PARTNER

Partnership for Air Transportation Noise and Emissions Reduction

An Observation and Model based-assessment of Hazardous Air Pollutants (HAPs) from a Medium-Sized U.S. Airport

Lakshmi Pradeepa Vennam

Ph.D. Candidate

Department of Environmental Sciences and Engineering

University of North Carolina, Chapel Hill

Advisors

Saravanan Arunachalam, Institute of Environment, UNC

William Vizuete, Department of Environmental Science and Engineering, UNC

THE UNIVERSITY *of* NORTH CAROLINA *at* CHAPEL HILL

Submitted to 9th Annual Joseph A. Hartmann Student Paper Competition

31 December 2012

Table of Contents

ABSTRACT

Efficient modeling of airport pollutants in the vicinity of airport is essential to study the impact on local air quality and to answer policy-related and health-based questions. Considering the knowledge gap that needs to be addressed regarding airport-related hazardous air pollutants (HAPs) and their air quality impacts, we performed a detailed source-based modeling of HAPs from T.F. Green airport in Providence, Rhode Island, and evaluated the model outputs against field-study data from monitors in and around the airport. The overall airport HAPs mean concentrations appear to be 40% lesser than urban sites except for formaldehyde. In terms of model performance, we observed Normalized Mean Error of 30 – 60% for all considered aviation prioritized HAPs in our simulations. Comparison between CMAQ and other local-scale dispersion and statistical models provided enhanced understanding of characterizing spatial-temporal patterns of HAPs near airport. We observed that National Air Toxics Assessment (NATA) census tract local scale modeling and CMAQ was unable to predict the highly emitted pollutant like formaldehyde in the vicinity of the airport, which can be improved by better emission characterization. In addition, many highly reactive pollutants are temporally variable and NATA provides annual concentrations, so we suggest that photochemical models such as CMAQ can provide better temporal predictions. Finally we demonstrated that Bayesian Maximum Entropy (BME) technique with available observed and modeled data as input can better predict concentrations at airport locations that lack monitoring data.

INTRODUCTION

Aviation has experienced proliferative growth in past few decades. Commercial aviation operations are rapidly increasing worldwide, with an operation growth rate of 61 percent, 40 percent and 22 percent in large, medium and small hub airports (FAA, 2011). The average annual growth rate is predicted to increase around 4.6 percent from 2010 to 2030 (FAA, 2010). FAA Aerospace 2012 forecast (FAA, 2012) also showed annual increase of 2.6 % and 2.9 % in system-enplanements from 2016-2032 for both baseline and optimistic cases respectively. These quantitative projections clearly indicate substantial aviation growth in past and future. This growth implicates potential increase in pollutants such as Nitrogen oxides (NO_x), Sulphur oxides (SO_x), Particulate matter (PM), Volatile Organic Compounds (VOC) and some other hazardous air pollutants both at ground level (Idling, Taxing and Landing -Take off (LTO)), and upper atmosphere (cruising > 90% of flight time). These aviation emissions could impact both air quality and human health locally and globally. Particularly during LTO conditions, these emissions vary with different aircraft thrust levels and emit various harmful pollutants at idling and taxiing condition that could reflect immediate local-scale impacts. There is thus a need to study impact of aviation emissions on local air quality particularly in the vicinity of an airport as first step to further assess their impacts on environment and human health.

MOTIVATION AND BACKGROUND

Among airport related air-quality studies, till-date most of them focused mainly on NO_x (Carslaw et al., 2006; Wood et al., 2008; Timko et al., 2010), $PM_{2.5}$ (Mazaheri et al., 2009) and CO due to their relatively higher contribution to the overall airport-related emissions (Schürmann et al., 2007). Prior air-quality modeling of airport emissions studies (Arunachalam et al., 2011; Woody et al., 2011; Unal et al., 2005) quantified in detail the contribution of present and future aviation related $PM_{2.5}$ and major airport emissions modeling at regional scale using chemical transport model such as CMAQ. Arunachalam et al., 2011 also discussed and quantified the effect of aviation related PM2.5 on population exposure at different model resolutions (36k, 12k CMAQ domain) near major airports. This shows that significant research and studies were performed on modeling and quantification of impacts from major pollutants such as $PM_{2.5}$, NO_x, O_3 near airports. However, assessment of less emitted pollutants such as HAPs has not been explicitly accounted for near airports. By definition, HAPs are pollutants that are known or suspected to cause serious

health effects specifically categorized from other air pollutants based on 1990 Clean Air Act (CAA). To our knowledge, limited studies have been performed with detailed model-based characterization of air quality due to HAP emissions from airports. Also a recent report (ACRP, 2008) clearly mentioned that inadequate attention was given to hazardous air pollutants (HAPs) modeling and gaps are associated with their scientific understanding, which further provides motivation for our investigation here.

