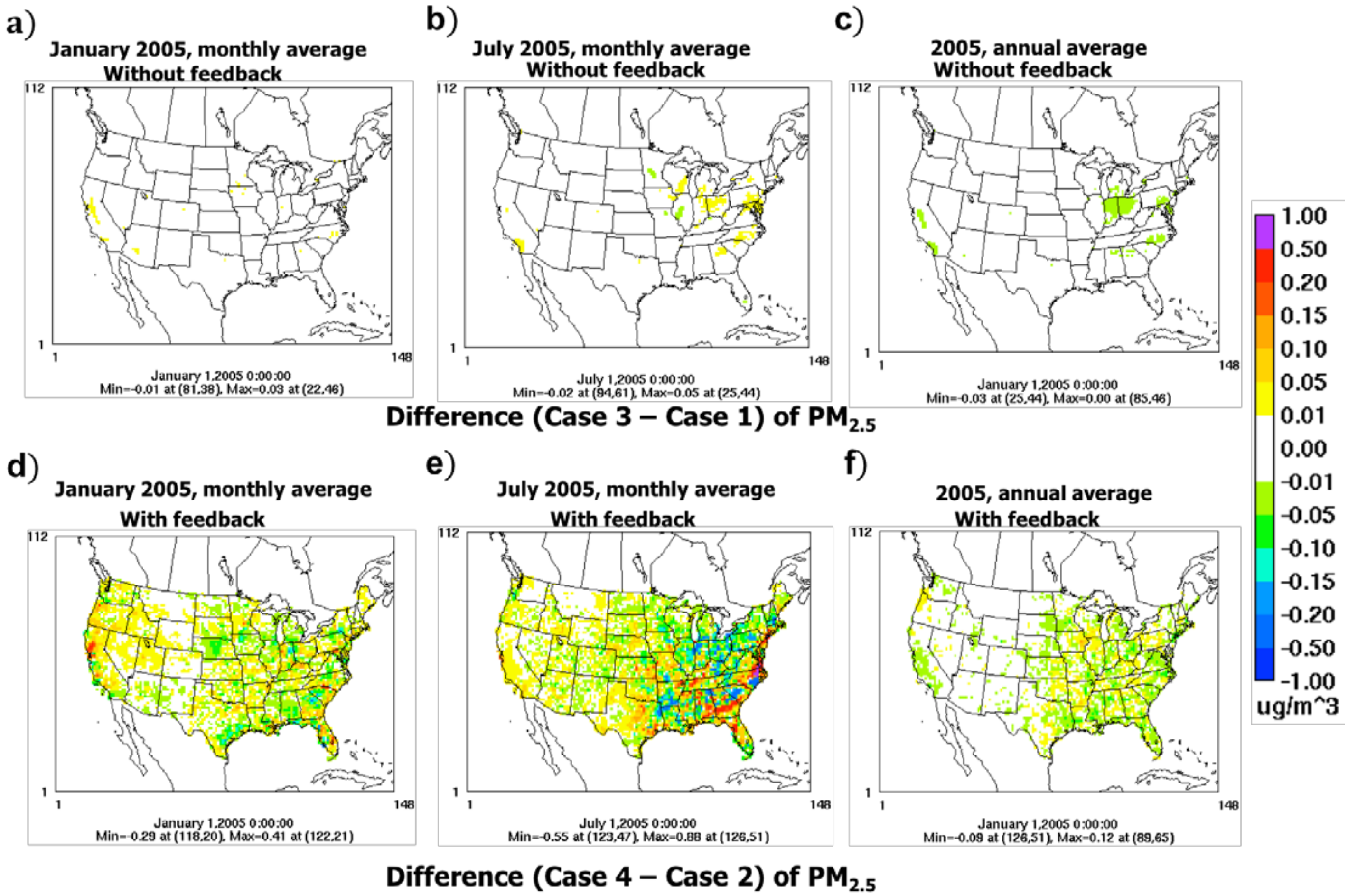

Figure 4-2: Effects of aircraft's LTO emission on surface layer $PM_{2.5}$ without feedback (top row): a) monthly average, January 2005, b) monthly average, July 2005 and c) annual average, 2005 and with feedback (bottom row): d) monthly average, January 2005, e) monthly average, July 2005 and f) annual average, 2005 predicted by the coupled WRF-CMAQ model.

