Project 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 Professor
- FAA Award Number: 13-C-AJFE-UNC Amendments 1 - 6
- Period of Performance: January 1, 2017 – October 31, 2017
- Task(s):
    - Perform NAS-wide impact assessment for 2011 and 2015
    - Perform airport-by-airport assessment using CMAQ-DDM
    - Develop generalized gridding tool for AEDT
    - Provide support for High fidelity weather in AEDT
    - Explore collaboration with NAU, Ukraine

Repeat for all participating universities.

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$212,494 from the FAA

Matching Cost-share provided by Transport Canada

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. Tools will be needed to rapidly assess the implications of alternative policies in the context of an evolving population and atmosphere. In the context of the International Civil Aviation Organization (ICAO)'s Committee on Aviation Environmental Protection (CAEP), additional tools are required to understand the implications of global aviation emissions.

The overall objective of this project is to continue to develop and implement tools, both domestically and internationally, to allow for assessment of year-over-year changes in significant health outcomes. These tools will be acceptable to FAA (in the context of Destination 2025) and/or to other decision-makers. They will provide 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). The project is performed as a coordinated effort with extensive interactions among the three institutions and will be evident in the reporting to the three separate projects (ASCENT 18, 19 and 20) by each collaborating university.

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 on previous efforts within Project 16 of PARTNER. This includes 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). We are continuing to adapt and refine the tools developed from that platform as part of ongoing work in this phase of the project.

In this project, the UNC-IE team is performing research on multiple fronts during the stated period of performance, and we describe them in detail below.

1. Perform NAS-wide impact assessment for 2011 and 2015
2. Perform airport-by-airport assessment using CMAQ-DDM
3. Develop generalized gridding tool for AEDT
4. Provide support for High fidelity weather in AEDT
5. Explore collaboration with NAU, Ukraine

[1] Boeing Commercial Airplane Market Analysis, 2010.

Task #1: Perform NAS-wide Impact Assessment for 2011 and 2015

University of North Carolina at Chapel Hill

Objective(s)

Using the most recent version of the Community Multi-scale Air Quality (CMAQ) model, develop an application for air quality simulation to investigate the trends of aircraft-attributable air pollutant concentrations at the surface for 2005, 2011, and 2015 years.

Research Approach

Introduction

The latest version of CMAQ, v5.2 was released in June 2017. UNC-IE previously used CMAQ v5.0.2 to quantify aircraft emissions impacts on surface air quality for 2005 in previous work. The most stable CMAQ version at the beginning of the year was v5.1. In CMAQv5.1 update from CMAQ v5.0.2, aerosol chemistry, homogeneous/heterogeneous chemistry, and planetary boundary layer scheme are improved (Appel et al., 2017). However, errors in wind-blown dust scheme have been found. Further, lightning NO_x calculation is still based on monthly total flash counts, while v5.2 has an algorithm to leverage the use of hourly data if available, and which we used.

In prior work under PARTNER and ASCENT, Woody et al. (2013) investigated secondary organic aerosols contributions from Atlanta airport (ATL) using CMAQ with three different resolutions (4, 12, and 36km). They concluded that different resolutions lead to different behaviors of organic chemistry. Huang et al. (in preparation) found that when using 36km resolution with CMAQv5.0.2 the 2005, landing and takeoff (LTO) attributable $PM_{2.5}$ is ~0.001 μg m^{-3} for domain average, and the highest increase was located in ATL (0.0029 μg m^{-3}).

Methodology

We modeled year 2011 at a new higher horizontal resolution of 12x12 km to assess aviation-attributable AQ impacts using CMAQ v5.1, meteorology from the Modern Era Retrospective Analysis for Research and Applications (MERRA) downscaled with WRF v3.8.1, background emissions from the National Emission Inventory (NEI) 2011 v6.3 processed through SMOKE v3.7, aircraft emissions from AEDT processed through AEDTProc, lightning NO_x, and inline photolysis.

The initial and boundary condition data for the main meteorology variables (except soil moisture and temperature, sea-surface temperature (SST) and snow height and snow-water equivalent) have been taken from NASA's MERRA data (Reienecker et al., 2011) which has 0.5 x 0.67 degree horizontal resolution with 72 vertical layers from surface to 0.01 hPa. The MERRA was chosen because it is a high resolution 3rd generation reanalysis dataset that includes high vertical and spatial resolution with 6-hourly data for entire globe which can be used in beyond CONUS domain such as northern hemispheric domain. MERRA does not provide soil data required for Weather Research Forecast (WRF) model (Skamarock et al., 2008) simulation. Soil moisture and temperature data for initial and boundary conditions were taken from National Centers for Environmental Prediction (NCEP) FNL (Final) Operational Global Analysis dataset which has 1x1 degree horizontal resolution with 6 hourly data. The sea-surface temperature data for WRF have been taken from the NCEP Environmental Modeling Center (EMC) real-time global SST dataset which has 0.5x0.5 degree resolution (Thiébaux et al., 2003). The snow height and snow water equivalent data have been taken from North American Mesoscale (NAM) model analyses datasets that were developed by the NCEP and obtained from the National Center for Environmental Information (NCEI) formerly known as National Climatic Data Center (NCDC). The model configurations for meteorology has been described in Table 1. The 2011year simulation has been performed using 3 months spin-up time.

We applied the Sparse Matrix Operator Kernel Emissions (SMOKE) v3.7 with the NEI 2011 v6.3 described at: https://www.epa.gov/air-emissions-modeling/2011-version-63-platform to estimate background emissions. We processed 19 emission sectors within 3 emission categories, including point, on-road, and area emissions to generate 2011 background emissions for the Continental United States (CONUS) 12km x 12km data. Biogenic emissions and wind-blown dust are not generated using SMOKE. They are calculated in CMAQ using inline modules. Aircraft emissions were removed in NEI v6.3 and generated using AEDTProc v1. We utilized the AEDT gridding processor called AEDTProc to process segmented aircraft emissions from the FAA's Aviation Environmental Design Tool (AEDT). AEDTProc has been used extensively for FAA in prior work by UNC for the production of regional scale modeling emission inputs like those needed for CMAQ.

We used CMAQ v5.1 to estimate aircraft-attributable ambient $PM_{2.5}$ and O_3 concentrations. CMAQ was built based on CMAQv5.1 with two modules from v5.2 which are windblown dust and lightning NO_x. Table 2 shows the configuration of CMAQ used for 2011 simulations. We updated windblown dust to v5.2 due to the incorrect calculation in v5.1 and lightning NO_x to v5.2 to take advantage of high time resolution of flash strike calculation (from monthly to hourly data). The CB05e51_AE6_AQ chemical mechanism was selected to be consistent with the potential available mechanisms in CMAQ v5.2 DDM. Initial and boundary conditions were downscaled from global MOZART-4/GEOS-5 simulations to 12km x 12km CONUS. After starting day, results from previous day were used as initial conditions. Base and sensitivity scenarios were conducted for 2011 and yearly simulations were trimmed into 4 seasons (Jan-Mar, Apr-Jun, Jul-Sep, and Oct-Dec). For each runtime period, simulations were spun up for a month with 3 months real simulations. Base scenario (base) includes non-aircraft emissions (SMOKE) and sensitivity scenario (sens) includes non-aircraft (from SMOKE) and aircraft emissions (AEDTProc). Aircraft-attributable ambient $PM_{2.5}$ and O_3 concentrations were calculated by subtracting base scenario concentrations from sens scenario.

Results

Meteorological Data (WRF) Processing

The model performance was evaluated with the observation database for winds, temperature, and water mixing ratio from National Oceanic and Atmospheric Administration (NOAA) Earth System Research Laboratory (ESRL) Meteorological Assimilation Data Ingest System (MADIS). The performance metrics used in the evaluation were bias and error for monthly average and diurnal value of 2-m temperature (T2), 2-m water mixing ratio (Q2), 10-m wind speed (WS10) and 10-m wind direction (WD10). Figure 1shows the soccer plot (mean absolute error vs mean bias) for 12 months for a) T2, b) Q2, c) WS10 and d) WD10. For 2-m temperature, there was a cold bias in winter and warm bias in summer shown in Figure 1a. The bias was less than ± 1 K except February when bias was ~ -1.2 K. The 11 months' biases were less (≤ 1.0 K) than the reference benchmark value (within outer rectangle in the figure). The temperature errors for all 12 months were between 1.75 K to 2 K in spring, summer, fall and 2.5 K in winter which were less (≤ 3.0 K) than reference benchmark value (within outer rectangle in the figure). Figure 1b shows the bias and error of 2-m mixing ratio in all 12 months. The biases and errors were within the reference benchmark value (within outer rectangle in the figure). Figure 1c shows the bias and error of 10-m wind speed in all 12 months which were within the reference benchmark value (within outer rectangle in the figure). Figure 1d shows the bias and error of 10-m wind direction in all 12 months which were also within the reference benchmark value (within outer rectangle in the figure).

Background Emission (SMOKE) Processing

Overall, emission data are consistent with the values reported by US EPA (<5% difference). However, some emission sectors showed significant differences, including wildfire, commercial marine vessels, and emissions outside lower 48 states. We confirmed with the US EPA emissions team that these discrepancies were due to the inconsistency of domain sizes.

Aircraft Emission (AEDTProc) Processing

Until recently, we have used AEDTProc for generating emissions at the 36km x 36km grid cell resolution across the CONUS. In the past, we have generated 36km x 36km emissions for the entire 2005 year's worth of AEDT data and January and July AEDT data for the years 2010, 2011, and 2015. We obtained new AEDT data for these recent years (2010, 2011 and 2015) from the U.S. DOT Volpe Center, and tested these new datasets with AEDTProc. We identified a few problems with these datasets and, working with Volpe, we fixed them. We have done extensive testing on the four years' worth of datasets to observe any trends over time and abnormalities in the data. Figures 2 and 3 shows the LTO versus full flight emissions for the three years' worth of data comparing monthly emission totals for January and February and for five different emission species. However, the goal of this task is to update our modeling platform and we have chosen to model at 12km x 12km grid cell resolution for the years 2011 and 2015.

The UNC team performed quality assurance by comparing our January and July 12km x 12km AEDTProc generated emissions to the January and July 36km x 36km generated emissions from the 2011 AEDT data. This comparison is meant to ensure that the overall trends are preserved between the two generated emission sets, while acknowledging that minor differences are unavoidable when gridding at different resolutions. Figures 4 and 5 show the monthly domain-wide total emissions between the two resolutions.

Emission totals are largely the same amongst grid resolutions, with two notable exceptions being POC and PEC species. This is due to the AEDTProc code that was run for the 36km x 36km some time back having a bug for the vertical allocation of the POC and PEC species. This has since been fixed and is represented correctly in the 12km x 12km grid resolution results.

We then looked at the vertical allocation of the monthly totals (Jan and Jul 2011) for six species across the grid resolutions. The vertical variations of emissions (CO, NO, NO_2, and SO_2) are matching between 12km x 12km and 36km x 36km, but POC and PEC show differences for the same reason explained above. Overall, air pollutant emissions contributed by aircraft in the North America are less than 5% (Table 3) from total emissions. These values are comparable to the numbers reported for Landing and take-off (LTO) 2005 emissions, and LTO aircraft emissions slightly increase (~10% for NO_x and SO_2) from 2005 to 2011, and this is explained by overall growth in aircraft activity.

Chemical Transport Model (CMAQ) Processing

CMAQ evaluations
Overall, the UNC team applied finer resolution and newer CMAQ configuration at 12x12 km for 2011 simulations, and covered full flight rather than LTO activity alone. We plan to run LTO-only next. We used the Atmospheric Model Evaluation Tool (AMET) v1.3 to evaluate CMAQ performance. O_3 error (40-70 % to 25-30%) and bias (40-70% to ~15%) have been significantly decreased for winter, summer and entire year (Table 4). CMAQ $PM_{2.5}$ performances for 2011 and 2005 are similar using these CMAQ configurations and it is worth to note that number of available sites for annual observations is small in 2005 and this could lead the performance bias. In general, errors and biases of most species are comparable with previous studies (Figure 6a) and domain wide annual average chemical composition highly matches between modeled results and field observations (Figure 6b). Based on above information, we conclude CMAQ performance for 2011 simulations is reliable to start to look at aircraft contributions.

Data analysis
Annual domain average of full flight attributable $PM_{2.5}$ is 0.003 ± 0.003 μg m^{-3}, and the contribution of 2005 LTO was ~0.001 μg m^{-3}. The highest impact (0.063 μg m^{-3}) is found in the San Francisco airport (SFO). Figure 7 shows the spatial variation of full flight attributable $PM_{2.5}$, the dark red hot spots are located in the airport grid-cells. There are regional dispersion areas in California Central Valley, Midwest, and Southeast, this regional dispersions have been reported (Woody 2011), secondary $PM_{2.5}$ formed when high NO_x aircraft emissions meet agricultural NH_3 emissions. Although, in 2005 simulations, only LTO was used, the spatial patterns between 2005 and 2011 are similar. Simulations of LTO impact for 2011 are still ongoing. Therefore, based on these evidences, LTO could have a greater impact on surface $PM_{2.5}$ concentrations than cruise emissions. Annual domain average full flight attributable O_3 concentration is 0.05 ± 0.04 ppb. However, in airport grid-cells, surface O_3 concentrations impacted by full flight are always negative due to NO_x titration. Similar to $PM_{2.5}$ hot spots, these O_3 depletion spots are concentrated in the grid-cells near airports (Figure 7). Ultimately, this provides additional evidence that even when full flight emissions are modeled; surface air quality is significantly impacted by aircraft activity during LTO rather than during cruise mode.

Looking into seasonal variation, secondary $PM_{2.5}$ contributions are changing by month (Figure 8). During summertime, the red areas are located in southeast section, whereas, during wintertime, California Central Valley and Midwest are important. Los Angeles Basin is an important full flight attributable secondary $PM_{2.5}$ region. Size of O_3 depletion (due to NO_x titration effects) change with seasons and there are some trajectories matching to regional flights. In general, larger O_3 depletion areas are seen in winter than summer near airports across the North America. These areas shrink in summer and are concentrated near airports (Figure 9). There are two hypotheses to explain this seasonal pattern. Planetary boundary layer is generally lower in winter than summer, which might enhance NO_x concentrations and NO_x titration could be more significant in winter. During summer time, humidity is higher than in winter, and this leads higher NO_3 deposition during nighttime and limits NO_x titration.