Though modeling of airport related HAPs still involves uncertainties, efforts have been increased in past few years to increase the knowledge of HAPs emissions near airport. Certain monitoring and health effect studies quantified the impact of airport related HAPs. Levy et al., 2008 discussed the health effects caused from air toxics locally and mentioned their serious health effects inspite of relative low quantitative percentages in total aviation emissions. Prior aviation emission and monitoring studies (Herndon et al., 2006; Anderson et al., 2006) investigated emissions of hydrocarbons (HC) from commercial aircraft during airport operations and quantified the emissions of formaldehyde, acetaldehyde, benzene, ethylene, propene and butenes + acrolein to be high during idle and taxiway conditions than take-off and approach. Spicer et al., 1994 also reported that these pollutants make up about 75 percent or more of the volatile organic compound (VOC) emissions that are being detected in the aircraft exhaust gas. APEX (APEX, 2009) and EXCAVATE measurement studies illustrated HAPs emissions for different aircrafts at ambient conditions and provided recent HAPs speciation profile for VOCs. In addition, according to Airport System Performance Metrics (ASPM) database, the average taxi time at mid- sized T.F.Green airport (PVD) was reported as 16.5 min, which is significant amount of time to emit harmful HAPs. Thus while HAPs are a subset of the various pollutants from aircraft activities at an airport, limited modeling efforts have been conducted to date to characterize their impacts. The limited HAPs modeling near airports could be due to sparse HAPs monitoring data near airports to validate the model predictions, and the uncertainty involved with HAPs specification in emission inventories. Despite these limitations, there is a necessity to develop a model to predict HAPs concentrations at airport locations that lack monitoring data. Also air toxics health risk assessments and expansion decisions by airport authorities based on predictions are still major concerns and demands investigation of models ability to predict airport-related HAPs. Therefore this paper aims to address the knowledge gap associated in the aviation related HAPs, by studying the assessment of HAPs near mid-sized airport using Chemistry Transport model like CMAQ at fine resolution (4km).

Further we analyzed the spatial, temporal variability of airport-related HAPs, evaluated model performance. Also compared CMAQ results from this study with another set of results from a national-scale assessment that relied on a local-scale dispersion model. Finally an alternate approach that relied on a statistical model was used to compare and contrast the various approaches in predicting and understanding HAPs contribution near a mid-sized airport.

STUDY FOCUS

In this study, we focused mainly on 8 major HAPs such as formaldehyde, acetaldehyde, 1-3 butadiene, acrolein, benzene, toluene, xylene and naphthalene that are considered as aviation health-risk prioritized pollutants (Levy et al., 2008). Among these based on toxicity, 2008 ACRP report ranked acrolein, formaldehyde, 1,3-butadiene, naphthalene and benzene as five major airport related HAPs. This study considered data from three different approaches to assess air quality impacts of HAPs from Providence T.F. Green (PVD) airport in Rhode Island for the year 2005.

1. Detailed measurements of HAPs conducted by the Rhode Island Department of Environmental Management (RIDEM) in and around the airport, and standard measurements at EPA's Air Quality sites (AQS),
2. Explicit source-based modeling using the Community Multi-scale Air Quality (CMAQ) model, and
3. National Air Toxics Assessment (NATA) performed by the EPA for 2005. This is the first study to take advantage of the recent 2005 NATA annual modeling data obtained from updated emissions inventory that considered detailed airport emissions.

Availability of observational data at urban, rural (AQS data) and airport (RIDEM) spatial locations enabled us to compare near-airport site HAPs concentrations with other urban and rural sites in the vicinity. We believe that above mentioned limitations for HAPs modeling near airport are minimized by considering RIDEM study observational data to evaluate the model predictions, highly resolved model for predictions and FAA-EPA generated new speciation profiles to characterize HAPs from VOC in the model input emissions. We also performed comparison of CMAQ with another local-scale dispersion model (used in NATA) and predictions from Bayesian Maximum Entropy (BME) (Christakos et al., 1990, Christakos et al., 2001) to study their ability in predicting HAPs at local scales. BME is a spatio-temporal interpolation

statistical technique used in the modeling community to predict concentrations at locations that lack monitoring data and discussed in detail further in the paper. Based on this enhanced knowledge of temporal, spatial variation and chemistry of airport-related HAPs, airport regulatory authorities would benefit in taking decisions regarding potential future airport expansion activities and health risk associated with the HAPs in the vicinity of an airport.

