Project 019 Development of Aviation Air Quality Tools for Airport-Specific Impact Assessment: Air Quality Modeling

University of North Carolina at Chapel Hill

Project Lead Investigator

Saravanan Arunachalam, Ph.D.
Research Associate Professor
Institute for the Environment
University of North Carolina at Chapel Hill
100 Europa Drive, Suite 490
Chapel Hill, NC 27517
919-966-2126
sarav@email.unc.edu

University Participants

University of North Carolina at Chapel Hill

- PI: Saravanan Arunachalam, Research Associate Professor
- FAA Award Number: 13-C-AJFE-UNC Amendments 1 - 3
- Period of Performance: September 13, 2013 – December 31, 2015
- 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. Consult with FAA and the ACCRI team of investigators to assess the surface air quality impacts of aircraft emissions during cruise mode.
    4. Develop High Fidelity Weather for Global Inventories using AEDT

Project Funding Level

$325,614

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

Investigation Team

Prof. Saravanan Arunachalam (UNC) (Principal Investigator) [Tasks 1-4]
Dr. Matt Woody (UNC) (Co-Investigator) [Tasks 1, 2]
Dr. Jared Bowden (UNC) (Co-Investigator) [Tasks 1, 4]
Dr. Mohammad Omary (UNC) (Co-Investigator) [Tasks 1, 4]
Mr. Alejandro Valencia (UNC) (Co-Investigator) [Task 1]
Ms. Pradeepa Vennam (UNC) (Graduate Research Assistant) [Task 1, 3]
Mr. Scott Boone (UNC) (Graduate Research Assistant) [Task 2]

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 EPA (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 PM2.5, 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. 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 Destination 2025 Air Quality Modeling Platform, for year-over-year modeling to achieve air quality (and health) goals.
2. Extend prototype modeling for CMAQ-DDM-3D to compute Airport-specific Sensitivities for the year 2005, and explore possibilities to extrapolate for a future year.

[1] Boeing Commercial Airplane Market Analysis, 2010.

3. Consult with FAA and the ACCRI team of investigators (MIT, Stanford, NCAR, Yale, NASA-Goddard and University of Illinois at Urbana Champaign) to assess the surface air quality impacts of aircraft emissions during cruise mode.
4. Develop high fidelity weather based 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 modeling platform using state-of-the-art tools such as WRF-SMOKE-CMAQ and assess efficacy of multiple emissions scenarios to achieve air quality (and health) goals under FAA's Policy initiatives.

Research Approach

The research approach for this task involved using three models, i.e., the Weather Research Forecast (WRF) model (for meteorology), Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (for emissions) and the Community Multiscale Air Quality (CMAQ) model to study US-wide aviation impacts on air quality for multiple years. Figure 1.1 shows the flow chart and the data used to run all three models. Here, we describe the updates incorporated in the methodology during our second round of modeling, after the project transitioned from PARTNER to ASCENT.

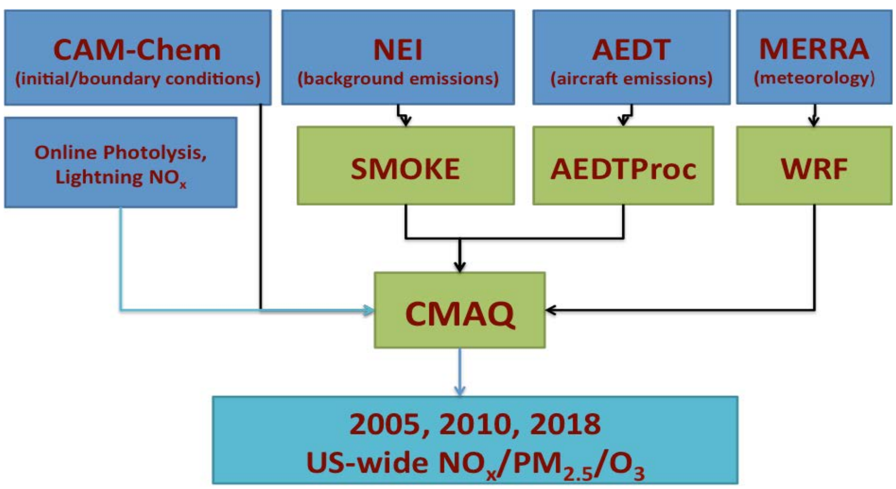


Figure 1.1: Flowchart representing the modeling methodology platform.

Meteorological Modeling

This research began with a review of global atmospheric datasets that can be used with the Weather Research and Forecasting Model (WRF) in near real-time for D2025 modeling efforts. Third generation reanalysis products provide significant improvements in both the data assimilation and temporal/spatial resolution and should be used for future modeling efforts. These datasets include:

- Climate Forecast System Reanalysis (CFSR),
- 40-yr ECMWF Re-Analysis (ERA-40),
- ECMWF Interim Re-Analysis (ERA-Interim),
- Japanese 25-year Reanalysis (JRA-25), and
- Modern Era Retrospective-Analysis for Research and Applications (MERRA).

At the time of selection, comparisons of these datasets were in their infancy, and MERRA was selected based on both data availability and discussion from prior studies (e.g. see special issue in Journal of Climate; http://journals.ametsoc.org/page/MERRA).

MERRA is a state-of-the-art global reanalysis dataset with a frozen data assimilation system. The data assimilation is frozen because MERRA is intended to provide a reanalysis dataset for climatological studies aimed to improve the representation of the hydrologic cycle. MERRA uses the GEOS-5 atmospheric general circulation model (AGCM) with a horizontal grid resolution of 0.5 deg. x 0.67 deg. with 72 vertical levels extending to 0.01hPa. A catchment-based land-surface model is used over more traditional regular latitude-longitude grids. A three-dimensional data assimilation algorithm called the Gridpoint Statistical Interpolator with an incremental analysis update is used to minimize the shock of the observation input. MERRA uses conventional observations, such as radiosondes and surface land observations, in addition to radiance data from many operational and research satellites.

A Fortran program, MERRA2WRF, is used to process the MERRA dataset into “WPS intermediate format”, a big-endian binary format used by the Weather Research and Forecasting Preprocessing System (WPS). WPS is responsible for collecting meteorological files needed as initial and later boundary conditions in the WRF model. The Fortran program can be downloaded from https://modelingguru.nasa.gov/docs/DOC-2242. The program requires the standard Unix ‘make’ program, plus a Fortran compiler (Intel’s ifort is recommended). In addition, the following third-party libraries are required, which must be built and installed using the same compiler (NETCDF, HDF4, JPEG, ZLIB, SZIP, HDF5).

When using MERRA2WRF, the following files and variables must be downloaded

1. Static fields (surface geopotential; lake and ocean fraction)
2. Instantaneous atmospheric fields (surface pressure, sea level pressure, temperature, winds, specific humidity, skin temperature, sea ice fraction).

An important caveat when using MERRA is that it does not process any soil data (temperatures, moisture), as the land surface model used with MERRA is not used by WRF. Soil conditions from the Global Forecast System are used as a substitute. The GFS soil fields are processed using a separate Vtable for soil temperature and moisture fields.

Numerous annual simulations were run to downscale MERRA to a 36-km horizontal resolution over the CONUS using WRF. These tests included using various physics options and nudging strategies, some of which became available with recent releases of WRF. Some of these tests improve near surface fields that are important for air quality modeling. They include recent advancements to the representation of sub-grid clouds and radiation feedbacks within the cumulus parameterization scheme and the treatment of lake temperatures using a mass and energy balance model.

Annual simulations were completed using WRF version 3.6.1 for 2005, 2010, and 2013 to support this task for ASCENT. The WRF configuration includes the Kain-Fritsch cumulus parameterization with modification for sub-grid cloud radiation feedback, lake treatment using the Community Land Model (CLM) lake module, Rapid Radiative Transfer for longwave and shortwave radiation (RRTMG), Noah land surface model, and Yonsei University (YSU) Planetary Boundary Layer. A 12-month spin-up period is used for each of these annual simulations and allows the atmosphere and lake surface temperatures to come into equilibrium.