Full flight attributable $PM_{2.5}$ concentrations are 0.04, 0.05, and 0.02 μg m^{-3} at ATL, LAX, and ORD, respectively (Figure 10). In this resolution, we are able to separate the $PM_{2.5}$ hot spots between ORD and Midway airport. In LAX, high full flight attributable $PM_{2.5}$ are under the landing trajectories, it extends 3 grid-cells (36km). O_3 depletions at ATL, LAX, and ORD are -0.78, -0.80, and -0.53 ppb, respectively. The O_3 depletion areas are varying at these three airports. In ATL, the depletion area only extends one grid-cell from airports. Inversely, for LAX and ORD, the areas extend to multiple grid-cells. Our conclusion, after looking into full flight contribution in detail, is even when full flight emissions are considered, air quality impacted by aircraft activities is generally limited to near-airport areas with secondary contributions alone dominating at downwind distances.

$PM_{2.5}$ chemical compositions change from airport grid-cell to domain wide average (Figure 9); at top three airports we observed high fraction of elemental carbon, and it decreases to a small fraction for domain average. This is due to the fact that elemental carbon is mostly from direct aircraft emissions as primary aerosols and diluted after dispersion. Figure 11 shows large fraction of NO_3 for domain average which is hypothesized to be due to secondary formation. However, in the top three airports, there are some inconsistencies of full flight attributable chemical compositions. In ATL, high SO_4 but low NO_3 fraction, however, in LAX and ORD, we see a larger fraction of NO_3 than the fraction in ATL. We believe this to be due to changes in local chemical regimes associated with inorganic PM formation.

Table 1– Model configuration for meteorological inputs

Name	Description
WRF model version	WRFv3.8.1(Skamarock et al., 2008)
Simulation period	2011 with 3 month spin-up
Domain	Continental US (CONUS)
Spatial grid size	12X12-km
Number of sigma vertical layers	35 (with top layer at 50 hPa)
Input meteorological data sources	NASA MERRA for most of the variables, NCEP-FNL GFS for soil moisture and temperature, NCEP EMC for SST and NAM for snow
Planetary boundary layer scheme	Asymmetrical Convective Model version 2 (ACM2) (Pleim, 2007)
Cloud microphysics scheme	Morrison 2-moment scheme (Morrison et al., 2009)
Land surface model	NOAH (Mitchell et al., 2001)
Cumulus parameterization	Kain–Fritsch scheme (Ma et al., 2009)
Land use	NLCD40 (NLCD, 2011)
Short wave radiation	RRTMG (Iacono et al., 2008)
Long wave radiation	RRTMG (Iacono et al., 2008)

Table 2 – CMAQ Model Configuration

Options	Description	Note
Mechanism	CB05e51_AE6_AQ v5.1	
CTM_WB_DUST	Windblown dust v5.2	On
CTM_LTNG_NO	Hourly lightning NO_x v5.2	On
CTM_ILDEPV	Inline dry deposition v5.1	On
CTM_MOSAIC	Landuse specific deposition v5.1	On
CTM_ABFLUX	Bidirectional NH3 v5.1	Off
CTM_HGBIDI	Bidirectional Hg v5.1	Off
CTM_SFC_HONO	Surface HONO interaction v5.1	On
CTM_BIOGEMIS	Inline biogenic emission v5.1	On
CTM_PT3DEMIS	Inline plume-rise for point emissions v5.1	Off
CTM_ACAERO	Specific aerosol emissions for aircraft v5.0.2	Off

Table 3 – AEDT-based aircraft emissions in North America

<table>
<tr><th></th><th>NO</th><th>NO_2</th><th>SO_2</th><th>Particulate SO4</th><th>Elemental carbon</th><th>Organic carbon</th><th>CO</th><th>TOG</th></tr>
<tr><td>2011 Aircraft full flight to total emission contribution (%)</td><td>3.6</td><td>4.1</td><td>0.7</td><td>1.3</td><td>0.3</td><td><0.1</td><td>0.21</td><td><0.1</td></tr>
<tr><td>2011 Aircraft full flight emission (tons)</td><td>614,579</td><td>72,197</td><td>60,713</td><td>1,858</td><td>1,605</td><td>1,444</td><td>177,525</td><td>29,501</td></tr>
<tr><td>2011 Aircraft LTO to total emission contribution (%)</td><td colspan="2">0.5</td><td><0.1</td><td colspan="3"><0.1</td><td><0.1</td><td><0.1</td></tr>
<tr><td>2011 Aircraft LTO emission (tons)</td><td colspan="2">96,187</td><td>7,874</td><td colspan="3">594</td><td>56,731</td><td>11,397</td></tr>
<tr><td>2005 Aircraft LTO emission (tons)</td><td colspan="2">83,248</td><td>7,217</td><td colspan="3">638</td><td>62,669</td><td>13,841</td></tr>
</table>

Table 4 – CMAQ evaluation for 2011

	O_3 (ppb)				**$PM_{2.5}$ (μg m^{-3})**			
	MEAN OBS	MEAN MOD	NME	NMB	MEAN OBS	MEAN MOD	NME	NMB
Jan_2005	19.1	33.7	75.0	70.7	11.1	12.1	57.1	12.7
Jan_2011 base	23.9	25.6	31.1	2.1	11.6	12.5	53.4	1.6
Jul_2005	34.1	45.9	43.6	36.9	12.8	7.62	49.2	-36.0
Jul_2011 base	34.9	40.5	25.4	15.5	11	5.8	50.4	-43.9
2005	30.4	41.8	45.5	39.2	12.8	11.3	36.7	-10.4
2011_base	31.6	36.4	24.1	12.8	9.87	7.71	47.7	-24.7
2011_sens	31.6	36.5	24.2	13.0	9.87	7.72	47.7	-24.6

OBS: observations, MOD: model results
NME and NMB: Normalized Median Error and Normalized Median Bias

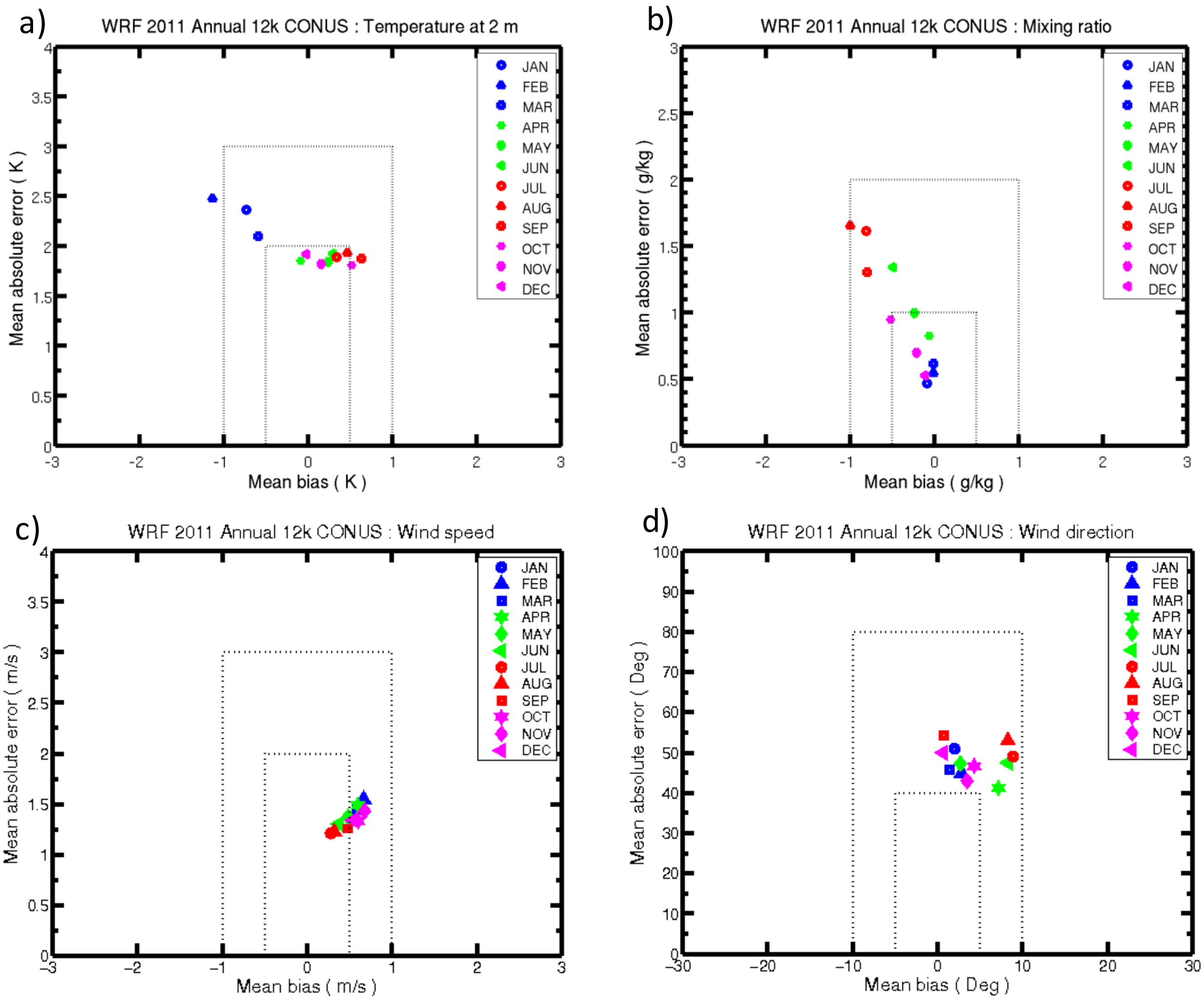


Figure 1 - Soccer plot for error vs bias of a) 2-m mixing ratio, b) 2-m mixing ratio, c) 10-m wind speed and d) 10-m wind direction averaged over the 12-km CONUS domain for all 12 months in 2011 [the inner dotted rectangle is the benchmark value limit for simple model and outer dotted rectangle is the benchmark value limit for the complex model (Moore, 2014)].

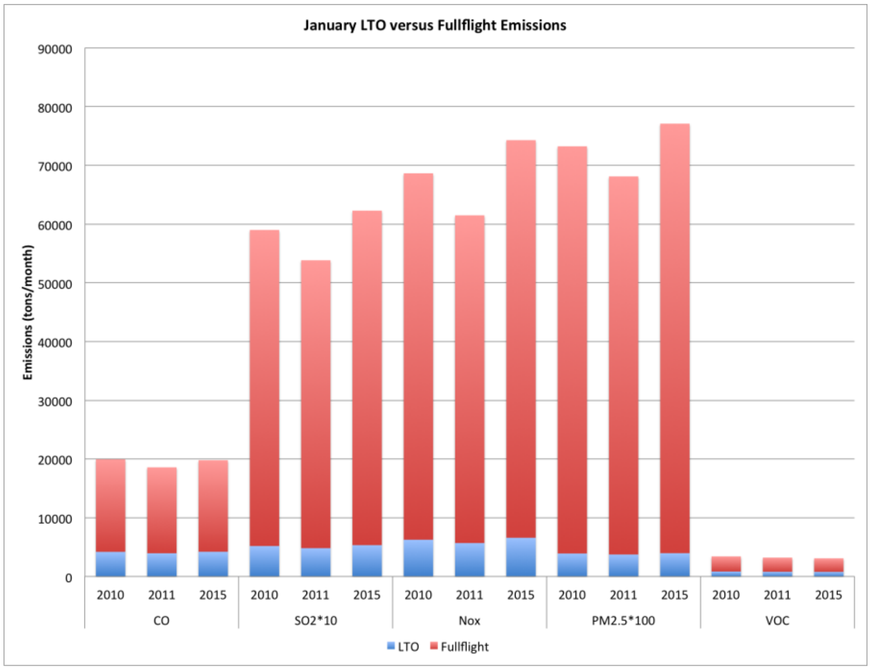


Figure 2 - LTO versus full flight January emission totals for five species across our three years' worth of data

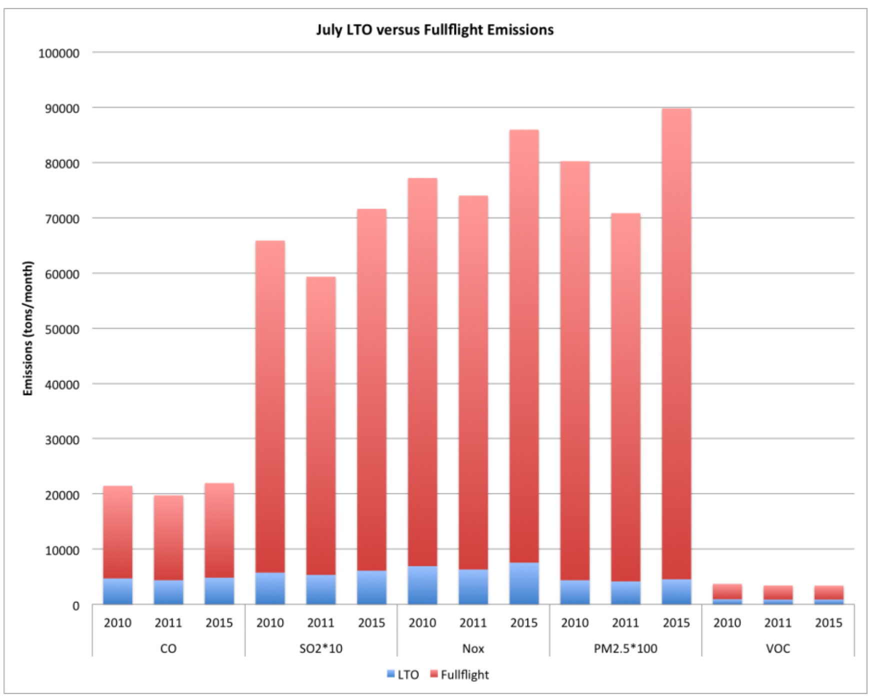


Figure 3 - LTO versus full flight July emission totals for five pollutants from AEDT across our three years' worth of data

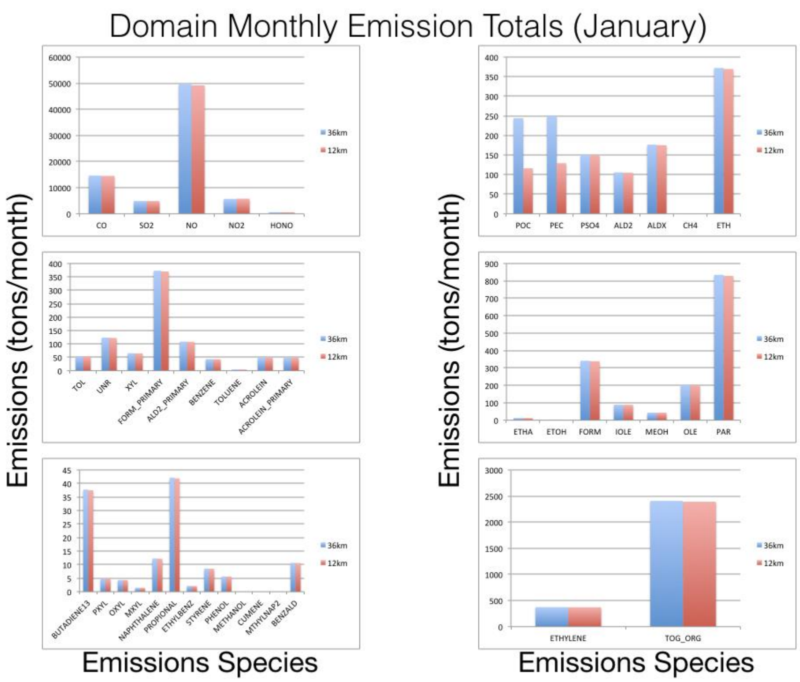


Figure 4 – Domain-wide Monthly Aircraft Emission Totals for January 2011 by model species.