The spatial $PM_{2.5}$ perturbations are shown in Fig. 4-2. With feedback, both positive and negative $PM_{2.5}$ perturbations were found in a majority of the states in January (Fig. 4-2d), in July 2005 (Fig. 4-2e), and in annual average (Fig 4-2f) caused by the T2 change (shown in Fig. 4-3a,b,c) and PBL changes (shown in Fig. 4-3g,h,i) in nearby grids but without feedback, in most states, it was either positive or negative or no change both in January (Fig. 4-2a), in July 2005 (Fig. 4-2b) and in the annual average (Fig. 4-2c). Perturbation of domain average values for with feedback for all 12 months and for annual average were different than that without feedback, which is not presented in this report, but will be presented in the final manuscript (under preparation).

One advantage of using the coupled WRF-CMAQ model is that it gives aviation LTO emission attributable perturbation of meteorological variables T2 (shown in Fig. 4-3a,b,c), SWR (shown in Fig. 4-3d,e,f) and PBL (shown in Fig. 4-3g,h,i) caused by PM radiative feedback. T2 perturbation is more in July (shown in Fig. 4-3b) than in January (shown in Fig. 4-3a) and both positive and negative perturbation occurs in adjacent grid-cells, which cancel each other when spatial summation is done for domain average (not shown in this report). SWR also shows similar perturbation which is higher in July (shown in Fig. 4-3e) than in January (shown in Fig. 4-3d) and also both positive and negative perturbation occurs in nearby grid-cells. Perturbation for SWR for annual average is smaller (shown in Fig. 4-3f) than in July (shown in Fig. 4-3e). PBL height affects dilution and dispersion of pollutants and also cloud formation. PBL is changed with the change in T2 caused by the change of short-wave radiation reaching the surface caused by aerosol's radiative effects. PBL height perturbation by aerosol feedback effects also shows that perturbation is higher in July (shown in Fig. 4-3h) than in January (shown in Fig. 4-3g) and both positive and negative perturbation occurs in nearby grid-cells which cancel each other when spatial summation is done for the domain average (not shown in this report).