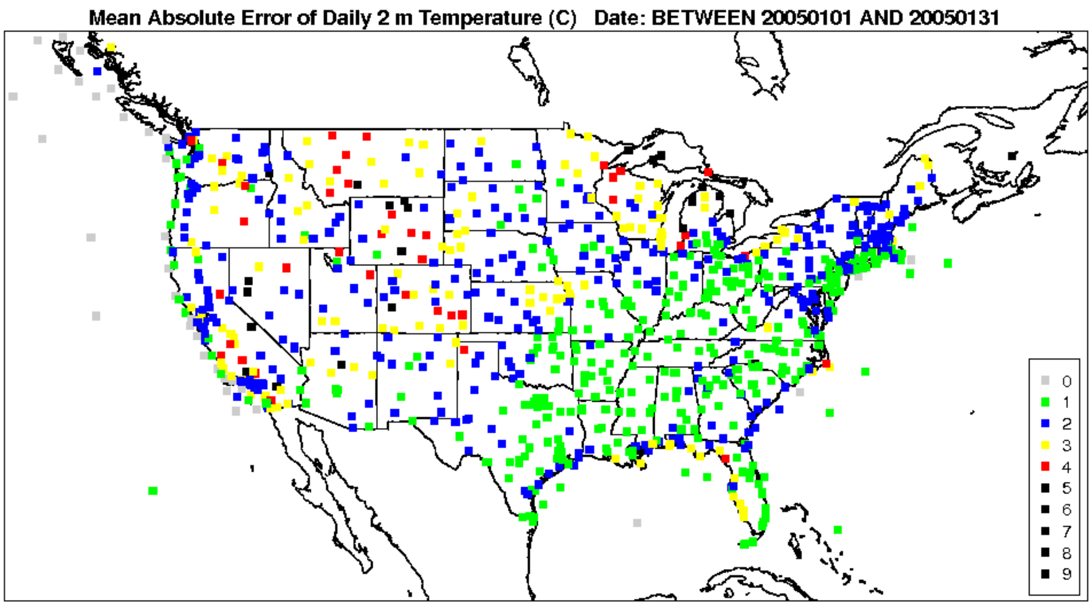
The meteorological model evaluation here focuses on temperature, precipitation, wind speed and direction for the 2005 annual simulation. Similar conclusions can be drawn for the additional years. A quantitative analysis for mean daily temperature is performed and compared against the observed National Oceanic and Atmospheric Administration (NOAA) Earth System Research Laboratory (ESRL) Meteorological Assimilation Data Ingest System (MADIS). We also use a qualitative approach to compare the model-estimated total monthly precipitation with the monthly Parameter-elevation Relationships on Independent Slopes Model (PRISM) precipitation.

Figure 1.2 compares January and July 2005 mean absolute error of daily 2-m temperature. The mean absolute error is typically less than 2˚C, with exceptions for the complex terrain over the intermountain West in some locations near the Great Lakes during the winter. The larger errors are likely a result of the limitation of the horizontal resolution and resolving sharp gradients in terrain and land-water interface. Figure 1.3 is the daily temperature error and bias average for each month over the CONUS. Most months have a slight cold bias (<1˚C) with a mean error between 2˚C-3˚C. The error and bias falls within the statistical benchmark suggested for meteorological modeling for air quality of ±1.0˚C for bias and 3.0˚C for error (McNally, 2009).[2]

Figure 1.4 is a comparison of PRISM monthly accumulated precipitation to the WRF-simulated precipitation. In both January and July, the WRF-simulated precipitation closely matches the PRISM observations throughout the CONUS. During the summer, there is a tendency to overestimate precipitation during July over the southeast US. The summer months are also when the mean absolute error and bias are largest on average for the CONUS (not shown). However, the error and bias of the 2-m mixing ratio during the summer months is within the suggested benchmark of 2 g/kg and 1 g/kg, respectively.

Figure 1.5 is the daily wind speed and direction error and bias average for each month over the CONUS. The root mean square error for wind speed in January and July, Figure 4, is largest in areas of complex terrain and near land-water boundaries. With exception of these locations, error is generally smaller than the recommended benchmark of 2 m/s. However, we find wind direction has the largest error and is the least reliable field evaluated. The average wind direction root mean square error is between 51–63 degrees for all months across the CONUS and typically larger than the wind direction error metric of 55 degrees. Despite the poorer performance for wind direction, the overall evaluation indicates the WRF-MERRA simulation provides reliable meteorology to support air quality modeling.

[2] McNally, D. E., 2009. “12km MM5 Performance Goals.” Presentation to the Ad-hoc Meteorology Group. 25-June, http://www.epa.gov/scram001/adhoc/mcnally2009.pdf.



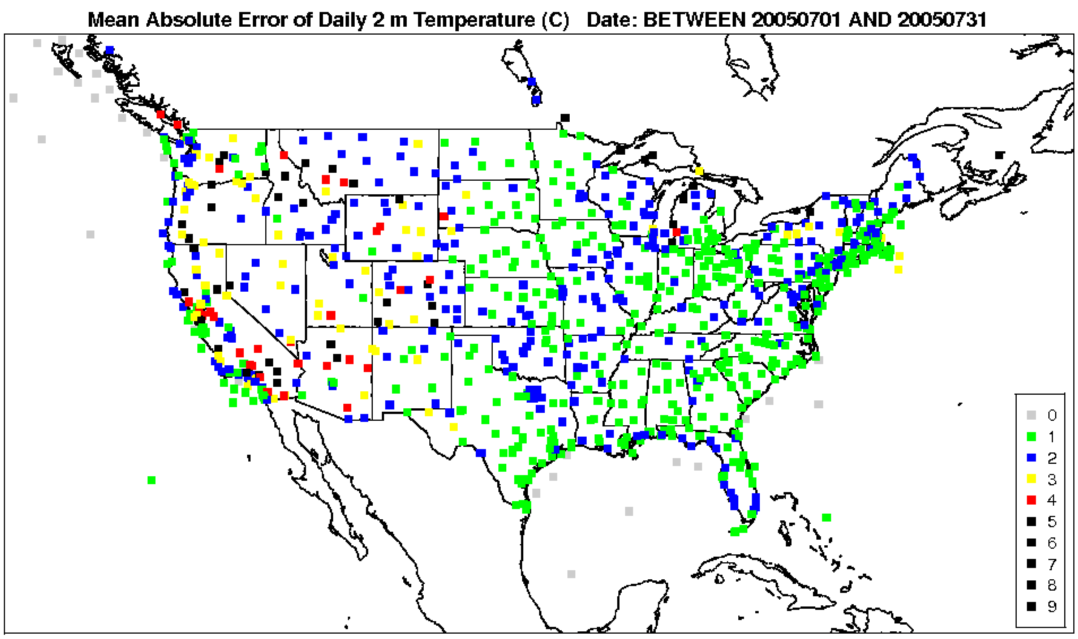


Figure 1.2: Mean absolute error of daily 2-m temperature (°C) for January (top) and July (bottom) 2005.