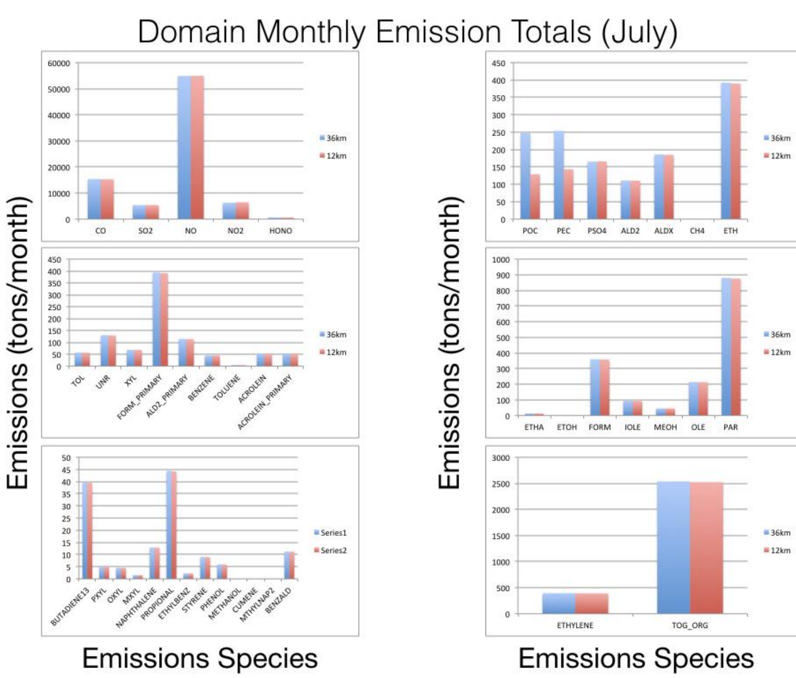
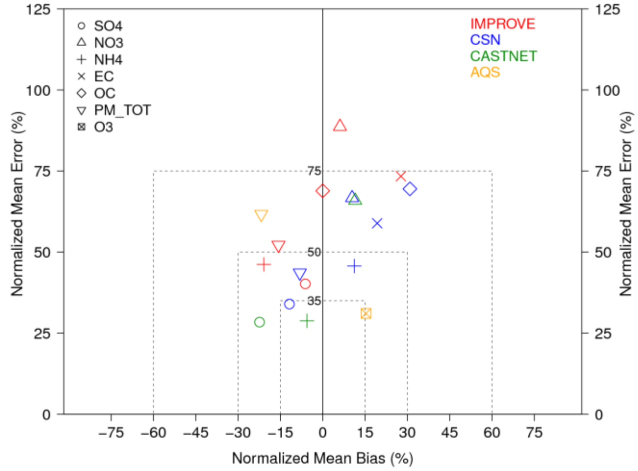


Figure 5 – Domain-wide Monthly Aircraft Emission Totals for July 2011 by model species.

a. Soccer plot for errors and biases by comparing CMAQ outputs with observations in 2011



EC: Elemental Carbon
OC: Organic Carbon
PM_TOT: total $PM_{2.5}$
IMPROVE: Interagency Monitoring of Protected Visual Environment
CSN: Chemical Speciation Network
CASTNET: Clean Air Status and Trends Network
AQS: Air Quality System

b. Stacked bar plot for annual domain wide average chemical composition between CMAQ outputs with observations in 2011

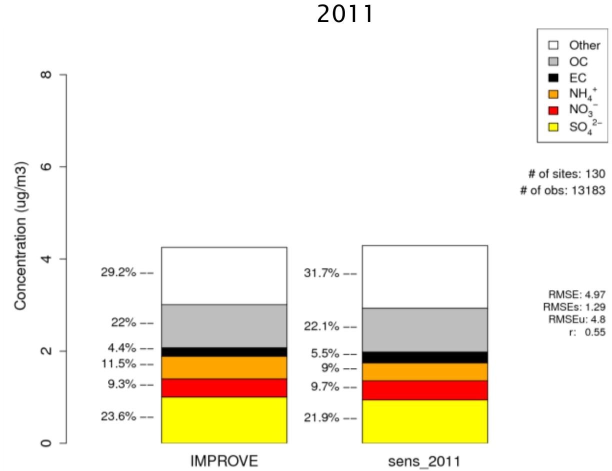


Figure 6 – Performance of CMAQ 2011 platform: a. soccer plot for errors and bias b. stacked bar plot for $PM_{2.5}$ chemical speciation.

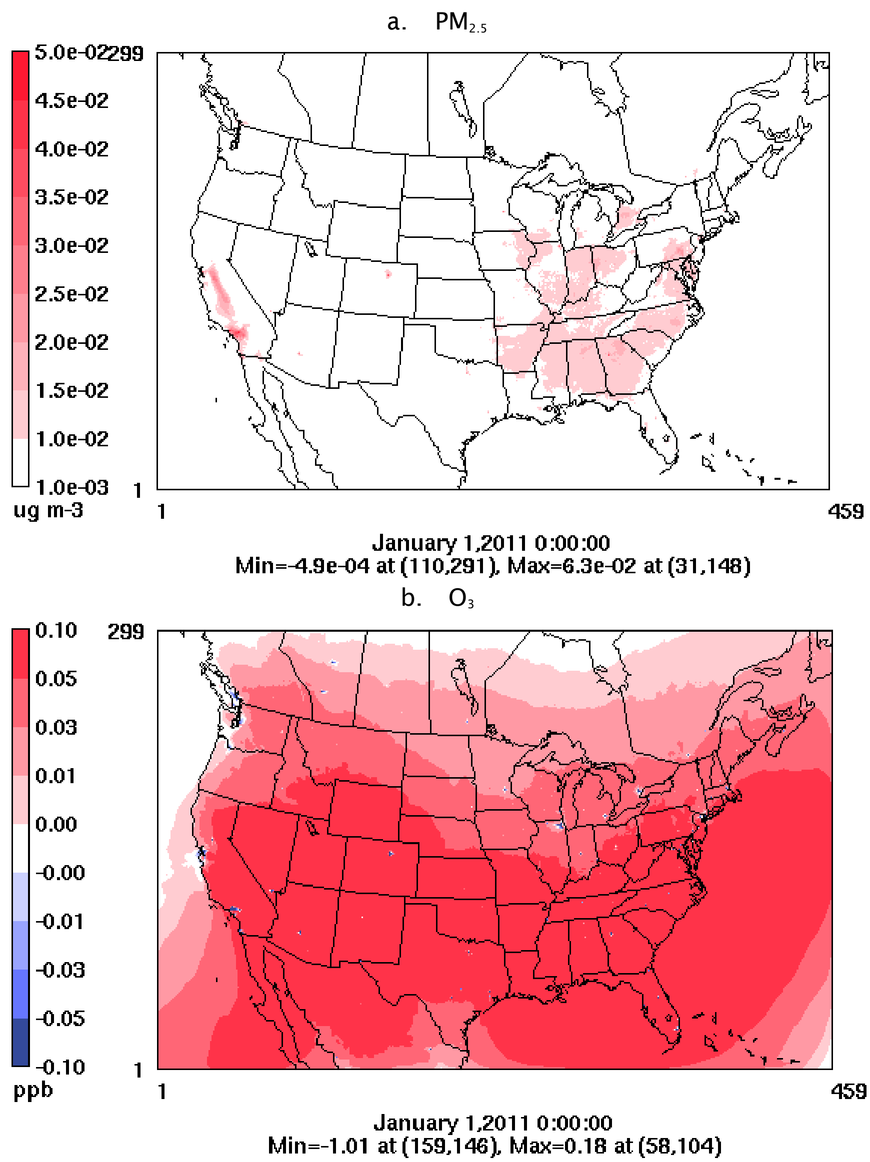


Figure 7 – 2011 Annual-average full flight attributable (a) $PM_{2.}$ and (b) O_3

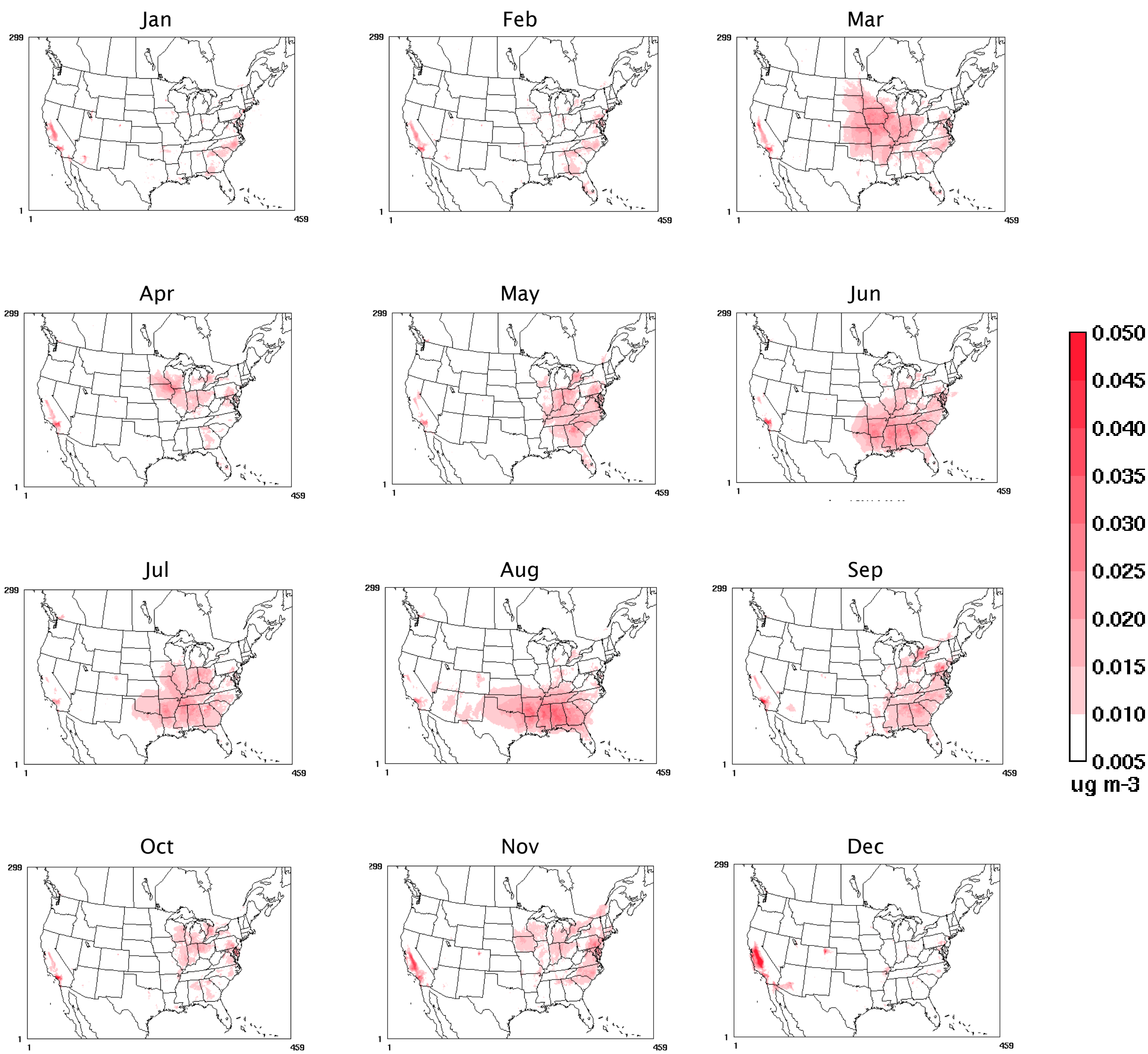


Figure 8 – 2011 Monthly average Spatial patterns of full flight attributable $PM_{2.5}$