METHODOLOGY

We used the National Emissions Inventory (NEI) for year 2005 to generate emissions for non-aviation sources, and emissions for aviation sources at PVD were based on outputs from the Emission Dispersion Modeling System (EDMS) (FAA, EDMS; Baek et al., 2007). EDMS is an analytical tool and queuing/sequencing model that models movement of aircraft along the taxiways, runways and gates. It includes emissions from aircraft, auxiliary power units (APU), ground supporting equipment (GSE), ground access vehicles (GAV) and other stationary sources in the vicinity of airport (FAA, EDMS). These non-aviation and aviation emissions are processed using Sparse Matrix Operator Kernel Emissions (SMOKE) model to generate grid-based emissions and meteorology input data were based upon the Mesoscale Meteorological (MM5) model (Grell et al., 1994).

Community Multiscale Air Quality (CMAQ) v4.6 model (Byun and Ching, 1999) with extended air toxics chemistry to actual Carbon Bond core mechanism was used for model simulations. CMAQ simulations are conducted on the Northeast U.S at 4-km horizontal grid spacing with 100 x 100 horizontal grid cells and emissions upto 22 vertical layers (10000 ft). Two model simulation cases are performed: 1) basecase - all sources except airport emissions 2) senscase - airport emissions combined with basecase emissions. Hence, the difference between senscase and basecase accounts for the incremental contribution to air quality from the airport emissions.

EMISSION ANALYSIS

On a national scale, the annual contribution of airport VOC emissions to the total anthropogenic emissions is about 0.02%. On a county scale (based on Kent county, PVD airport location) the annual contribution of airport VOC to the total non-highway VOC is about 5.4% and this value is subjected to change in a county with large airport. In our modeling domain, emissions of GSE (ground supporting equipment), GAV (ground auxiliary vehicles) are considered along with the aircraft emissions. But we

should note that majority of airport HAPs emissions come from aircraft, almost (>90%) occurs during idling and taxing stage.

The Pie chart (figure 1) illustrates the percentage contributions of major HAPs to the annual total airport VOC emissions at PVD based on mass (kg) basis. Formaldehyde, acrolein, acetaldehyde appear to be the major contributors to the annual HAPs emissions that are mainly emitted from aircraft. It should be noted also that 1,3-butadiene, benzene majorly come from non-aircraft sources and more toxic than toluene, xylene. In general, formaldehyde and benzene are the key pollutants that contribute to the cancer-risks and acrolein contributes mainly to non-cancer risks (NATA 2005).

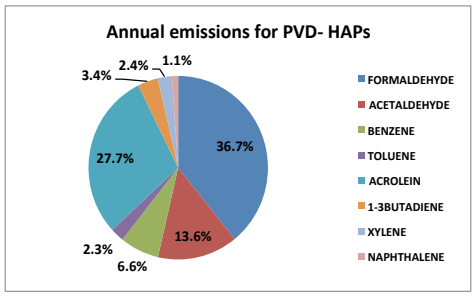


Figure 1: Pie chart representing the percentage contribution from HAPs to annual airport VOC emissions

The daily time series plots (Figure 2, included only two quarters plots for illustration) represent the domain total gridded airport emissions for CMAQ 4km domain obtained from SMOKE model. These plots help us to understand the individual HAP pollutants daily variation and the magnitude difference among airport HAPs species. Throughout the year, we observed same species order in terms of highly emitted to less emitted species. Formaldehyde was consistently highly emitted followed by xylene, toluene, acetaldehyde and other remaining species. We should note that though toluene, xylene are highly emitted, their toxicity levels are less according to EPA's Integrated Risk Information system (IRIS database) when compared with other less emitted acrolein, 1,3-butadiene species.