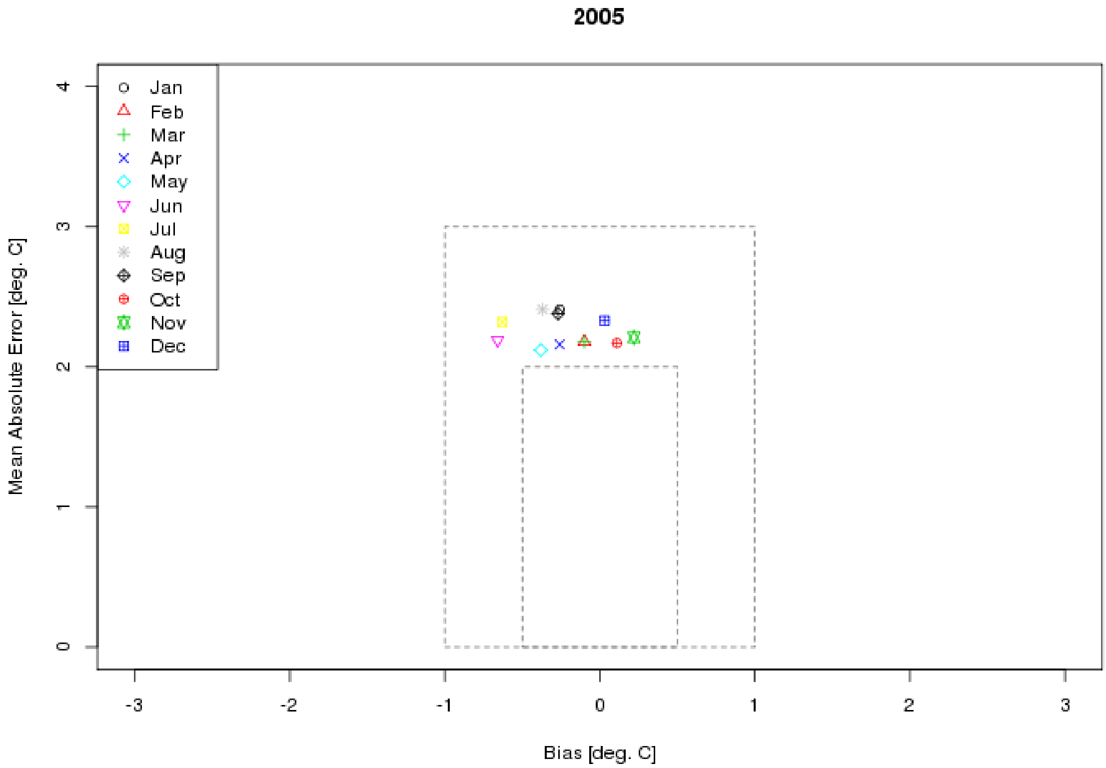


Figure 1.3: Mean absolute error and bias of daily 2-m temperature (˚C) with benchmark metrics.

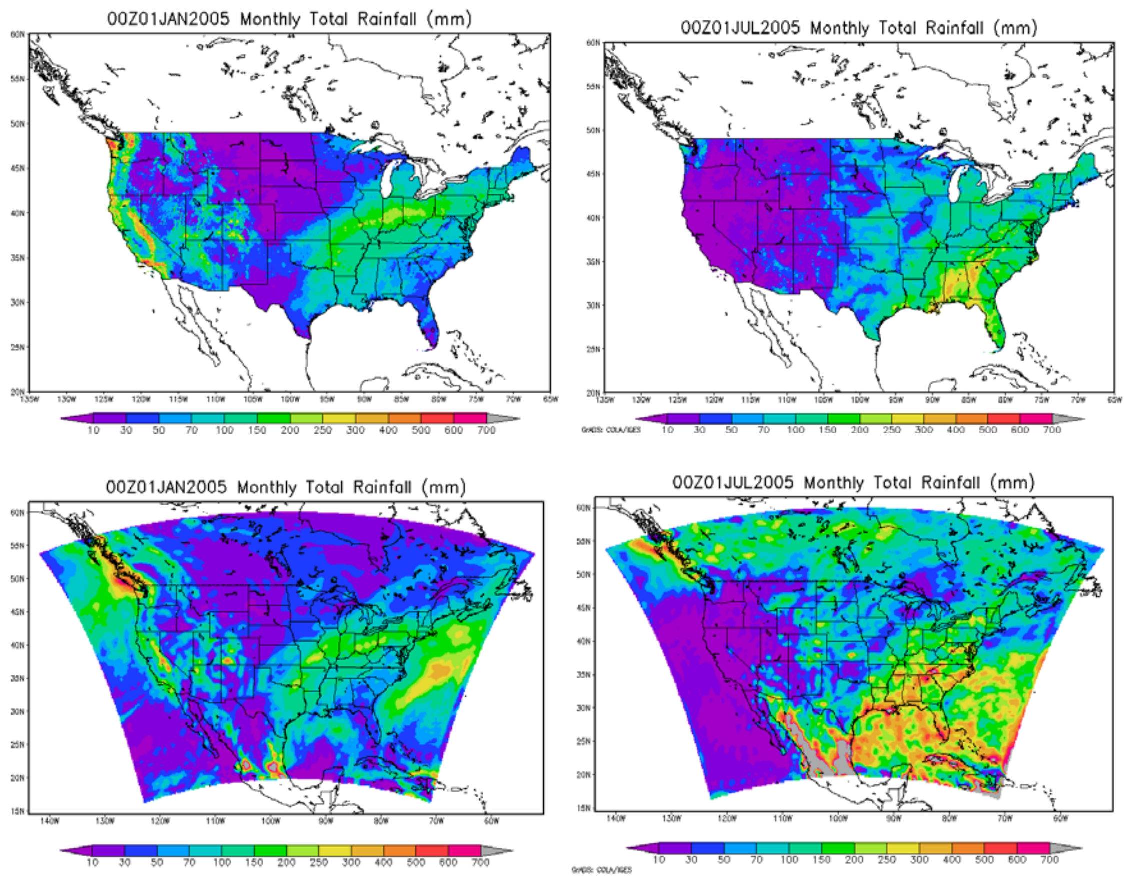
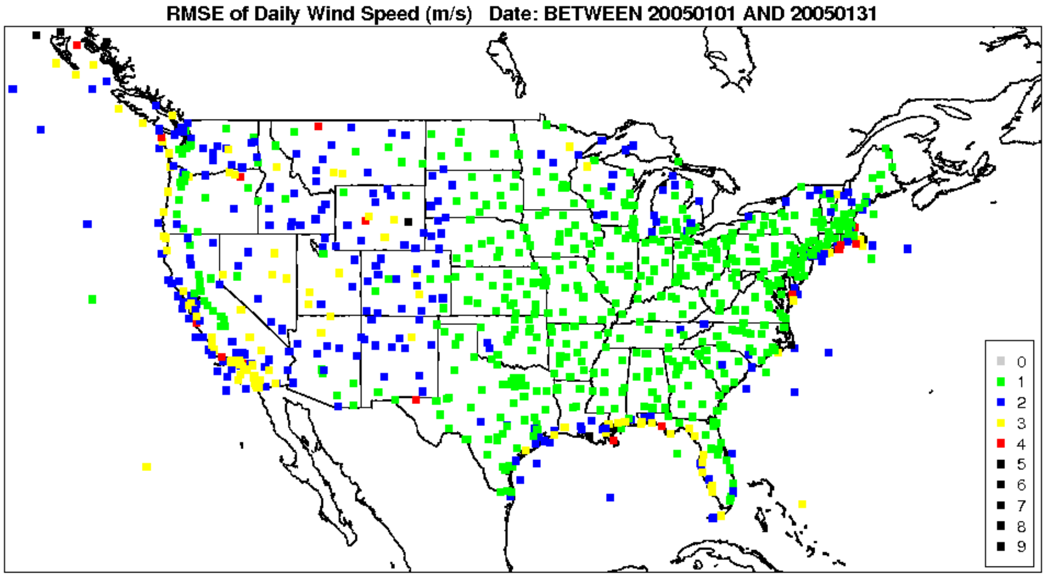


Figure 1.4: Accumulated monthly precipitation for January (left) and July (right) 2005.
PRISM is on top and WRF simulation is on the bottom.