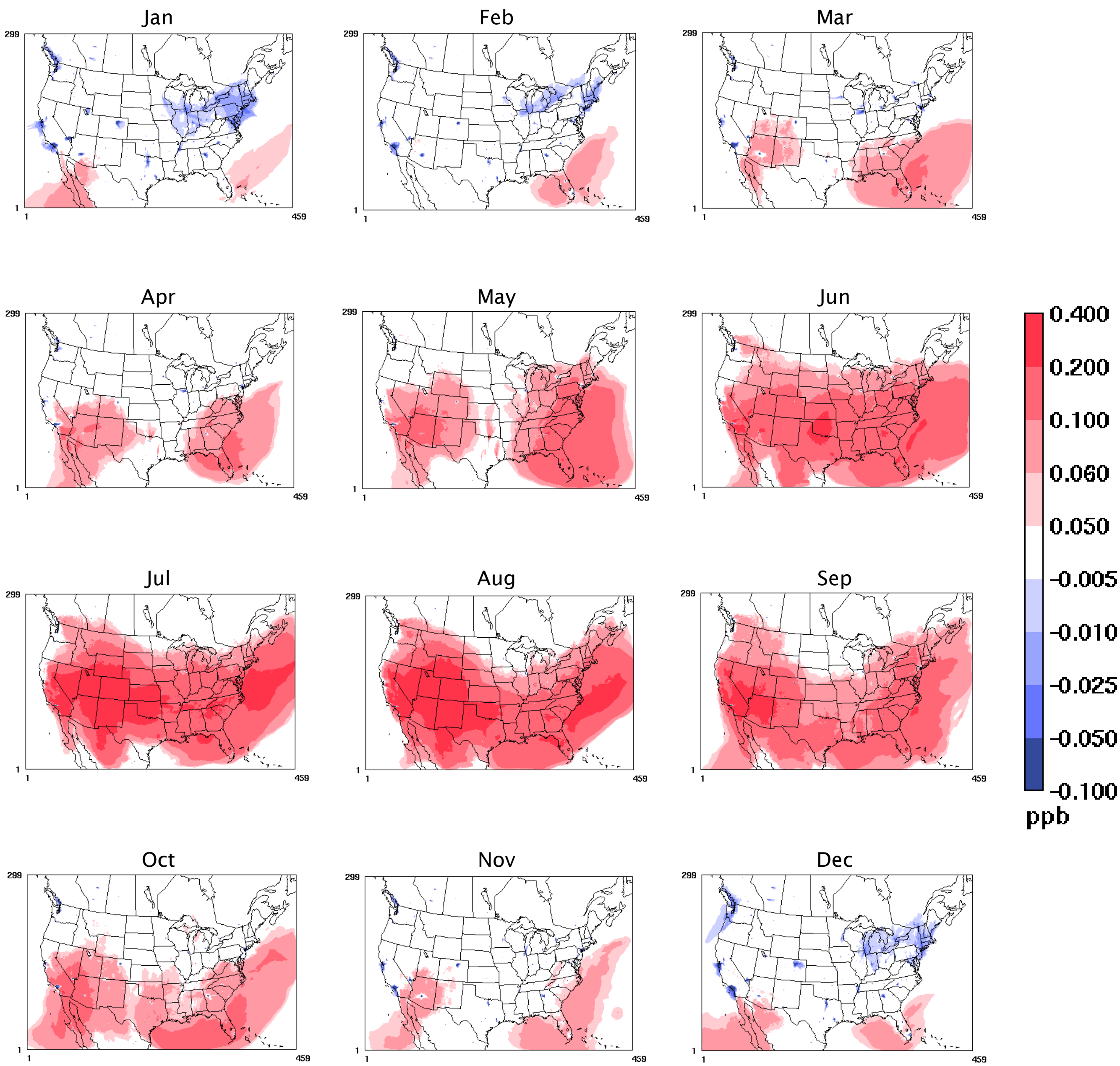


Figure 9 – 2011 Monthly average Spatial patterns of full flight attributable O_3

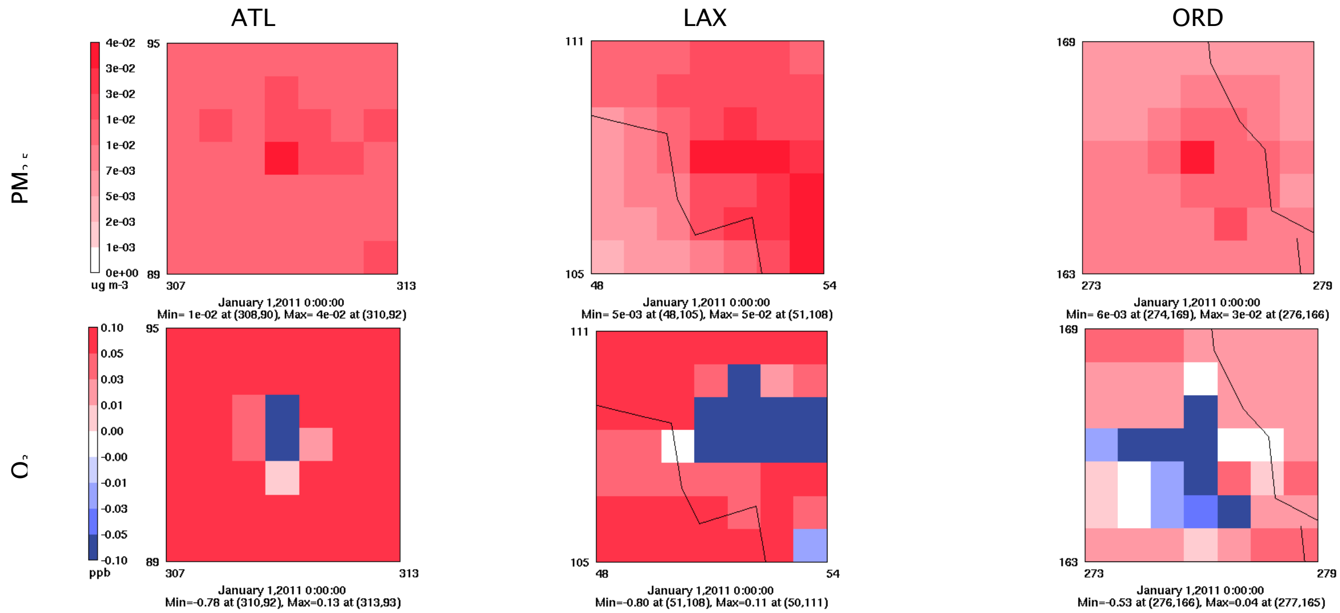


Figure 10 – 2011 Annual average full flight attributable $PM_{2.5}$ and O_3 for top three airports. Each square panel contains 7 × 7 grid-cells (84km × 84km), with airport located in the center of each square.

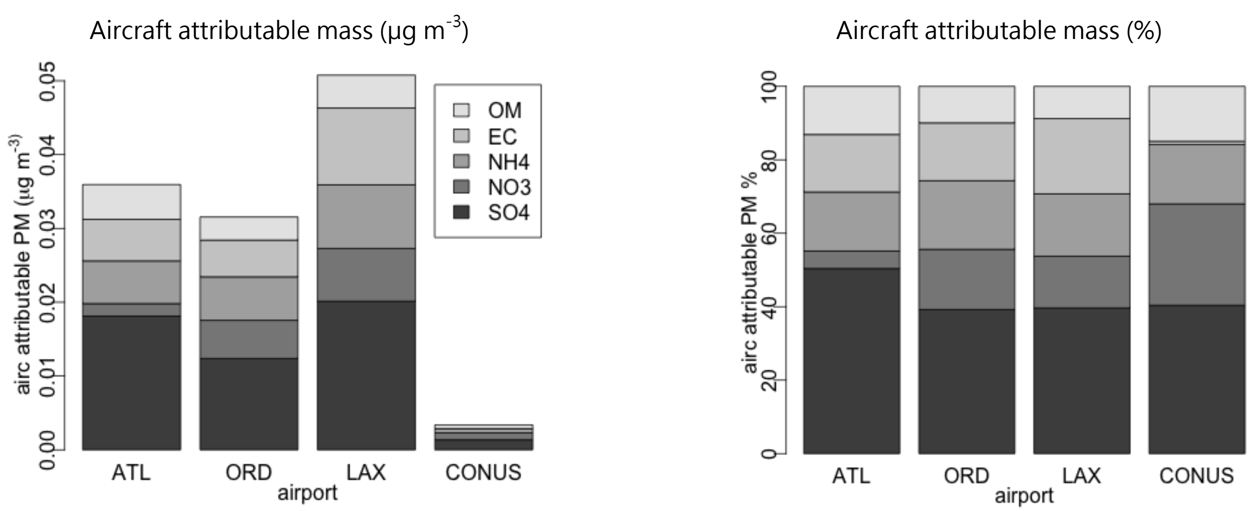


Figure 11 – Chemical composition of $PM_{2.5}$ at top three airports using domain average values.

Milestone(s)
Sep, 2017 – Completed running WRF for the 2011 using the finalized configuration
Sep, 2017 – Completed processing 2011 background emissions and full flight emissions
Sep, 2017 – Completed simulating 2011 base (non-aircraft emissions) scenario with CMAQ
Oct, 2017 – Completed simulating 2011 sensitivity (non-aircraft and aircraft emissions, full flight) scenario with CMAQ
Oct, 2017 – Completed assessment of aircraft-attributable impacts for new 12-km platform

Major Accomplishments
Quantified surface $PM_{2.5}$ and O_3 concentration contributed by full flight emissions for 2011, and performed extensive spatio-temporal analyses.

Publications
None

Outreach Efforts
Presentation at bi-annual ASCENT stakeholder meetings

Awards
None

Student Involvement
Calvin Arter is a Ph.D. student helping AEDT data preparation and evaluating 2011 full flight emissions.

Plans for Next Period
To complete surface air quality impacts from LTO for 2011
To simulate surface air quality impacts from LTO and full flight for 2015

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Task #2: Perform Airport-by-Airport Assessment Using CMAQ-DDM

University of North Carolina at Chapel Hill

Objective(s)

In addition to this NAS-wide assessment, to further refine the individual airport-by-airport modeling framework using the CMAQ v5.0.2 enhanced with the Decoupled Direct Method in Three Dimensions (DDM-3D), UNC-IE will use an advanced sensitivity tool to perform seasonal simulations. Previous work used this tool in CMAQ v4.7.1 to compute first order sensitivities. We will enhance this to use second order sensitivities in the latest CMAQ v5.0.2 and use these to perform quantitative analyses to assess the number of airports that will be needed to transition an area in attainment of the U.S. EPA's National Ambient Air Quality Standards (NAAQS) to non-attainment.

Research Approach

Introduction

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. 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).

Our aim for this work was to quantify the amount of emission reductions needed at five individual airports to reduce the concentration of O_3 by 1 ppb and the concentration of $PM_{2.5}$ by 0.1 μg/m^3 at the grid cell containing the airport.

In order to choose the five individual airports, UNC-IE began with a list of all the airports located in the U.S. that are currently located in regions of attainment (nonattainment status of maintenance, marginal, or nonattainment) of the NAAQS for O_3 and PM. We selected from a list all airports that had at least 0.05% of annual passenger boardings designated as being a small hub according to the FAA's Voluntary Airport Low Emissions (VALE) program (FAA 2016). The final selection involved choosing airports across the country that represented the greatest geographic and climatic diversity while servicing major metropolitan areas (MSA population > 1,000,000 people). Table 5 shows the airport hub type (FAA 2016) and its description and Table 6 shows the tier status as defined by Woody et al. 2016, and its description. Figure 12 shows the 17 candidate airports from which we then selected our final five. Table 7 shows the list of 17 airports with various climate, traffic, and pollutant statistics. In consultation with the FAA, we chose Raleigh Durham International Airport (RDU), Boston Logan International Airport (BOS), Kansas City International Airport (MCI), Tucson International Airport (TUS), and Seattle-Tacoma International Airport (SEA) from the list of 17 candidate airports to model with HDDM.

Table 5 - Hub type descriptions

Hub Type	Percentage of Annual Passenger Boardings
Large	1% or more
Medium	At least 0.25%, but less than 1%
Small	At least 0.05%, but less than 0.25%

Table 6 -Tier number descriptions

Tier Number	Number of operations per month
I	Greater than 40,000
II	At least 20,000, but less than 40,000
III	Less than 20,000

Table 7 - List of candidate airports and criteria regarding climate, flight operations, and other pollutant NAAQS

	Size			Attainment Status		Population	Distance	Climate				
	Hub		The Emplaments	CO	SO2	MSA 2016	(km)	Average annual min temp © 1961 to 1990	Average annual max temp © 1961 to 1990	January 2016 Temp © (min, max, ave)	July 2016 Temp © (min, max, ave)	Average annual precipitation (in) 2005 to 2009
MSP	Large	1	16,972,678	Maintenance	Nonattainment/ Maintenance	3,551,036		0.11-2.93	10-15	-11.66, -4.32, -7.94	19.08, 28.87, 23.98	21-35
RDU	Medium	3	4,673,869	Maintenance		1,302,946		8.92-12.46	20-25	-0.84, 8.98, 4.07	22.4, 33.28, 27.76	36-50
MCI	Medium	3	4,982,722			2,104,509		5.86-8.92	15-20	-6.38, 3.80, -1.29	20.83, 30.91, 25.87	36-50
BOS[a]	Large[a]	2[a]	15,507,561[a]	Maintenance[a]		4,794,447[a]		2.93-5.86[a]	15-20[a]	-3.52, 4.18, 0.39[a]	19.69, 29.28, 24.48[a]	51-80[a]
MHT[b]	Small[b]		1,032,964[b]	Maintenance[b]		407,761[b]	72[a-b]	0.11-2.93[b]	10-15[b]	-5.49, 3.75, -1.37[b]	17.7, 30.02, 23.86[b]	51-80[b]
PVD[c]	Small[c]	3	1,764,828[c]			1,614,750[c]	79[a-c]	2.93-5.86[c]	15-20[c]	-4.51, 4.8, 0.15[c]	19.06, 29.8, 24.43[c]	51-80[c]
ABQ[d]	Medium	3[d]	2,354,184[d]	Maintenance[d]		909,906[d]		2.93-5.86[d]	20-25[d]	-3.17, 8.59, 2.71[d]	19.39, 35.37, 27.38[d]	0-20[d]
TUS[e]	Small[e]	3[e]	1,597,247[e]			1,016,205[e]	516[d-e]	8.92-12.46[e]	25-30[e]	3.8, 19.0, 11.4[e]	25.57, 39.16, 32.36[e]	0-20[e]
BUF[f]	Medium	3[f]	2,378,469[f]			1,132,804[f]		0.11-2.93[f]	10-15[f]	-6.65, 1.12, -3.76[f]	18.55, 28.31, 23.38[f]	36-50[f]
ROC[g]	Small[g]	3[g]	1,173,933[g]			1,078,879[g]	88[g-f]	2.93-5.86[g]	10-15[g]	-6.79, 1.76, -2.52[g]	17.64, 29.9, 23.77[g]	21-35[g]
SYR[h]	Small[h]	3[h]	987,169[h]	Maintenance[h]		656,510[h]	126[g-h]	2.93-5.86[h]	10-15[h]	-7.67, 0.96, -3.36[h]	17.22, 28.71, 22.97[h]	36-50[h]
SAT[i]	Medium	3[i]	4,046,856[i]			2,429,609[i]		12.46-19.43[i]	25-30[i]	4.38, 17.56, 11.02[i]	24.85, 36.21, 30.53[i]	21-35[i]
AUS[j]	Medium	3[j]	5,219,982[j]			2,056,405[j]	107[i-j]	12.46-19.43[j]	25-30[j]	2.12, 17.17, 9.64[j]	23.95, 36.53, 30.24[j]	21-35[j]
SEA	Large	2	17,888,880	Maintenance		3,798,902		5.86-8.92	20-25	3.54, 9.47, 6.51	14.24, 24.43, 19.33	36-50
MIA[k]	Large[k]	2[k]	19,471,456[k]							15.78, 23.49, 19.64[k]	35.7, 32.86, 29.28[k]	
FLL[l]	Large[l]	2[l]	12,031,860[l]			6,066,387[l]	34[k-l]	12.46-19.43[l]	25-30[l]	15.67 23.55, 19.61[l]	26.63, 32.5, 29.58[l]	51-80[l]
PBI[m]	Medium	3[m]	2,926,243[m]				68[l-m]			14.15, 23.05, 18.6[m]	28.8, 33.68, 30.13[m]	