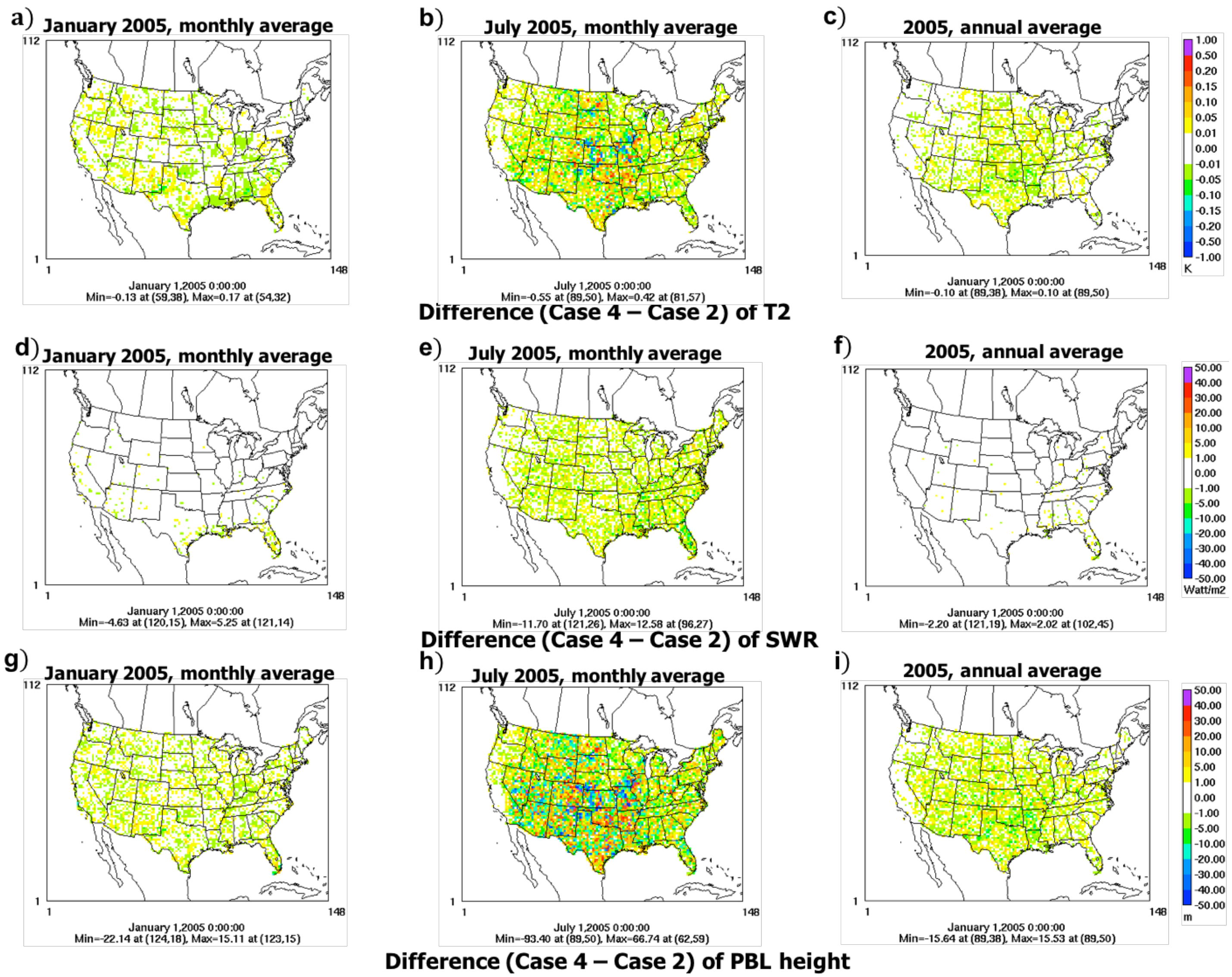

Figure 4-3: Effects of aircraft's LTO emission on temperature at 2 m (T2) (top row): a) monthly average, January 2005, b) monthly average, July 2005 and c) annual average, 2005, short-wave radiation(SWR) (middle row): d) monthly average, January 2005, e) monthly average, July, 2005 and f) annual average, 2005 and planetary boundary layer (PBL) height (bottom row): g) monthly average, January 2005, h) monthly average, July, 2005, and i) annual average, 2005 predicted by the coupled WRF-CMAQ model.

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Milestone(s)

July 2016: Simulation of January 2005 with 11-day spin-up completed
August 2016: Simulation of July 2005 with 11-day spin-up completed
October 2016: Simulation of entire 2005 year with 6-month spin-up completed
December 2016: Post processing, data analysis and model evaluation have been completed

Major Accomplishments

1. Quantified the effects of aerosol feedback in estimating the aircraft LTO emission attributable change in surface O_3 and $PM_{2.5}$ in CONUS grid for entire year of 2005 which was missing in the output of traditional uncoupled air quality model where meteorology is used as input to CTM, and is not changed by chemistry.
2. Quantified the aircraft LTO emission-attributable change to meteorology in CONUS grid for entire year for 2005 which was missing in the output of traditional uncoupled meteorology model.

Publications

Moniruzzaman, C. G., Bowden, J., Arunachalam, 2016. Effects of aerosol feedback on aircraft-attributable surface O3 and PM2. 5 concentrations using the two-way coupled WRF-CMAQ modeling system. Presentation at the 15th Annual CMAS Conference, October 24-26, 2016 Chapel Hill, NC, available online at: https://www.cmascenter.org/conference/2016/slides/monir_effects_aerosol_2016.pdf.

Outreach Efforts

Research findings were presented in a poster session at the 15th Annual CMAS conference held on October 24-26, 2016, at Chapel Hill, NC.

Awards

None

Student Involvement

Pradeepa Vennam, a PhD student, provided the CMAQ emissions, initial and boundary conditions files and post processing scripts and helped in numerous steps of the research.