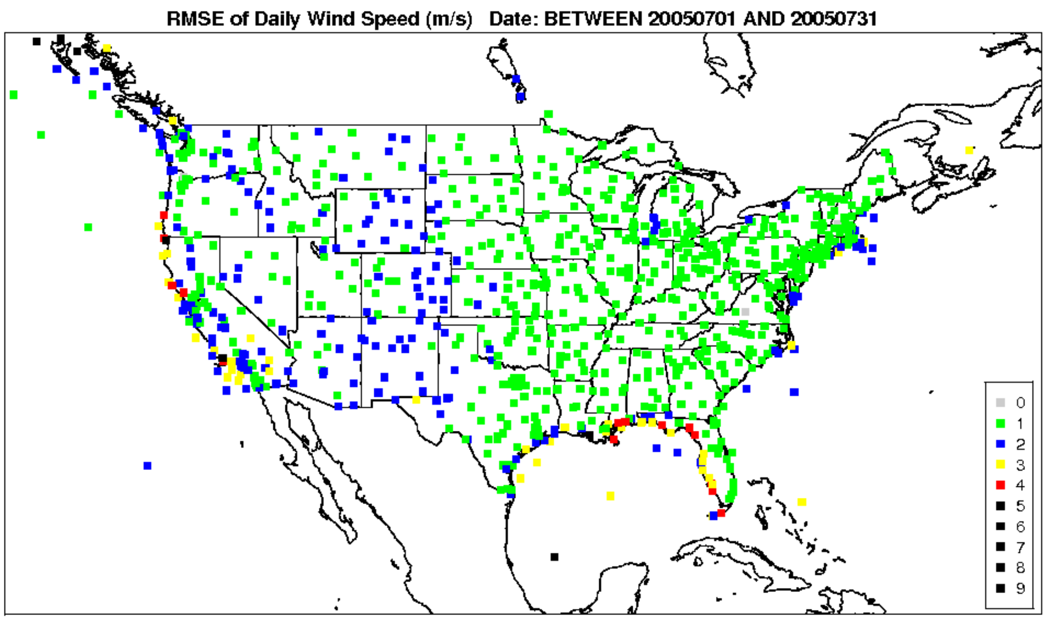


Figure 1.5: Root mean square error of daily wind speed (m/s) for January (top) and July (bottom) 2005.

1) **Emissions:**
   a) **Background:** In our previous modeling, we used the NEIv05_4.2 version for 2005 background emissions. In these new simulations, we are using the latest NEIv05_4.3 emissions, subsequently released by the US EPA. Major changes in these new background emissions were observed mainly in the on-road and non-road sectors. The 2010 emissions were based upon an interpolation of the 2008 and 2013 future year projection years available at that time.
   b) **Lightning NOx:** Based upon prior sensitivity modeling of lightning NOx (LNOx) emissions, we found some issues with a mismatch of emissions layers processing due to a bug in CMAQ. While background emissions and aircraft emissions (from LTO) are only within the planetary boundary layer (lowest 3 km of the atmosphere), lightning

NOx emissions are typically distributed through the entire model column. We developed a fix for this problem in our prior efforts, and will continue to use this in the new round of modeling.

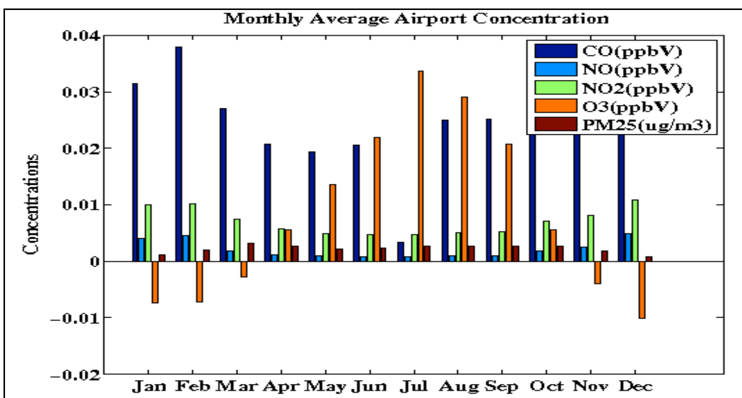
CMAQv5.0.1/5.0.2 takes National Lightning Detection Network (NLDN) based flash count observational data and allocates emissions based on convective precipitation. EPA released 2011-2013 gridded NLDN flash counts for 12km recently; we downloaded the data and regridded them to 36km to use in the present year CMAQ modeling. Regridding was performed using the spatial allocator tool by area weighted average approach. Overall, we have 5 years (2005, 2010, 2011, 2012, 2013) of NLDN data for the 36-km CMAQ domain.

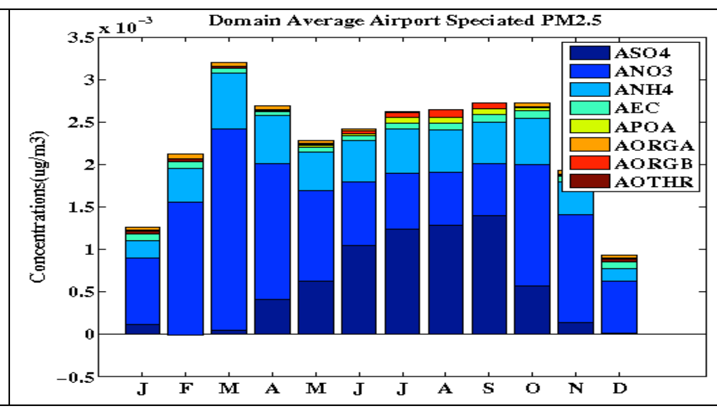
We are also trying to develop a method to calculate LNOx emissions from convective available potential energy (CAPE) based on the recent paper (Romps et al., *Science*, 2014). This approach might be beneficial to use particularly for future year simulations, as we will not have lightning flash rate measurements to generate LNOx emissions. So a simple empirical proxy approach is the suitable way to estimate future year LNOx emissions.

2) **Downscaled Boundary conditions:** We updated CMAQ species mapping with CAM4 (an earlier version) and CAM5 global data and also made new SOA species mapping. As CMAQ needs other SOA species, such as AXYLJ, ATOLJ, ABNZJ, AALKJ, AISO2J, ASQT, and AOLBGJ (xylene, toluene, benzene, alkane, sesquiterpene), we incorporated mapping of these SOA precursor species to the bulk SOA aerosol in the CAM5 model. We obtained CAM5 simulations from collaborators at the University of Illinois at Urbana Champaign (used in the ACCRI modeling) for the years 2005 and 2050 (two alternate emissions scenarios). Using this approach, we downscaled CAM5-based boundary conditions for use in CMAQ. The 2050 BCs will be used to extrapolate from 2005 BCs and create CMAQ inputs for other in-between years such as 2010, 2013, 2018 and 2025.
3) **CMAQ Model:** Previously we used CMAQv5.0.1 to perform 2005 and 2010 annual runs. With the latest release of CMAQv5.0.2 (few updates and corrections made in chemistry and transport algorithms) we built and tested the new v5.0.2. Using this new build, we performed an annual basecase model simulation. For this second round of modeling, we finished annual simulations for the following scenarios:
   - Base05b_KF – CMAQv5.0.1, met update, BC update, without aircraft.
   - Sens05b_KF – CMAQv5.0.1, met update, BC update, without aircraft.
   - Base05c – CMAQv5.0.2, background emissions update, including base05b_KF updates.

Results

Based on the aircraft-attributable concentrations presented in Figure 1.6, overall the US annual aviation perturbation is ~0.02% (max: 0.08%). For NO_2 and $PM_{2.5}$, the US annual aviation perturbation is ~0.25% and ~0.035% (max: 3.72% and 0.26%) in 2005. In 2010 the aircraft-attributable perturbations are similar to 2005 but 2010 shows slight increases in NO_2 (max: 0.02 ppbv) and $PM_{2.5}$ (max: 7.6 ng/m^3) concentrations near airports (based on the spatial plots that are not presented here). From Figure 1.7 we can observe that the maximum hourly O_3 aviation perturbation average is ~0.5ppbV but can also be as high as 2.5ppbV in a few grid cells. In the case of $PM_{2.5}$, maximum aviation perturbation mean is below ~0.5μg/m^3 but it can be as high as 7μg/m^3. The diurnal profile of O_3 shows higher contributions during late evening hours. In the case of $PM_{2.5}$ we are observing a uniform trend throughout the day. We also looked at the number of exceedance events in 2005, as shown in Table 1.1. We note that 735 grid-cells exceed the daily maximum 8-hr O_3 standards and 12 grid-cells exceed the 24-hr average $PM_{2.5}$ standards due to NAS-wide aircraft emissions.