Figure 12 - Locations of the 17 candidate airports (MHT and PVD underneath BOS with labels not shown)

CMAQ-DDM simulations instrumented to compute first and second order sensitivities were performed for the five airports for the months of January and July, 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. First order sensitivities were of the form:

$$S_{i,j}^{\mathbf{1}} = \frac{\partial C_i}{\partial E_j} \quad \text{Eq. 2.1}$$

While second order sensitivities were consisting of two forms:

$$S_{i,j}^{\mathbf{2}} = \frac{\partial^2 C_i}{\partial {E_j}^2} \quad \text{Eq. 2.2}$$

$$S_{i,j,k}^{\mathbf{2}} = \frac{\partial^2 C_i}{\partial E_j \partial E_k} \quad \text{Eq. 2.3}$$

Eq. 2.2 represents second order sensitivities to one emission species, while Eq. 3 represents second order cross sensitivities to two emission species.

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). Sensitivities were calculated in the first model layer alone, to reflect where people live and are exposed to air pollution.

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

We present spatial plots for one airport (SEA) as an example of the sensitivities we calculated for first and second order with respect to NO_x aircraft emissions. Figure 13 shows the first order (top row) and second order (bottom row) sensitivities of O_3 with respect to NO_x emissions from LTO activity at SEA for the months of January and July. Figure 14 shows the same but for $PM_{2.5}$ sensitivities to NO_x.

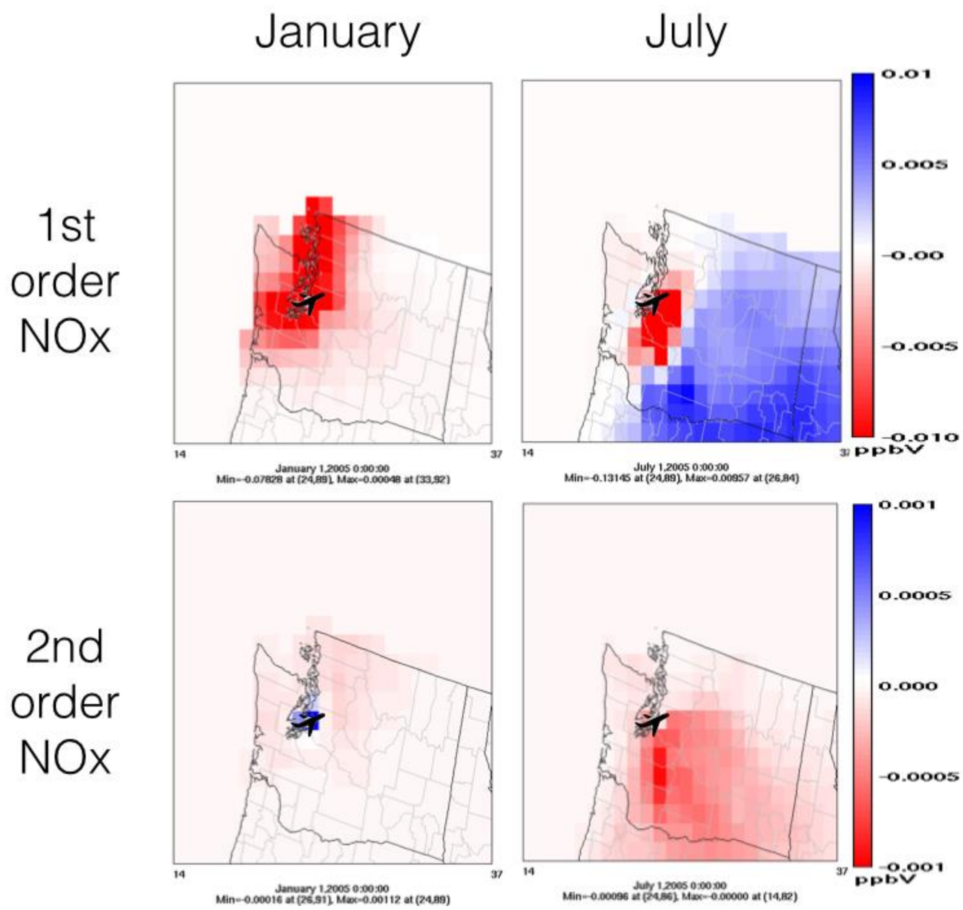

Figure 13 - O_3 first and second order sensitivity coefficients with respect to NO_x emissions at Seattle

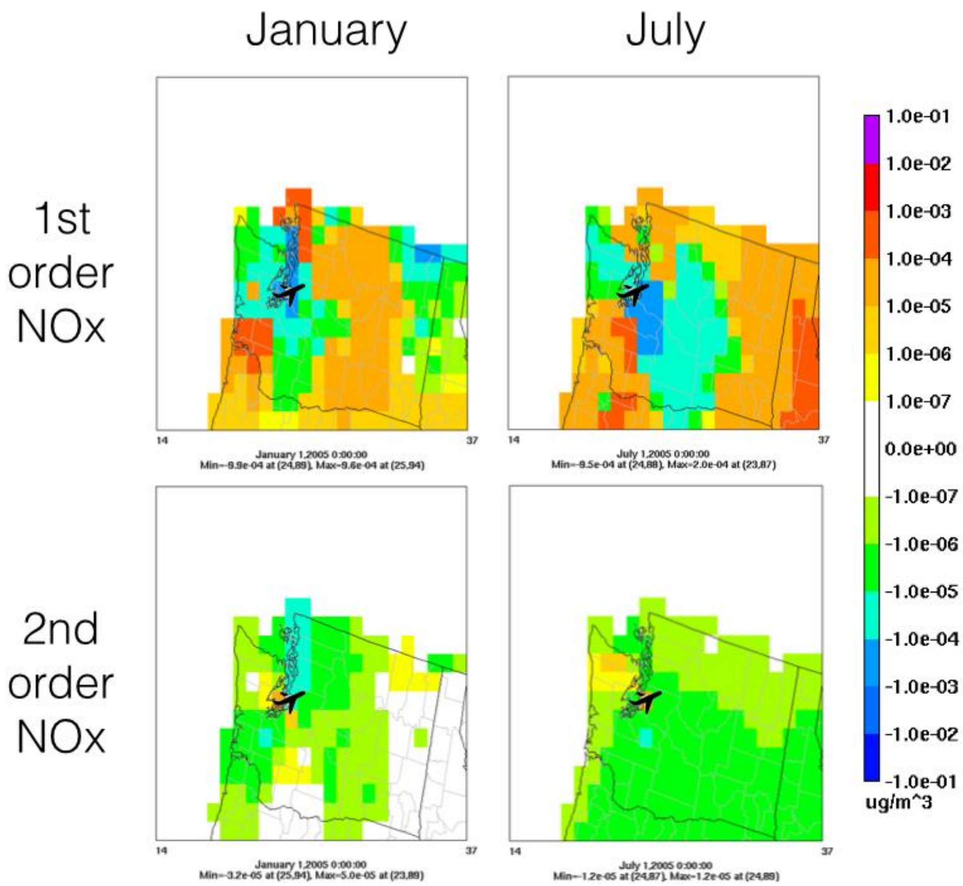

Figure 14 - $PM_{2.5}$ first and second order sensitivity coefficients with respect to NO_x emissions at Seattle

Spatial plots reveal how the emissions at the airport may impact regions downwind with sensitivities calculated at each model grid cell. However for our reduction analysis, we looked at emission reductions in the grid cell containing the airport. Figure 15 shows the pseudo-annual average (January and July averaged) sensitivities of O_3 with respect to NO_x and VOC emissions at each of the five airports. Figure 16 shows the pseudo-annual average sensitivities of $PM_{2.5}$ to NO_x, VOC, SO_2, PSO_4, POC, and PEC emissions at the five airports.

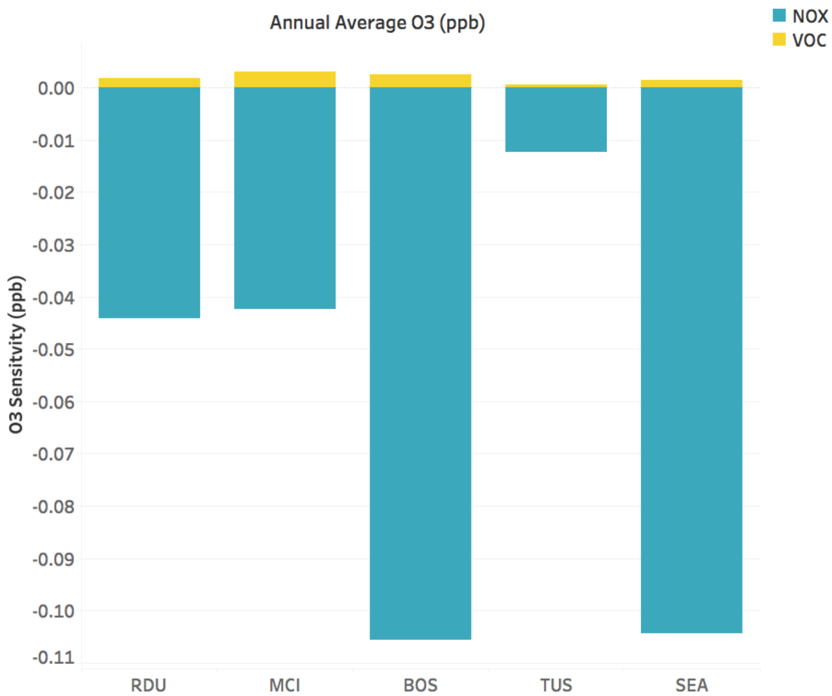

Figure 15 - O_3 sensitivities disaggregated by precursor species at grid cell containing airport

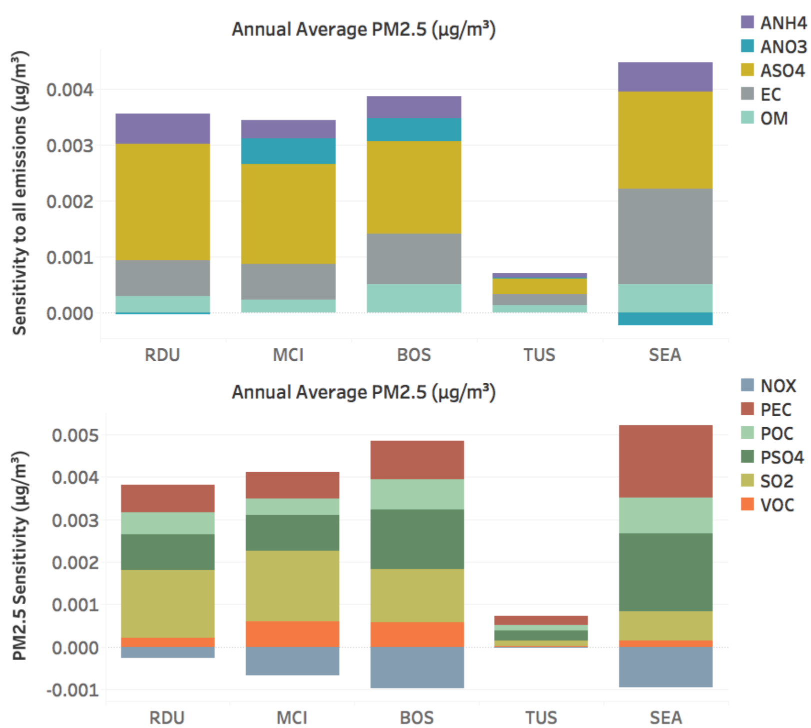

Figure 16 - $PM_{2.5}$ sensitivities disaggregated by output species (top) and precursor species (bottom) at grid cell containing airport

We can utilize Taylor series expansions with only first order sensitivities (Eq. 2.4) and with first and second order sensitivities (Eq. 2.5) to calculate the emission reductions needed to reduce concentrations of O_3 by 1 ppb or $PM_{2.5}$ by 0.1 μg/m^3 at the grid cell containing the airport.

$$\sum_{j=1}^{n} C_{\epsilon_j} = C_0 + \Delta\epsilon_j S_j^{\mathbf{1}} \quad \text{Eq. 2.4}$$

$$\sum_{k=1}^{n}\sum_{j=1}^{n} C_{\epsilon_j} = C_0 + \Delta\epsilon_j S_j^{\mathbf{1}} + \frac{\Delta\epsilon_j{}^2}{2} S_j^{\mathbf{2}} + \Delta\epsilon_j \Delta\epsilon_{j\neq k} S_{j,j\neq k}^{\mathbf{2}} \quad \text{Eq. 2.5}$$

(n is the number of precursors, for O_3 $n = 2$, for $PM_{2.5}$ $n = 6$)

Figure 17 shows the emission reductions needed at each airport to reduce the concentration of O_3 at the airport grid cell by 1 ppb. The left side of the figure shows the emission reductions while the right side shows O_3 monitor values for 2005 and 2016 at the monitor closest to the respective airport. The positive reduction values indicate that a large disbenefit is seen in the airport grid cell. This indicates an *increase* in NO_x emissions is needed at the airport to decrease concentrations of O_3 by 1 ppb. Clearly, it is due to the large negative sensitivities at the location of the airport, indicative of a VOC-limited chemical regime in which NO_x emission controls result in more O_3 being produced.