Plans for Next Period

Effects of aerosol feedback on estimating aircraft's cruise emissions' contribution to both vertical profile of O_3, $PM_{2.5}$, temperature and also the surface O_3 and $PM_{2.5}$ and surface temperature will be quantified by the coupled WRF-CMAQ model for northern hemisphere domain. 80% aviation black carbon (BC) emission occurs during climb and cruise (non LTO) operation (Lee et al. 2013) and it will be interesting to see aerosol feedback effects in estimating cruise emission effects on both surface air quality and meteorology and their vertical profile.

APPENDIX A

Additional results

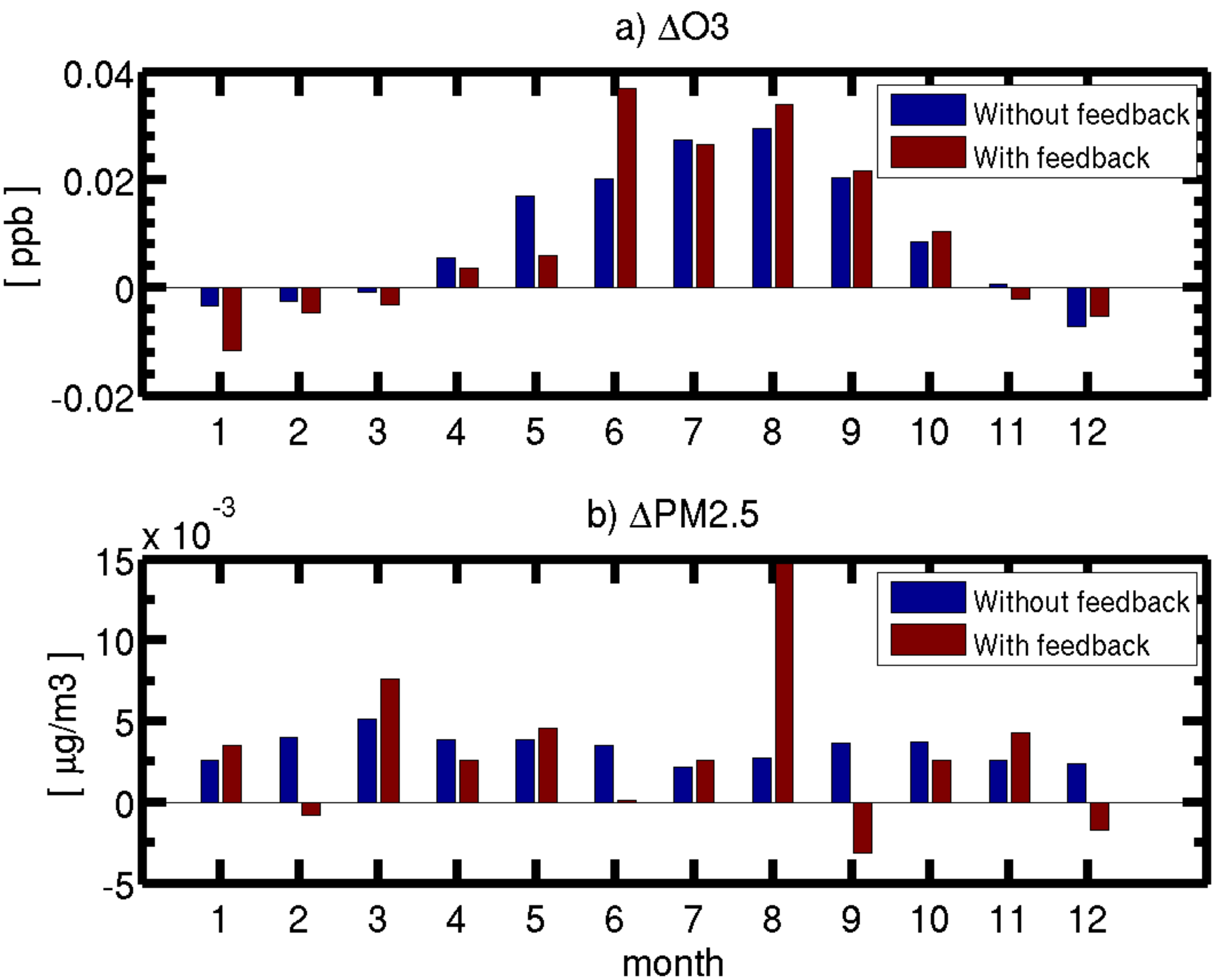

Figure 4-A1: Effects of aircraft's LTO emission on domain average of monthly average of surface a) O_3 and b) $PM_{2.5}$ for without feedback and with feedback in 2005.