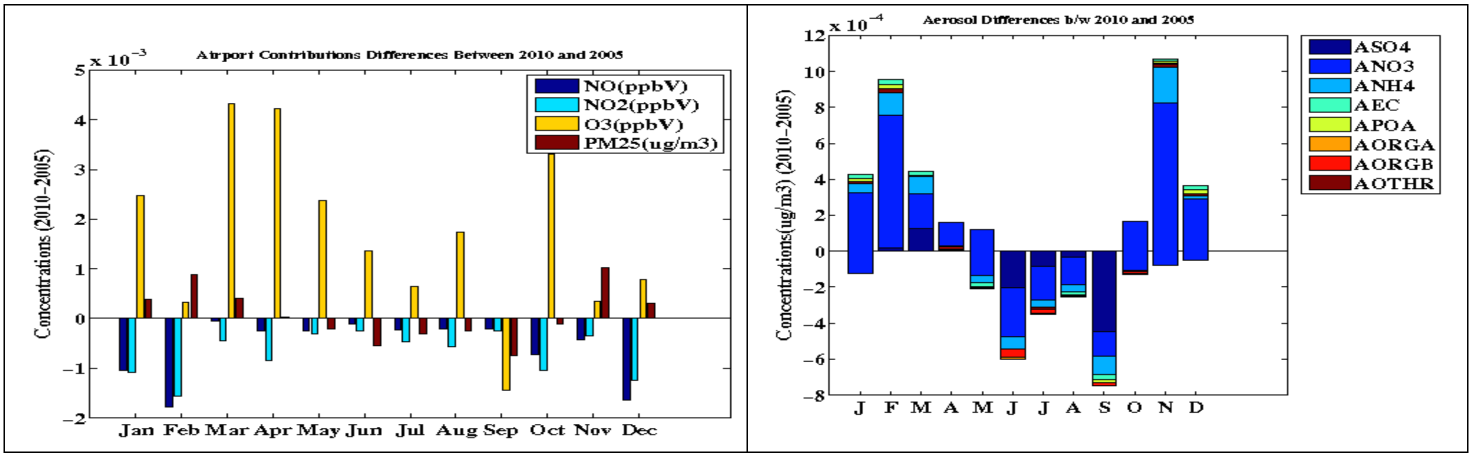


Figure 1.6: Monthly average aircraft-attributable perturbations for key pollutants (top, left), speciated aerosol species (top, right) in 2005, differences between 2010 and 2005 concentrations for key pollutants (bottom, left) and speciated aerosol species (bottom, right).

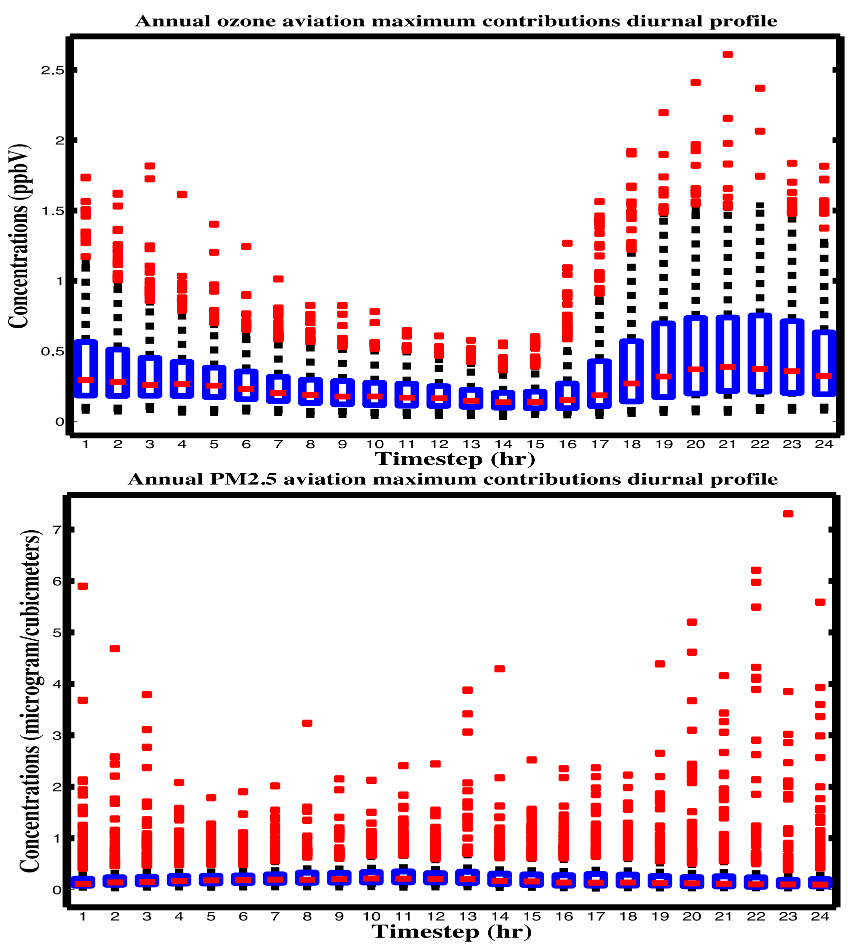


Figure 1.7: Diurnal Profile of maximum aviation contributions of Ozone and $PM_{2.5}$ in 2005.

Table 1.1: NAAQS exceedances for O_3 and $PM_{2.5}$ standards for senscase (with aircraft emissions) and basecase (without aircraft emissions) model scenarios

O3(> 75ppbV (8hrmax))	Sens	Base	NAAQS (8hr max) 75ppbv
Number of exceedances events (grid cells)	65268	64533	
Number of days	235	235	
PM2.5 (> 35ug/m3)			
Number of exceedances events	9123	9111	NAAQS 35 ug/m3
Number of days	289	288	
PM2.5 (annual average)	110	110	NAAQS 12 ug/m3

Based upon discussions with FAA, we will model 4 to 5 specific years to assess aviation-attributable AQ impacts. Possible candidate years are 2005, 2010, 2013, 2018 and 2025. Each year will include a 2-week spin-up period.

Note that the previously modeled 2005 and 2010 emissions from AEDT did not use high fidelity weather in its processing. UNC is assisting Volpe to process AEDT emissions using MERRA-based meteorology. It is anticipated that UNC will get a revised set of AEDT outputs for the proposed modeling years. If AEDT emissions based upon high fidelity are not available in a timely manner, it is anticipated that FAA will provide AEDT outputs from the “Goals and Targets” project. Thus, while redoing the CMAQ simulations, if time permits, we will also upgrade WRF to use the latest version (V3.6),[3] and repeat the meteorological downscaling. This version of WRF has an updated lake scheme from the Community Land Model (V4.5) that will address problems we saw with earlier versions of WRF around the Great Lakes region.

Milestone(s)

We have achieved multiple milestones during this performance period, listed below.

- Completed 2005, 2010, 2013 annual WRF simulations
  - Post-processed these simulations using MCIP for CMAQ, including changes to MCIP code for additional lake category
- Completed 2005 and 2010 annual basecase and senscase modeling simulations (with CMAQv5.0.1) with latest updates and performed 2005 basecase annual simulations using new CMAQv5.0.2 build.
- Evaluated model predictions extensively with surface observation data (AQS, CASTNet, IMPROVE, CSN) and in-situ aircraft observational (MOZAIC) data.
- Refined the AEDTProc tool previously developed to process AEDT emissions inventories in a form for use in CMAQ
- Performed analyses of AQ results to predict 2005 and 2010 annual US aircraft impacts; simultaneously studied the annual aviation impacts differences between these years.
- Updated background emissions, meteorology data and boundary conditions in our second round of modeling.
- Sub-grid scale clouds, radiation scheme and lake scheme updated in WRF modeling.
- SOA mapping updated in boundary conditions downscaling tool.
- Generated boundary conditions from recent ACCRI project related CAM5 data for 2005 and 2050 annual years.
- Fixed high aircraft-attributable O_3 issues (particularly in summer months) observed in our first round of modeling due to lightning NOx emissions.

Major Accomplishments

- Substantially improved the modeling platform using the WRF-SMOKE-CMAQ
- Models configured and ready for use
  - Once revised AEDT-based emissions inventories are made available by the FAA, UNC is prepared to perform the modeling for each year of interest and assess the aviation-attributable trends from current to future years.

[3] http://www2.mmm.ucar.edu/wrf/users/wrfv3.6/updates-3.6.html

David M. Romps, Jacob T. Seeley, David Vollaro, and John Molinari, 2014. Projected increase in lightning strikes in the United States due to global warming. Science 14 November 2014: 346 (6211), 851-854, [DOI:10.1126/science.1259100].