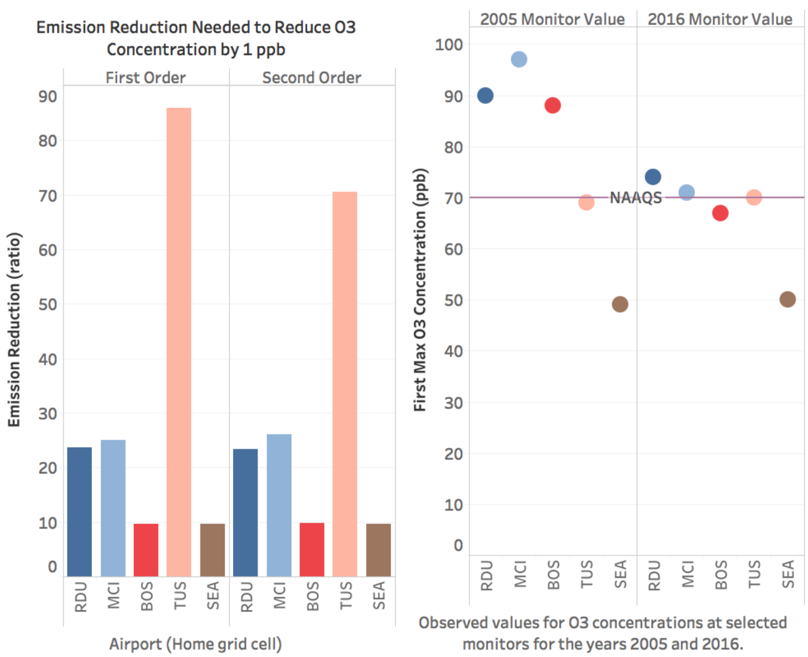

Figure 17 - O_3 reductions analyses (left) and 2005, 2016 observations (right).

Figure 18 shows the emission reductions needed at each airport to reduce the concentration of $PM_{2.5}$ at the airport grid cell by 0.1 μg/m^3. As in Figure 17, the right side of the figure shows the emission reductions needed and the right side displays $PM_{2.5}$ monitor values for reference. Negative reduction values indicate that a reduction in precursor emissions at each of the airports will result in a reduction in ambient $PM_{2.5}$. The numbers are scaled relative to the total emissions at each airport with BOS needing for example, approximately 20 times less total emissions at the airport to reduce concentrations of $PM_{2.5}$ by 0.1 μg/m^3.

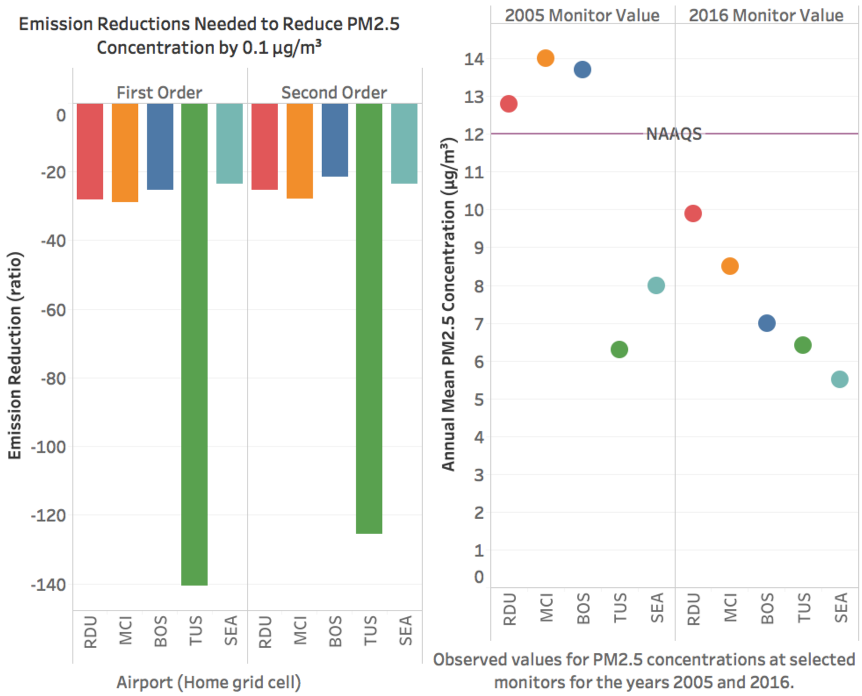

Figure 18 - $PM_{2.5}$ reductions analyses (left) and 2005, 2016 observations (right).

For both O_3 and $PM_{2.5}$ the differences between using only first order sensitivities and using both first and second order sensitivities are very small. The first order sensitivities dominate at the location of the airport and the non-linear chemistry, which the second order sensitivities will help describe, occurs downwind of the airport. We performed an analysis to look at the impact of LTO emissions downwind of Seattle-Tacoma International Airport.

We first looked to define regions where nonlinearity will be important. We utilized a nonlinearity ratio as described in Wang et al. (Wang et al. 2011). The ratio is defined as:

$$R_{C_i} = \frac{|0.5S^2|}{|S^1| + |0.5S^2|}$$

Eq. 2.6

Figure 19 shows the nonlinearity ratio plotted for sensitivities to NO_x emissions. NO_x was the only emission species to show nonlinear response with respect to both O_3 and $PM_{2.5}$ concentrations. The nonlinearity ratio results in a value from 0 to 1 where 1 describes a region that is highly sensitive to nonlinearity. We then selected grid cells with higher values of the nonlinearity ratio (approximately greater than 0.33) as well as the grid cell containing Seattle-Tacoma International Airport. Starting at a hypothetical $PM_{2.5}$ base concentration of 12 μg/m³, we utilized our first and first and second order Taylor series expansions (Eq. 4 and 5, respectively) to calculate the $PM_{2.5}$ response to an approximately 75% increase in NO_x emissions and approximately 50% increase in VOC emissions from Seattle-Tacoma International airport. Figure 20 shows the concentration response at each downwind location as shown in Figure 19 using only first order sensitivities (top) and using both first and second order sensitivities (bottom). It is clear that some locations downwind exhibit a different response when including second order sensitivities; with nonlinearity leading to a decrease in $PM_{2.5}$ from our base value while using only first order sensitivities shows an increase in $PM_{2.5}$ at those same locations.

In addition to the above analyses for airports in attainment areas, we expanded the framework to perform modeling and analyses at four of the largest airports in the nation and that are in non-attainment for O_3 and/or $PM_{2.5}$ - Atlanta (ATL), Chicago O'Hare (ORD), Los Angeles (LAX), New York (JFK) and computed 1st and 2nd order sensitivities for O_3 and $PM_{2.5}$, with the goal to assess changes in emissions needed to reduce O_3 by 1 ppb or $PM_{2.5}$ by 0.1 μg/m³ in the airport grid-cell.

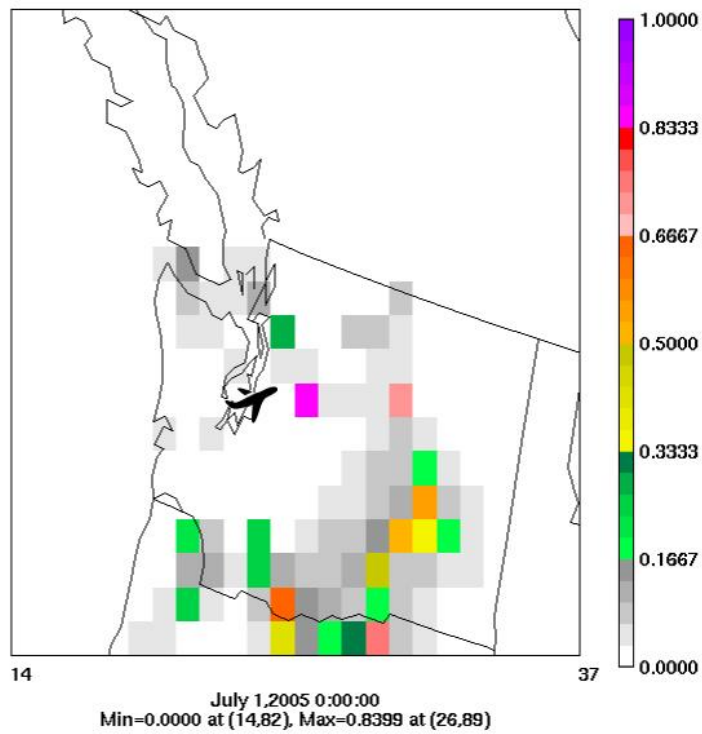

Figure 19 - Nonlinearity ratio plotted for Seattle-Tacoma International airport

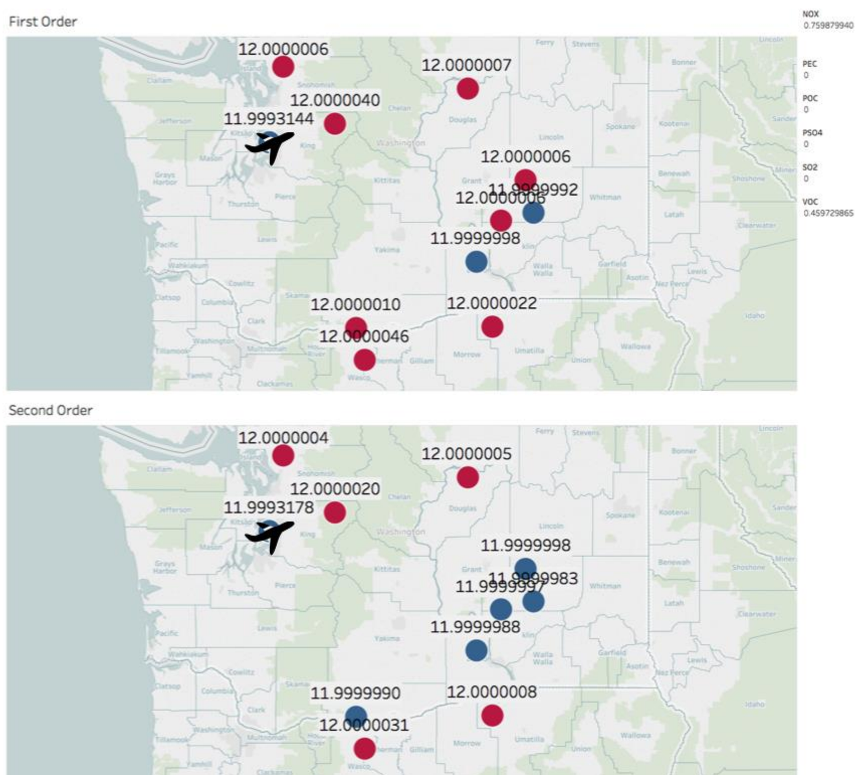

Figure 20 - $PM_{2.5}$ concentration response to increased NO_x and VOC emissions at Seattle-Tacoma International airport

Milestone(s)
Developed candidate short-list of airports for attainment analyses
Computed first and second order sensitivities for O_3 and $PM_{2.5}$ due to 5 airports in attainment areas, for the first time
Expanded framework to look at four additional large airports that are currently in non-attainment areas too.
Developed a novel approach using CMAQ with HDDM to quantify the impacts of airport-specific aircraft emissions on potential O_3 and $PM_{2.5}$ non-attainment.

Major Accomplishments
This is the first use of higher order sensitivities with respect to airport-specific aircraft emissions. We have demonstrated that higher order sensitivities are important for describing nonlinear effects and paint a more accurate picture with regards to the atmospheric chemistry that may be occurring in downwind regions of emission sources. Insights from this novel approach can be used for larger emission sectors to allow for more accurate emission reduction strategies.

In addition to the above 5 airports in attainment areas, we also expanded this work to look at four additional large airports that are in non-attainment areas – Atlanta (ATL), Chicago O'Hare (ORD), Los Angeles (LAX), New York (JFK) to look at 1st and 2nd order sensitivities for O_3 and $PM_{2.5}$.

Publications/Presentations
Arter, C. A. & Arunachalam, S. (2017). *Calculating Second Order Sensitivity Coefficients for Airport Emissions in the Continental U.S. Using CMAQ-HDDM.* Presented at the 2017 ASCENT Advisory Board Meeting, Washington, D.C.
Arter, C. A. & Arunachalam, S. (2017). *Calculating Second Order Sensitivity Coefficients for Airport Emissions in the Continental U.S. Using CMAQ-HDDM.* Poster session presented at the 2017 North Carolina BREATHE Conference, Raleigh, NC.
Arter, C. A. & Arunachalam, S. (2017). *Calculating Second Order Sensitivity Coefficients for Airport Emissions in the Continental U.S. Using CMAQ-HDDM.* Poster session presented at the 2017 University of North Carolina Chapel Hill Climate Change Symposium, Chapel Hill, NC.
Arter, C. A. & Arunachalam, S. (2017). *Using Higher Order Sensitivity Approaches to Assess Aircraft Emissions Impacts on O_3 and $PM_{2.5}$*. Poster session presented at the 2017 Annual CMAS Conference, Chapel Hill, NC.