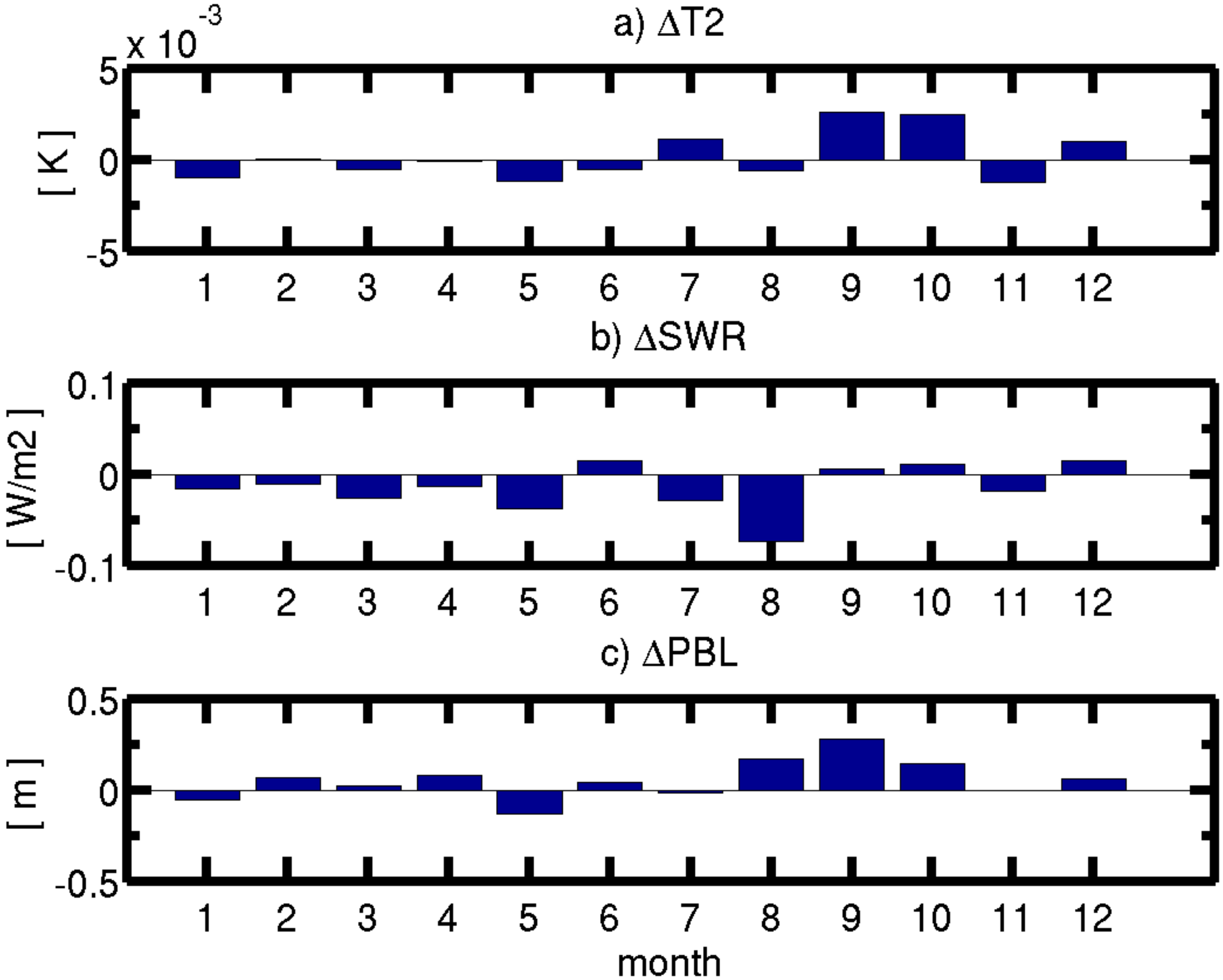

Figure 4-A2: Effects of aircraft's LTO emission (Case 4 – Case 2) on domain average of monthly average of a) temperature at 2 m (T2) b) short-wave radiation (SWR) at surface and c) planetary boundary layer (PBL) height in 2005 with aerosol feedback.