Publications

1) Arunachalam, S., M Woody, J. Rissman, F.S. Binkowski, H.-W. Wong, S. Jathar, A. Robinson (2014). An Enhanced Sub-grid Scale Approach to Characterize Air Quality Impacts of Aircraft Emissions, Air Pollution Modeling and its Application XXIII, D.G. Steyn and R. Mathur (eds.), ISBN: 978-3-319-04378-4 (Print) 978-3-319-04379-1 (Online), Springer, The Netherlands, 2014.
2) Vennam, L.P., S. Arunachalam, B.H. Baek, M. Omary, F.S. Binkowski, S. Olsen, R. Mathur, W. Vizuete, G. Fleming (2014). A Multiscale Modeling Study to Assess Impacts of Full-Flight Aircraft Emissions on Upper Troposphere and Surface Air Quality, Air Pollution Modeling and its Application XXIII, D.G. Steyn and R. Mathur (eds.), ISBN: 978-3-319-04378-4 (Print) 978-3-319-04379-1 (Online), Springer, The Netherlands, 2014.
3) Vennam. L.P., Arunachalam. S., Vizuete. W., Baek. B.H., Omary. M., Bowden. J., and Olsen. S. " Modeled Trends in Impacts of Landing and Takeoff Emissions on Surface Air Quality in US for 2005, 2010 and 2018", *Oral presentation at 13th Annual CMAS Conference held at Chapel Hill, NC from Oct 5-7, 2014.*
4) Vennam. L.P., Arunachalam. S., Vizuete. W., Baek. B.H., Omary. M., Bowden. J., and Olsen. S. " Modeled Trends in Impacts of Landing and Takeoff Emissions on Surface Air Quality in US for 2005, 2010 and 2018", Poster presentation *at 2014 AGU Fall meeting held at San Francisco, CA from Dec 15-19, 2014.*
5) Woody, M. C., West, J. J., Jathar, S. H., Robinson, A. L., and Arunachalam, S. (2015): Estimates of non-traditional secondary organic aerosols from aircraft SVOC and IVOC emissions using CMAQ, Atmos. Chem. Phys., 15, 6929-6942.

Outreach Efforts

- Multiple presentations to ASCENT Advisory Board and to the FAA during the Weekly Tools telecons.

Awards

- None.

Student Involvement

- Pradeepa Vennam, Ph.D. student in the Department of Environmental Sciences and Engineering is leading the air quality modeling efforts for this task. She is expected to graduate in 2016.

Plans for Next Period

- Rerun the multi-year modeling with the updated platform and study the incremental US-wide impacts.
- Perform model evaluation for additional years that have observational data available.
- We will repeat all previous US-wide analyses and also study O_3 and $PM_{2.5}$ sensitivity changes in major urban areas, or by other appropriate divisions of the US.

Task 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

University of North Carolina at Chapel Hill

Objective(s)

The overall objective of this task is to extend the WRF-SMOKE-CMAQ Modeling platform from Task 1, described above, that incorporates the latest modeling science, datasets and tools, and helps address the aspirational goals of Destination 2025, to compute sensitivity coefficients that link changes in atmospheric $PM_{2.5}$ concentrations to perturbations in aircraft emissions on an individual airport-basis.

Research Approach

The approach involved using the D2025 modeling platform with the CMAQ v4.7.1 instrumented with the Decoupled Direct Method (DDM) – a sensitivity analysis technique to perform multiple simulations. Note that the CMAQ v5.0.2 version with DDM was available much later during the past year, and in the interest of getting a first order implementation complete, we used an earlier version of CMAQ instrumented with DDM. Using a smartly designed grouping technique to separate AQ and health impacts from individual airports, we clustered 66 individual airports into 30 groups, each containing 1 – 4 individual airports, and performed 30 simulations during January and July 2005 with an appropriate spinup period. We then post-processed these results to tease out the individual airport AQ impacts and performed multiple types of analyses to assess / quantify individual airport AQ impacts at various spatio-temporal scales.

In addition to the above, we also performed 3 more simulations on a NAS-wide basis:

- CMAQ v4.7.1 with background emissions alone from all other sources
- CMAQ v4.7.1 with background emissions and NAS-wide aircraft emissions
- CMAQ-DDM v4.7.1 with NAS-wide aircraft emissions

Use of the DDM-3D allows a single model run with hourly sensitivity coefficients to take the place of "brute force" sensitivity analysis, where discrete model runs compare varying scenarios with an unperturbed base case.
DDM-3D outputs sensitivity coefficients of chemical concentration Y in grid cell i to sensitivity parameter X_j as:

$$C_{ij} = \frac{\partial}{\partial X_j} Y_i$$

where X_j is, in our case, emissions of a species (or group of species) from a specific airport. Thus, given unperturbed concentrations of Y_i,

$$Y_i^{'} = Y_i + \Delta E \times C_{i,j}$$

where ΔE is the multiplicative change in X_j. The base case would be represented as ΔE = 0; the effect of 50% reduction in emissions category j would be calculated using ΔE = -0.5.

During the previous year's work, we first short-listed a set of 139 major airports from the US. This list included the 99 airports from Woody et al, 2011, with additional airports used for geographical representativeness (at least one airport in each state), and to leverage comparisons with other airport-related health studies, such as the retrospective study for aircraft noise and hospital admissions related to cardiovascular diseases (Correia et al, 2013). We then used the CMAQ and health impact results from the two-week long simulations of 99 individual airports to develop an empirical concentration threshold below which airport impacts were not meaningful. Using this threshold, we developed a design of experiments, which was the foundation of the work performed here.

We explicitly modeled 66 large airports in the US in about 30 different CMAQ simulations. Each CMAQ simulation contained between 1 – 4 airports. Airports that do not significantly overlap in influence were grouped together to save processing power and reduce model runtime. For example, one CMAQ simulation will have the IAH (Houston, TX), BUR (Burbank, CA), and ALB (Albany, NY) airports chosen using the empirically driven concentration threshold. CMAQ-DDM-3D will be able to track the model's sensitivity for each output species (such as O_3 and various $PM_{2.5}$ chemical components) to six aircraft-emitted precursors, namely NO_x, VOC, SO_2 and the three $PM_{2.5}$ primary components (PEC, POC and PSO4). These 66 airports capture about 61% of flight activity and 77% of fuel burn on a NAS-wide basis. This intense modeling required over 200,000 CPU-hours and generated 8 terabytes of model outputs; however during the model simulations, we generated hundreds of terabytes of data that were then discarded. Resources permitting, we will model another 15 airports explicitly to capture up to 92% of fuel-burn. We leveraged the extensive testing and benchmarking performed under last year's funding to perform this task. Our collaborators at BU then developed regression-based approaches to assess AQ and health impacts for all the non-modeled airports in the US.

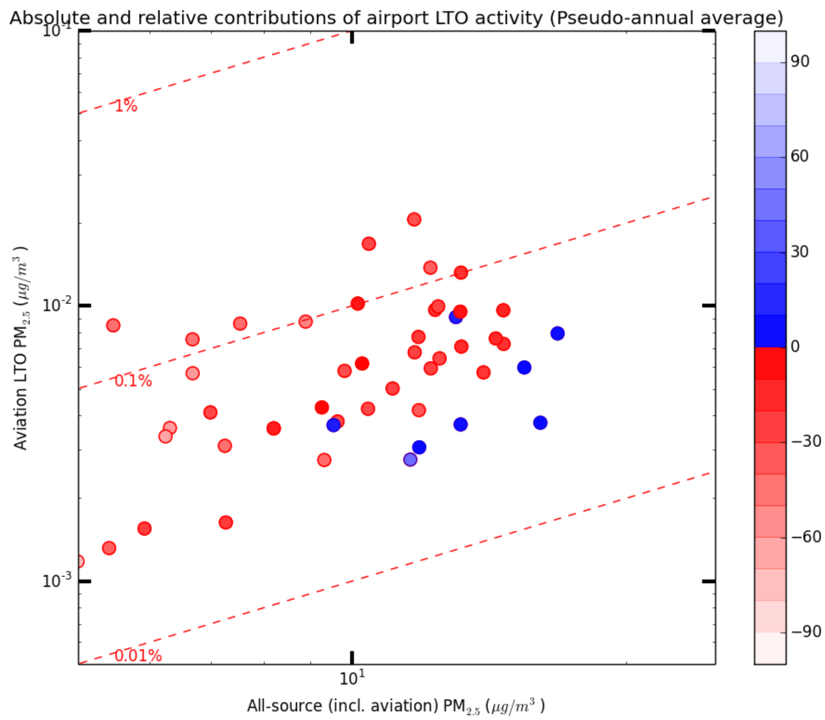
We post-processed the CMAQ simulations to extract daily average $PM_{2.5}$ (total mass and chemical components) and daily maximum 8-hr O_3 fields to assess aviation impacts, and shared the results with collaborators at Boston University to perform the health risk analyses.