Outreach Efforts
Presentation at bi-annual ASCENT stakeholder meetings in Spring and Fall 2017, Alexandria, VA.
Presentation to FAA and investigators during monthly Tools telecons
Presentation to New York City Metro Area Energy and Air Quality Data Gaps Workshop, organized by NYSERDA, Columbia University, May 2017

Awards
Calvin Arter – 1st prize ASCENT's Joseph A. Hartman Student Paper Competition 2017

Student Involvement
All of the work in the task has been performed by 2nd year PhD student, Calvin Arter

Plans for Next Period
The next steps for this research will be investigating the chemistry surrounding the second order sensitivities with the goal of explaining the nonlinearities we are seeing. This work will then be incorporated into a manuscript with the goal of publication within the next few months.

The HDDM methods will be used for a new modeling platform with a state of the science model. We will utilize the most recent version of CMAQ (v5.2) with HDDM and a model application for the continental U.S. at a 12km x 12km horizontal grid cell resolution, and using 2011 AEDT emission data.

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Models.

Boone, S., & Arunachalam, S. (**2014**). Calculation of sensitivity coefficients for individual airport emissions in the continental U.S. using CMAQ-DDM/PM. In *ACM International Conference Proceeding Series.* [10] Association for Computing Machinery. 10.1145/2616498.2616504

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Task #3: Develop Generalized Gridding Tool for AEDT

Objective(s)

The objective of this task is to develop a generalized emissions gridding processor that can take AEDT chorded outputs and create inputs for any global or regional-scale model.

Research Approach

Introduction

The Federal Aviation Administration (FAA)'s Aviation Environmental Design Tool (AEDT) is a software system that dynamically models aircraft performance in space and time to produce fuel burn, emissions and noise. Full flight gate-to-gate analyses are possible for study sizes ranging from a single flight at an airport to scenarios at the regional, national, and global levels. AEDT is currently used by the FAA to consider the interdependencies between aircraft-related fuel burn, noise and emissions. Currently, AEDT outputs are used by multiple regional-scales and additional global air quality and climate models for various purposes. However, the process to take the AEDT outputs and grid them to the model's native resolution is not streamlined. In many cases, different modeling groups develop their own custom approach and "reinvent the wheel" that leads to inconsistency in methods.

To address this concern, the FAA has identified a need to develop a generalized emissions gridding processor that can process the Aviation Environmental Design Tool (AEDT) emissions to meet the needs of multiple models, including and not limited to CMAQ, GEOS-Chem, CAM5, CAMChem, MOZART, GOCART, NASA GISS-E, etc. Ideally, the generalized gridding processor should process the AEDT emissions for uniformly structured as well as unstructured variable grid models. It will process the AEDT segment level aircraft emissions data in dimension of x, y, z, and t, and assign the emissions to any types of modeling grid structures. It has the ability to grid emissions at various spatial resolutions from global to local, to temporally allocate emissions for variable time steps, and to chemically speciate emissions for various modeling platforms. FAA has informed us that the current gridding processor developed by the U.S. DOT's Volpe Center does not meet these specifications, and that it requires many duplicated intermediate output dataset files such as ASCII-formatted segmented aircraft emissions from AEDT Microsoft SQL Databases (DBs) to support various modeling platforms.

Objective

The overall objective of this task is to develop a generalized emissions gridding processor that can support all the specifications desired by FAA without compromising the computational speed and processing efforts. In 2012, UNC-IE developed the AEDT gridding processor called AEDTproc to process the segmented aircraft emissions from AEDT for use in CMAQ, the regional-scale air quality model used in various other FAA projects. AEDTProc has the capability to process emissions only during Landing and Takeoff (LTO), during cruise, etc. for a custom CMAQ modeling domain. UNC-IE will update/enhance the latest AEDTproc program to expand its capabilities beyond current CMAQ modeling needs, and to meet the needs of various regional and global-scale air quality and climate models. The enhancements for AEDTproc for Version 2 (AEDTProc V2 hereafter) include the following:

- Support various modeling projections (i.e., Latitude-Longitude, Polar Stereographic, Lambert Conformal, Mercator, UTM, etc.)
- Support structured (uniform) and variable (non-uniform) modeling grids
- Support altitude-based vertical coordinates layer structure
- Support multiple scale modeling domains (i.e., global, regional, and local scales)
- Support various temporal resolutions (i.e., hourly, daily, weekly, monthly, and so on)
- Support multiple chemical mechanisms (mole-based and mass-based emissions), along with using the FAA/EPA TOG speciation profile
- Support direct access AEDT segment level aircraft emissions from Microsoft SQL server
- Enable to read in the NetCDF format emissions and export the output data in NetCDF Climate and Forecast (CF) compliance format to support various air quality and climate models
- Optimization of AEDTproc to reduce the memory usage as well as the computational time
- Parallelization of AEDTproc Fortran code to take advantage of multiple processors on the servers
- Support of AEDTproc to run on both Linux OS and Windows OS platforms

Approach

To implement all of these capabilities into current AEDTproc, we divided the task into three stages.

<u>Stage 1:</u> First, we implemented the most of technical enhancements, such as multi-scale modeling domains, various map projections, structured/unstructured grids, various chemical mechanisms, various temporal allocations, and optimization and parallelization into the latest Linux-based AEDTproc program.

Stage 2: Second, we implemented the direct accessibility to Microsoft SQL Server on Windows OS into Linux-based AEDTproc to avoid generating any unnecessary intermediate output files from SQL databases prior to the AEDTproc runs.
Stage 3: In the third and final stage, we developed the Windows-based AEDTproc that can directly access MS SQL AEDT DBs on Window OS.

With all three stages completed, FAA or others users can run AEDTproc program on Windows OS machine to generate temporally/chemically/spatially allocated AEDT emissions to support various modeling platforms without generating external segment-level aircraft AEDT emissions files. During each stage of the AEDTproc development, we performed testing with various use cases provided that were identified (which include models with both structured and unstructured grids) along with implementing various QA procedures. The specific use cases we tested were:

- Models with structured grids: e.g. GEOS-Chem for global and CMAQ for regional to hemispheric scales.
- Models with unstructured grids: e.g. Model for Prediction Across Scales (MPAS) [See https://mpas-dev.github.io/ for more information]. The U.S. EPA is developing a Next Generation Model for Air Quality, that will use MPAS as the meteorological driver, and that will provide the horizontal and vertical grid structure.

The latest version of Linux-based AEDTproc has been developed to process only ASCII-formatted segmented AEDT aircraft emissions to create hourly gridded speciated emissions for CMAQ modeling runs. It obtains the modeling grid domain information (x, y, z), and temporal resolution (t) through MCIP (Meteorology-Chemical Interface Processor) meteorology input file for CMAQ model. So, the current version reads the MCIP outputs in NetCDF formats and the text-based AEDT segmented data, and outputs NetCDF format emissions file that can be directly read by CMAQ.

In the following sections, we describe the detailed methods UNC-IE used for the AEDTproc enhancements.

Stage 1: AEDTproc Enhancements on Linux OS
Prior to any development of AEDTproc on direct access to Microsoft SQL Server, UNC focused on implementing all the following specifications into our latest Linux-based AEDTproc program.

1) Various Input/output Format Support

Depending on the formats of three use case emissions input files, we updated AEDTproc program to read accordingly and output the results in NetCDF CF-compliant format to support various modeling platforms other than CMAQ model. Unlike CMAQ, GEOS-Chem, MOZART, and CAM-Chem are global 3-D chemical transport models (CTM) for atmospheric composition driven by meteorological inputs from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling Assimilation Office (GMAO). The GEOS-Chem option will be used for all of the global 3-D models. To create the global CTMs-ready 3-D aircraft emissions file, a user needs to provide the NetCDF-formatted GEOS meteorological input data file to the AEDTPROC program.

2) Various Map Projections Support

Although AEDTproc has been fully tested to support Lambert conformal, Universal Transverse Mercator (UTM), and Latitude/Longitude projections, it has not been applied to other map projections like polar stereographic and Mercator. To support these other projections, UNC-IE obtained polar stereographic and Mercator projection-based CMAQ input file for this update in AEDTproc.

3) Various Output Temporal Resolution Support

As mentioned earlier, current AEDTproc output temporal resolution is based on temporal resolution in MCIP input file. In this update, we updated AEDTproc for users to define their own temporal resolution of output emission values (i.e., hourly, daily, weekly, and so on) to support various modeling platforms.

4) Various Chemical Speciation Allocation Support

We updated AEDTproc to support more than CMAQ-ready chemical speciation profiles (such as Carbon Bond 2005) to support other regional or global-scale models. For CMAQ, the speciation profile is based upon the FAA-EPA Total Organic Gases (TOG) speciation profile developed in 2009 (U.S. EPA, 2009). The tool is now designed to read a specific input list of chemical species and the associated mass fractions as a stand-alone text input file. It then reads the input VOC emissions from AEDT, converts to TOG and then speciates based on the assigned mass fractions, thus providing complete flexibility to the user depending on the modeling system.

5) Unstructured Modeling Grid Support

We implemented this feature into AEDTproc to support unstructured/variable grids, specifically based on the MPAS file structure. This is a significant update to AEDTproc's capability to read and grid unstructured grids, as opposed to uniform grids. The defining features of MPAS are the unstructured Voronoi meshes and C-grid discretization which are used as the basis for many of the model components. The unstructured Voronoi meshes, formally Spherical Centroidal Voronoi Tesselations (SCVTs), allow for both quasi-uniform discretization of the sphere and local refinement. Figure 21 shows an example of horizontal and unstructured grids that are used by CMAQ and MPAS respectively.

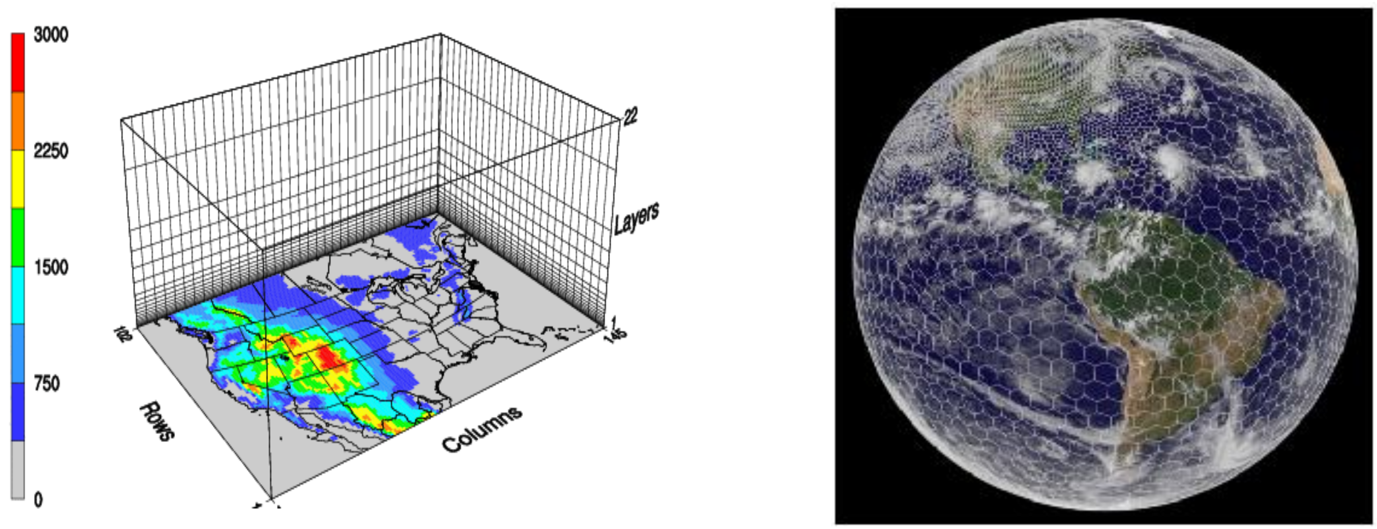

Figure 21 - Uniform horizontal grid structure (left) and unstructured grid structure (right) [Right figure courtesy NCAR]

Stage 2: Linux-based AEDTproc Direct access MS SQL on Windows OS

Once Linux-based AEDTproc development in Stage 1 was completed, UNC added a critical new feature in this task, which allows AEDTproc direct access to Microsoft SQL server to extract AEDT segment-level aircraft emissions directly from the SQL database. This will eliminate the preprocessing steps in current approach, which generates the ASCII-formatted segment-level aircraft emissions AEDT model using the FAA's Power Shell scripts prior to AEDTproc runs. These scripts read the AEDT SQL database, and output ASCII files to be read by AEDTProc.

Because the MS SQL Server that holds AEDT segment-level aircraft emissions is installed on Windows OS, two additional drivers for Fortran-based AEDTproc program are required to directly connect to MS SQL server. Figure 22 shows the schematic of this approach between two different OS (Linux and Windows). First, one needs to install the open source Fortran ODBC driver, called FLIB. FLIB allows Fortran compiled program to directly access standard SQL DBs using ODBC (Open Database Connectivity) which is a standard programming language middleware application programming interface (API). However, since MS SQL Server is not compatible with ODBC, we installed the ODBC driver for MS SQL server on RedHat Linux OS developed by Microsoft. This driver allows FLIB library to directly access MS SQL AEDT DBs through ODBC.

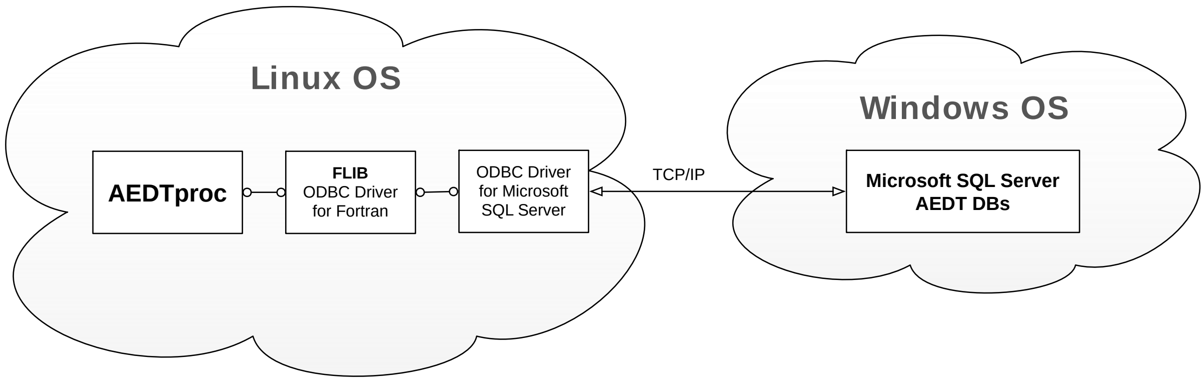

Figure 22 - Schematic of Connectivity between AEDTproc on Linux OS and MS SQL Server on Windows OS

Stage 3: AEDTproc direct access MS SQL on Windows OS

Once the stage 2 work was completed, the UNC team compiled the updated AEDTproc program on Windows OS with windows-based Fortran compiler using Cygwin that provides similar functionalities and environment of Linux on Windows OS. Unlike Stage 2, AEDTproc program now runs on the same Windows OS where MS SQL Server is installed. Based on our testing, we did see some level of computational speed-up due to a faster connectivity between ODBC driver and MS SQL Server.