Task 5: Support for High Fidelity Weather

University of North Carolina at Chapel Hill

Objective(s)

Provide support to FAA (ATAC and Volpe Center) in processing high fidelity weather for AEDT.

Research Approach

In this task, UNC assisted FAA contractors ATAC and Volpe Center in the identification, acquisition and implementation of high fidelity weather data from global scale datasets for use in the Aviation Environmental Design Tool (AEDT) for developing aviation emissions inventories. Specifically, UNC worked with ATAC and U.S. DOT's Volpe Center for implementing the Modern Era Retrospective Analyses for Research and Applications (MERRA)[2] (Rienecker et al., 2011) dataset to derive meteorological fields in AEDT's calculations. Prior to this, UNC reviewed all available datasets with global coverage and recommended that MERRA be the choice of data for driving AEDT with high fidelity weather. Once we learned that NASA was in the process of migrating from MERRA to MERRA-2 (Bosilovich et al., 2015), we recommended that FAA move to MERRA-2, and we will continue to engage with NASA developers as necessary and assist both ATAC and Volpe in developing and implementing the prototype tool for use in AEDT. UNC's assistance to the FAA contractors included the following:

a) Identifying appropriate datasets

b) Developing scripts for data downloads from NASA servers

c) Assist with QA of AEDT processing, and troubleshooting as necessary

d) Assist with evaluation of results

At the end of this performance period, we collaborated with ATAC in preparing a joint final report covering the process for creating high fidelity weather full flight environmental analyses for global inventories using AEDT, using both great circle routes and radar flight tracks as input. This report included a description of the optimal high fidelity weather data sources for this purpose, instructions on how to use the optimal weather data within AEDT, validation of its use using Cockpit Flight Data Record (CFDR) data, and issues and recommendations of high fidelity weather usage in AEDT 2b. This report did not cover actual AEDT enhancement implementation in the form of software development, but identified multiple issues, and provided suggestions for improvements. The summary of the issues is provided below, and the reader is referred to the actual final report for further details.

1. Database-related issues
    a. UTC Time
    b. Inconsistent Runway Effective & Expiration Dates
    c. Unusable Airports through Importation
    d. Runway ends with null elevations
    e. Null airport weather
2. Performance module issues fixed in AEDT 2b
    a. Track distance disagreements
    b. Weather reading altitude in the FPPM
    c. Weather reading times in the FPPM
    d. Incorrect Location for Controlled-Point Weather Readings
    e. Altitude AFE in ANP Thrust Equations
3. Outstanding Performance Module Issues
    a. Fuel Burn in the Terminal Area
    b. Sampling Rate of High-fidelity Weather
    c. General Airspeed to Groundspeed Conversion
    d. Inconsistent High-fidelity Weather Sampling Rates
    e. Wind Perpendicular to Airplane Course
    f. Enroute Groundspeed/True-Airspeed Conversions

[2] http://gmao.gsfc.nasa.gov/merra/

   g. Modeling Failures Due to Extreme Weather Conditions
4. Weather Module Issues
   a. International Dateline
   b. Minimum Amount of Weather Data
   c. Peculiar Interpretation of MERRA Time Data
   d. Missing Values in MERRA Data
   e. Negative Latitudes
   f. Single Day Limit
   g. Specific Humidity
   h. MERRA Version 2

Milestone(s)
September 2016 - Research Approach for Hi-Fi Weather in AEDT, with ATAC

Major Accomplishments
Completed prototyping an approach for use of MERRA in AEDT and developed a report that summarizes various issues that need to be resolved, with our recommendations.

Publications
None

Outreach Efforts
Multiple presentations to FAA and Volpe Center during this performance period

Awards
None

Student Involvement
None

Plans for Next Period
We will continue working with Volpe to migrate from MERRA to MERRA-2, and also with the implementation of BADA4 in AEDT. In addition, we will also assist Volpe in processing WRF data directly in AEDT (instead of MERRA or MERRA-2). This will assist in additional consistency in meteorological fields for regional-scale air quality applications.

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