We analyzed the model AQ results to explore developing specific metrics related to airport-specific impacts for future policy use. We performed this analyses both at the airport grid-cell, and at increased distances for O_3 and primary and secondary components of $PM_{2.5}$. Possible candidates for this metric are radial influences of air pollutants at increasing distances.

Finally, we are also collaborating/coordinating with other FAA-funded research activities to cross-compare our regional-scale CTM results (such as CMAQ) with global-scale model simulations (such as GEOS-Chem) at multiple scales, using both forward and inverse source attribution techniques.

The differences between scenarios (a) and (b), called the Brute-force approach, were then compared with results from (c) to evaluate the efficacy of the DDM technique for various $PM_{2.5}$ species and O_3.

Figure 2.1 shows the aviation-attributable $PM_{2.5}$ concentrations as a function of total all-source $PM_{2.5}$ concentrations in both absolute and relative terms, and as a function of model performance when compared to $PM_{2.5}$ monitors (top) and fuel burn in millions of gallons (bottom). As can be seen from this figure, there are 9 airports that contribute at least 0.01% of the total $PM_{2.5}$ in the airport's home grid-cell. But not all of these 9 airports have the highest fuel-burn in the nation, highlighting the fact that there are potentially smaller airports that could have a higher contribution to $PM_{2.5}$ than larger airports. Figure 2.2 shows the aviation-attributable $PM_{2.5}$ concentrations from each of the 66 airports as a function of distance from the airport. From this figure, there are at least 23 airports with at least 1E-3 $\mu g/m^3$ of aviation-attributable $PM_{2.5}$ at distances of up to 150-200 km from the airport's home grid-cell. The bulk of these concentrations at downwind distances are due to secondary $PM_{2.5}$ formed by the atmospheric interactions between aircraft-emitted gas-phase precursors with background emissions at downwind distances.



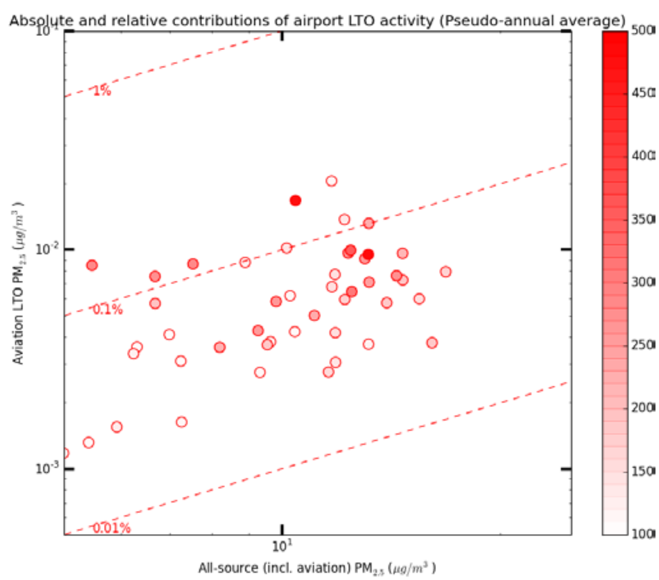


Figure 2.1: Aviation-attributable $PM_{2.5}$ concentrations compared to total $PM_{2.5}$ concentrations from all sources, in absolute and relative terms. The intensity of the dots represent bias in model performance compared to observations (top) and as a function of fuel burn at the airport (bottom).

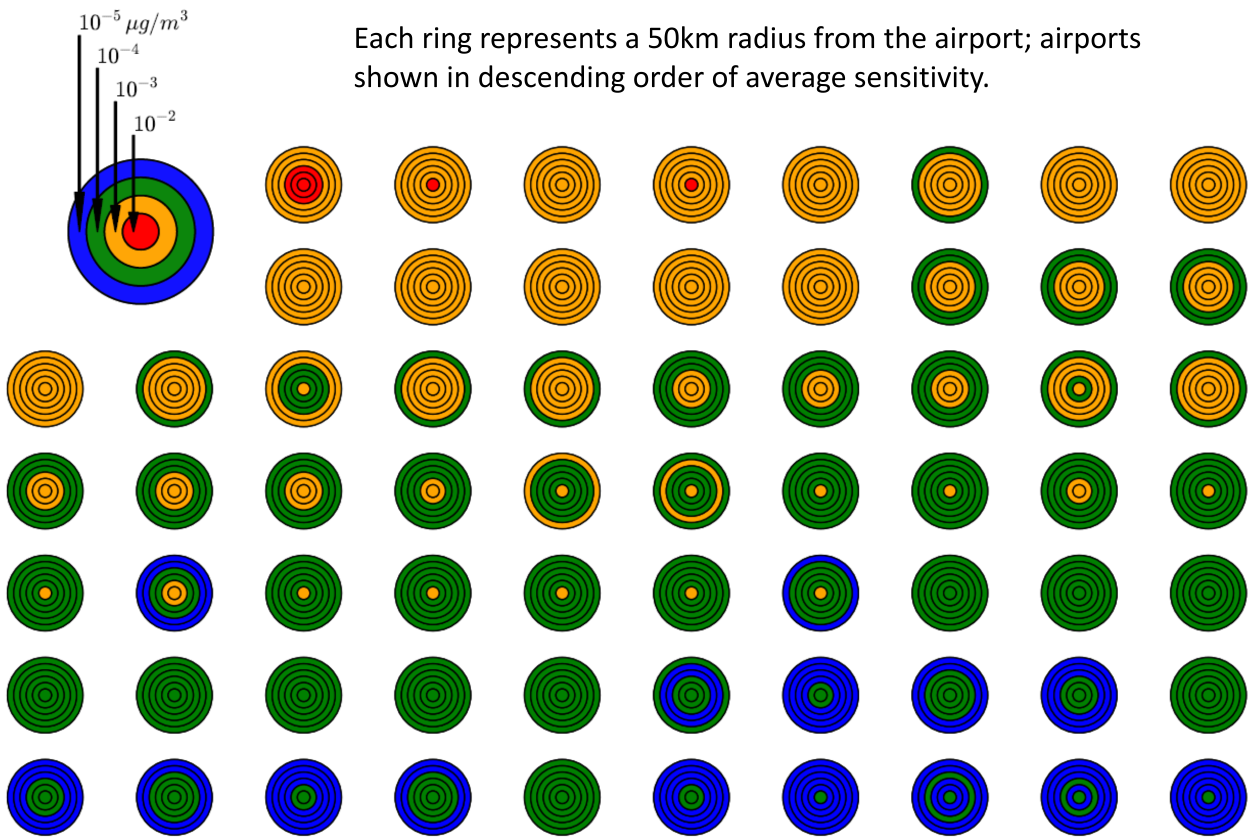


Figure 2.2. Airport-specific aviation-attributable $PM_{2.5}$ concentrations from each of the 66 individual airports as a function of distance from the airport.

Milestone(s)

We have achieved multiple milestones during this performance period, listed below.

- Completed January+July modeling for 66 individual airports with CMAQ-DDM v4.7.1.
- Post-processed these simulations and shared with BU for health-risk analyses.
- In parallel, performed extensive analyses of AQ results to tease out airport-specific impacts.
- Manuscript in final stage of preparation before submission to the Journal.