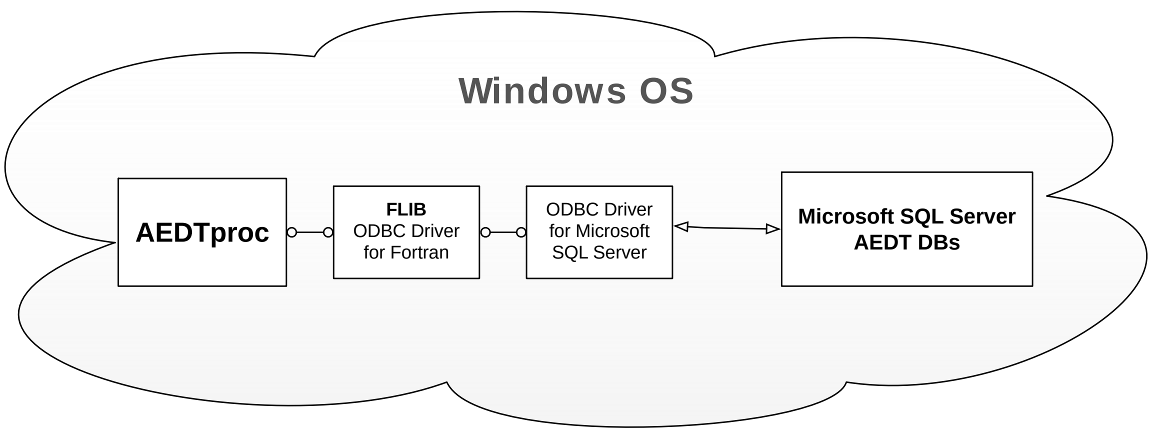

Figure 23 - Schematic of Connectivity between AEDTproc and MS SQL Server on Windows OS

Results

AEDTProc for GEOS-5 gridding

To perform emissions magnitudes QA, UNC-IE first used AEDTProcv2 to grid for a global domain using GEOS-5 meteorology, and then windowed for the continental U.S. We then compared aircraft emissions for a single day in 2011 January 2 generated using AEDTProc v2 with GEOS-5 to the data generated using AEDTProc v2 with MCIP for CONUS total (Table 8). Overall, differences between these two versions are relatively low (up to 11%), and are likely explained by small differences in the domain extents as well as different assumptions in vertical grid structure between the two models.

Table 8 - Differences in CONUS aircraft emissions for 20110102 using GEOS-5 (AEDTProc V2) and MCIP (AEDTProc) V1)

	(AEDTProc V2 for 2011 GOES5 – AEDTProc V1 for 2011 MCIP)/AEDTProc V2 for 2011 MCIP (%)
CO	-11
NO	-3.7
SO2	-8.8
Black carbon	-9.0

AEDTProc for CMAQ gridding: UNC-IE tested AEDTProcv2 versus AEDTProcv1 for one day's worth of AEDT flight data. Domain emission mass totals generated by AEDTProcv2 are comparable to emissions generated from the same day's worth of AEDT data with AEDTProcv1. Figure 24 shows the emissions as a function of model layer for AEDTProcv2 and two different versions of AEDTProcv1 (one version has a correction to the POC/PEC allocation). The results are quite comparable across the two versions.

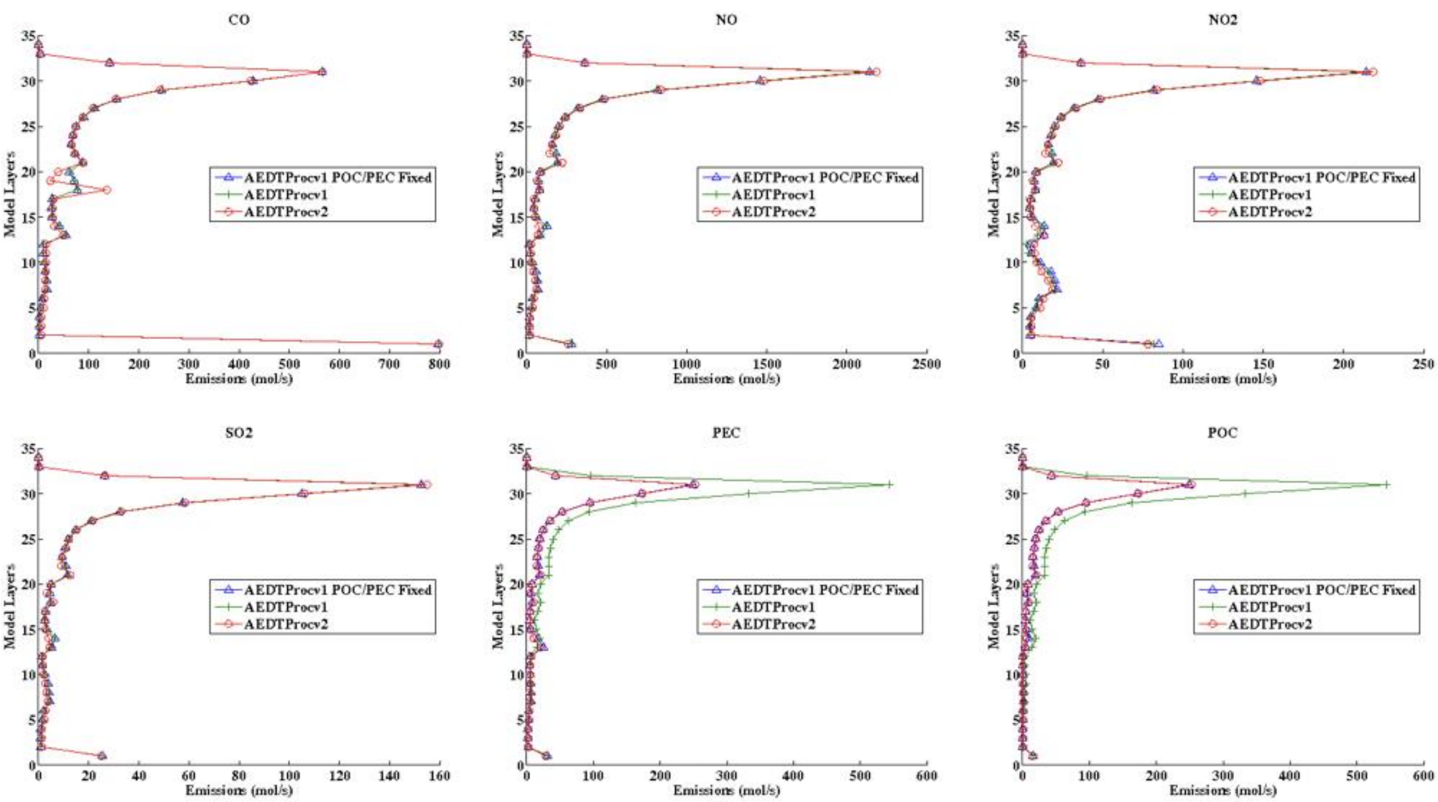

Figure 24 - Vertical profiles for CO, NO, NO_2, SO_2, POC, and PEC emissions from one day's worth of full flight emissions

Milestone(s)
AEDTProcv2 enhanced to support additional features
AEDTProcv2 support now includes both structured and unstructured grids
AEDTProc v2 now can read SQL database directly from AEDT and create gridded emission files for regional-scale and global-scale air quality models.
User's Guide and Demonstration given to the FAA AEE

Major Accomplishments
UNC-IE developed AEDTProc V2 with several substantial enhancements as initially scoped, and delivered tool, user's guide and demonstration to the FAA AEE.

Publications
None

Outreach Efforts
Presentation at bi-annual ASCENT stakeholder meetings in Spring and Fall 2017, Alexandria, VA.

Awards
None

Student Involvement
Calvin Arter, 2nd year Ph.D. student played a key role in testing AEDTProcv2 for CMAQ domain, and performing various QA steps.

Plans for Next Period
None

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Task #4: Provide Support for High Fidelity Weather in AEDT

Objective(s)
The objectives of this task are to assist U.S. DOT Volpe Center to modify AEDT to use appropriate high fidelity weather data, such as from NASA's MERRA or MERRA-2, and to modify AEDT to directly use outputs from the Weather Research Forecast (WRF) model.

Research Approach
In this continuation task from last year, UNC-IE assisted FAA contractor 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, we worked with U.S. DOT's Volpe Center (and ATAC) 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 also recommended that

FAA move to MERRA-2. UNC-IE continued to engage with NASA developers as necessary and assisted Volpe in developing and implementing the prototype tool for use in AEDT. In addition to using MERRA-2, we also assisted Volpe to adapt AEDT to process higher resolution meteorological fields from the Weather Research and Forecast (WRF) model. WRF is a limited-area model typically used to prescribe meteorology for CMAQ – the regional scale air quality model that UNC-IE has used for several years in support of FAA's PARTNER and ASCENT COE-related research, and other ongoing activities.

Through these enhancements in AEDT, we aim to achieve the following:

a) Consistent large-scale forcings from MERRA used to drive both global-scale (and sometimes regional-scale) air quality applications and emissions estimation from AEDT
b) Consistent regional-scale forcings from WRF used to drive regional-scale air quality applications and emissions estimation from 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

Milestone(s)
AEDT enhanced to process high fidelity weather from MERRA-2
AEDT enhanced to process high fidelity weather from WRF for limited-area regional scale applications.

Major Accomplishments
UNC-IE assisted FAA/Volpe Center to use high fidelity weather from a new global reanalysis product (MERRA-2) or prognostic model (WRF) for the AEDT calculations. This was summarized in two reports that were led by the Volpe Center.

Publications
Volpe Reports 1 and 2 for MERRA and WRF

Outreach Efforts
Presentation at bi-annual ASCENT stakeholder meetings in Spring and Fall 2017, Alexandria, VA.
Presentation to FAA and investigators during monthly Tools telecons.

Awards
None

Student Involvement
None

Plans for Next Period
None

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Task #5: Explore Collaboration with NAU, Ukraine

Objective(s)

To explore collaboration with the National Aviation University of Ukraine for local-scale air quality models in support of the nVPM standard.

Research Approach

The National Aviation University of Ukraine in Kyiv has historically performed research related to aviation noise, emissions and operations. FAA identified a need for ASCENT investigators to participate in a technical exchange and reciprocal site visit with NAU. The purpose of the technical exchange and site visit was to continue to discuss the participation of NAU in ASCENT Center of Excellence research, related research, and to assess NAU capabilities.

During a 2.5-day period in July 2017, Dr. Sarav Arunachalam of the University of North Carolina (UNC) and Dr. Vic Sparrow of the Pennsylvania State University (PSU) participated in a technical exchange and site visit with National Aviation University (NAU) of Ukraine in Kyiv. In return, Dr. Kateryna Synylo of NAU visited UNC Chapel Hill during a 10-day visit in October 2017.

From ASCENT 19's perspective, the closest area of interest for collaboration with NAU was the PolEmiCa local-scale dispersion model developed and applied by NAU for several case studies. NAU has applied PolEmiCa for the CAEPport database maintained by the ICAO-CAEP, and submitted model evaluation white papers to the CAEP Modeling and Database Task Force.

PolEmiCa model is based upon OND-86. It has similarities to the AERMOD code in the U.S. However it is antiquated since being first published by Berland in 1987. It is a diffusion equation solution which can determine plume rise, etc. One interesting addition in recent research is to include wing-tip vortices in the distribution of PM. This is a natural methodology for aircraft emissions inventory and it uses a large eddy simulation using the FLUENT CFD code. Recently, NAU conducted a measurement campaign at the Kyiv Borispol airport, and where they compared PolEmiCa output with real airport operations from Ukraine-Germany cooperation (with the University of Wuppertal) during 2012. There they made measurements at moveable stations and found higher NOx at takeoff compared to landing. This is where they noticed a difference in the modeling and experimental data regarding whether they included the wing-tip vortices or not. NAU is planning another field campaign in the Kyiv Zhulyany airport, and UNC-IE provided some inputs for parameters to be measured during this campaign.

During Dr. Arunachala's visit to NAU, he presented a summary of emissions and air quality related research in UNC and ASCENT and toured the NAU facilities which included a fuel testing lab, ICAO training facility for airport operators on safety issues, large hangar with multiple aircraft and helicopters, and worked with NAU researchers to understand the PolEmiCa model and its features.

During Dr. Synylo's visit to UNC, she presented the PolEmiCa model at the 16th Annual CMAS conference in Chapel Hill, and worked with the UNC-IE team to explore how to adapt the PolEmiCa model to apply for the Los Angeles Airport Air Quality Source Apportionment Study (LAX AQSAS). UNC-IE has shared these datasets with NAU.

Milestone(s)

Site visit by UNC to NAU in July 2017
Reciprocal site visit by NAU to UNC in October 2017

Major Accomplishments

Through multiple telecons and the two site visits, UNC has an understanding of the NAU's capabilities in local-scale dispersion modeling.

Publications
None

Outreach Efforts
Presentation at bi-annual ASCENT stakeholder meetings in Spring and Fall 2017, Alexandria, VA.
Presentation at NAU on ASCENT research during site visit in July 2017.

Awards
None

Student Involvement
None

Plans for Next Period
None

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