Major Accomplishments

- Completed modeling and analyses, with a manuscript nearly ready for submission.
- Master's thesis summarizing these results submitted to UNC's Department of ESE.

Publications

1) Boone, S., S. Napelenok, and S. Arunachalam, 2013. Calculation of sensitivity coefficients for airport emissions in the Continental United States using CMAQ DDM-3D/PM, *Presented at the 12th Annual CMAS Conference*, Chapel Hill, NC, October 28-30, 2013.
2) Boone, S. and S. Arunachalam (2014). Calculation of Sensitivity Coefficients for Individual Airport Emissions in the Continental US using CMAQ-DDM/PM, *In Proceedings of the Extreme Science and Engineering Discovery Environment (XSEDE) 2014 Conference*, July 2014, Atlanta, GA.
3) Boone, S., S. Penn, J. Levy and S. Arunachalam (2015). Calculation of sensitivity coefficients for individual airport emissions in the continental United States using CMAQ-DDM3D/PM. *Presented at the 34th International Technical Meeting (ITM) for Air Pollution Modeling and Applications*, Montpellier, France, May 2015.

Outreach Efforts

- Multiple presentations to ASCENT Advisory Board and to the FAA during the Weekly Tools telecons.

Awards

1) "**Best Student Paper of the 2014 Conference**"
   Boone, S. and S. Arunachalam. Calculation of Sensitivity Coefficients for Individual Airport Emissions in the Continental US using CMAQ-DDM/PM, In Proceedings of the Extreme Science and Engineering Discovery Environment (XSEDE) 2014 Conference, July 2014, Atlanta, GA.

Transition of Research Results

- None.

Student Involvement

- Scott Boone, who did the bulk of the work under this task, obtained his dual M.S. in Environmental Sciences and Engineering and in Transportation Planning, and has graduated from UNC.

Plans for Next Period

- Finalize two manuscripts – one led by UNC on air quality impacts, and the other led by BU on health risk analyses.
- Extend work to look at additional "damage/ton" metrics over multiple geographic regions – such as Census divisions, metroplex, airshed, etc.
- Explore computing 2nd order sensitivities with DDM, and compare/contrast with adjoint-based methods.

Task 3. Consult with FAA and the ACCRI team of investigators to assess the surface air quality impacts of aircraft emissions during cruise mode

University of North Carolina at Chapel Hill

Objective(s)

Assess surface air quality impacts of cruise emissions using multiple global-scale modeling systems.

Research Approach

This task includes a multi-model assessment including GEOS-Chem, NASA GISS-E, GATOR-GCMOM, CESM, CAM-Chem, and GMI. UNC's role was to provide guidance for using consistent sets of input meteorology and emissions, and post-processing to facilitate comparison between the models, and against ongoing modeling and analyses, specifically relevant to health impacts from a NAAQS perspective.

The UNC PI participated in several conference calls with the ACCRI team to provide guidance on model analyses and evaluation to be consistent with D2025 modeling platform, focused on O_3 and $PM_{2.5}$ air quality and health impacts. This task is now complete. The lead investigators in the ACCRI team are finalizing their project reports to the FAA and developing manuscripts.

Milestone(s)

None.

Major Accomplishments

The project team completed the modeling and analyses and a final report was submitted to the FAA.

Publications

None.

Outreach Efforts
None.

Awards
None.

Student Involvement
None.

Plans for Next Period
We are exploring a follow-on task to obtain the multi-model datasets and work with investigators at BU to perform health risk analyses of these air quality impacts of full-flight global emissions.

Task 4. Develop High Fidelity Weather for Global Inventories using AEDT
University of North Carolina at Chapel Hill

Objective(s)
The primary objective of this project is to assist ATAC's development of a 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 will include a description of the optimal high fidelity weather data sources for this purpose, instructions on how to use the optimal weather data within AEDT, and validation of its use using CFDR data. (Note that ATAC was funded separately, and not through ASCENT.)

Research Approach

AEDT and WEATHER DATA
This research provided a detailed description of weather data sources as input into AEDT. This description complements and extends upon the information available about weather data in the AEDT2a Technical Manual and User Guide, and helps justify the selection of an appropriate weather data source from those currently available (RUC, NCEP-NCAR Reanalysis, GEOS-5, MERRA). Comprehensive review of this data by UNC concluded MERRA should be used for future development with AEDT. However, recent developments with MERRA must be considered for future development. MERRA will soon transition to MERRA-2, but no decision has been made to cease its forward production. MERRA-2's format will be slightly different from MERRA. The global grid will change from 540x360 to 576x360. There will no longer be a coarse resolution for certain variables, all will be written at the native resolutions. Most variables remain with some to be added. The MERRA-2 data is being written to netCDF format directly, and not the HDF-EOS format that MERRA used. MERRA-2 will use an updated form of the GEOS-5 atmospheric model and analysis scheme, and assimilate meteorological and aerosol observations not available to MERRA.

MERRA as input into the weather module with AEDT
The version of AEDT 2b used to model operations using high-fidelity MERRA weather was built in June 2014 and reflects the AEDT 2b development code base from around that time. ATAC and UNC worked together to identify problems within AEDT when using the MERRA weather data as input. Fixes and improvements were recommended for each encountered issue. UNC compared raw MERRA data values for select flights with AEDT output. The comparison revealed several fundamental issues within the AEDT weather module that were also independently confirmed by ATAC through the code. The issues UNC identified and the recommended solutions provided to ATAC are discussed below.

- Temporal interpolation issue within AEDT: AEDT currently requires hourly data for a single day.
  Recommendation: Update the weather module to be completely flexible on the temporal duration of weather data files. The current interpolation algorithm assumes 1-hour duration. Update the weather module to use weather data from the following day when performing interpolations whenever it is appropriate to do so.
- Missing MERRA values near the surface.
  Recommendation: Missing values may exist because MERRA does not extrapolate below ground. To fill between lowest model pressure level available and valid pressure surfaces below this surface, an extrapolation routine is

needed. Update the methodology employed by the weather module when loading AEDT-readable binary into memory in order to minimize the amount of invalid pressure levels. This would reduce recalculating geo-potential heights and temperature for pressure levels marked as invalid. For these pressure levels, wind values would be made equal to those of the highest (pressure-wise) valid pressure level.

- The weather module in the version of AEDT 2b used in MERRA analysis interprets weather reading requests with negative latitudes as errors. Therefore, the weather module is not able to take weather readings south of the equator.
  Recommendation: The weather module should be updated to ensure correct interpretation of negative latitudes in the high-fidelity weather use-case.
- The MERRA-capable version of AEDT 2b is limited to using only one day of MERRA weather data. If a user were to provide two or more days of MERRA weather data, and make a weather reading request for one of the days following the temporally first day, the weather reading request would default to using the first day's weather data.
  Recommendation: Update the weather module to ensure that it can access all dates of its loaded weather data, making sure to avoid the issue encountered in the MERRA-capable version of AEDT 2b.
- The MERRA-capable version of AEDT only uses airport-relative humidity in acoustics computations. Relative humidity coming from high-fidelity weather would have no impact on these computations
  Recommendation: Update the weather module to calculate relative humidity from the specific humidity contained in MERRA data

Milestone(s)
We have achieved multiple milestones during this performance period, listed below.
- Determined optimal weather data sources for AEDT.
- Identified methodologies that need updating to improve MERRA based AEDT high fidelity weather modeling.
- Recommended changes to AEDT methodology for processing meteorological fields.

Major Accomplishments
This research provided a report with a priority of recommendations for improving high fidelity weather within AEDT. A final report that will include a detailed description of MERRA and other meteorological inputs (RUC, NCEP-NCAR Reanalysis, GEOS-5, as well as a methodology to download meteorological fields will be provided in this report.

Publications
- None.

Outreach Efforts
Presentation to the FAA during the Weekly Tools telecons.

Awards
- None.

Student Involvement
- None.

Plans for Next Period
The next step is to implement the recommended changes within AEDT. A similar comparison will be made between raw MERRA and AEDT output to ensure the AEDT output is consistent with the input.