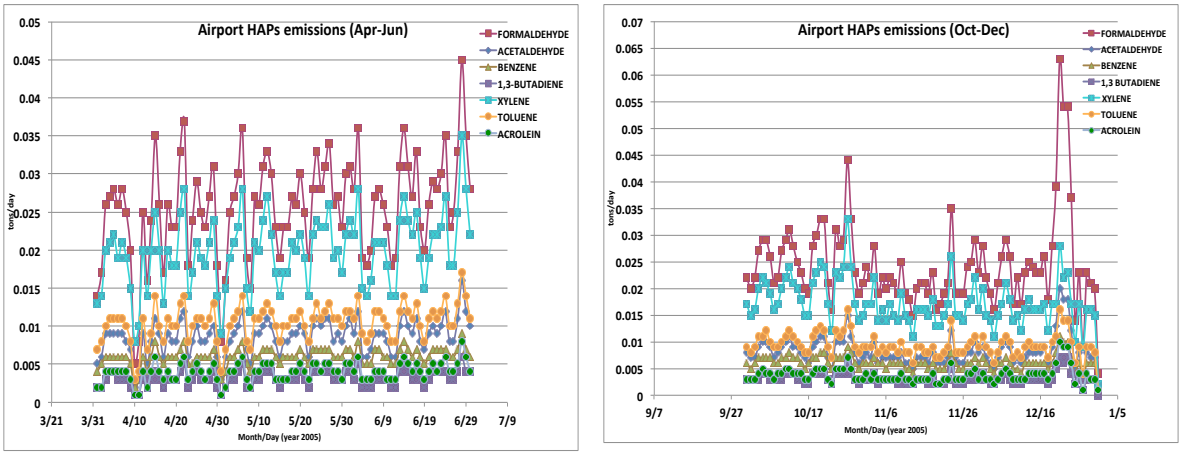


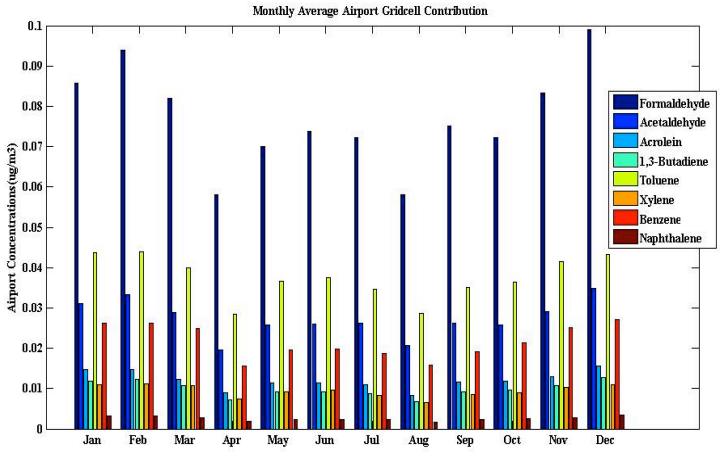
Figure 2: Daily time series of emissions for all HAPs species for Apr-Jun (left) and Oct-Dec (right)

There is no significant difference between winter and summer month's emission values but one could observe an increase of 0.017 tons/day (37%) with comparison of highest day emission value of both seasons. The monitoring and measurement data studies (Timko et al., 2010) indicated that emission rates from aircraft are temperature dependent and relatively higher during low ambient temperatures. Recent report (ACRP, 2012) also found that the VOC emission indices for aircraft are twice in cold conditions than warm conditions. But we did not observe any significant temperature dependency nature among emissions and this was also pointed out in the ACRP report (2008). Therefore this inability of not reflecting temperature dependency in the emission inventories can further introduce uncertainty in model predictions.

RESULTS AND DISCUSSION

Temporal and Spatial Analysis

We studied the temporal and spatial variability of HAPs near the airport to illustrate how varied are the concentrations with change in time and space and compared the concentrations with observational values (from RIDEM and AQS) to study the model performance in capturing the variability. Figure 3 represents the variability in airport-related HAPs concentrations (senscase minus basecase) by month and their contribution to the airport grid cell. The concentration levels are higher during winter months than summer months, that could be related to the incomplete combustion of fuel, which results in emissions of these harmful unburned hydrocarbons such as formaldehyde, acetaldehyde and some other HAPs species.



Species	Jan	July
Formaldehyde	7 %	5 %
Acetaldehyde	3 %	1.3 %
Acrolein	34 %	49 %
1,3- Butadiene	8.3 %	20 %
Benzene	1.8 %	3 %
Naphthalene	6 %	15 %
Toluene	0.3 %	0.7 %
Xylene	0.5 %	1 %

Figure 3: Monthly average airport concentrations (left) and their contribution for summer and winter months (right) in the airport grid cell.

We also present percentage contributions (Figure 3, right) for two months to demonstrate the airport concentrations when compared with background sources. It is evident that formaldehyde and

acetaldehyde contributions are 2% higher during January than July, whereas for remaining species the July month contributions appear to be higher than January. This could due be to the huge decrease among other sources concentrations from January to July and less decrease in the case of airport concentrations (could notice from bar plot that there is no significant difference from January to July in the case of these species) that made airport percentages to be relatively higher in July. We also want to point out that the airport contribution in the case of acrolein is relatively high in the airport grid cell.

Spatial variability was studied by comparing modeled (senscase) and observational data at the available monitoring sites. Figure 4 illustrates the variation among different spatial locations for few species (included only Benzene, Toluene, Acetaldehyde & Formaldehyde to limit space). The urban site (Pawtucket, Providence) concentrations appear to be higher than the airport sites for all species except for formaldehyde where the airport site (Field view) shows higher concentrations. From figure 4, the model comparison with observed data also indicates the model performance in predicting spatial variability.

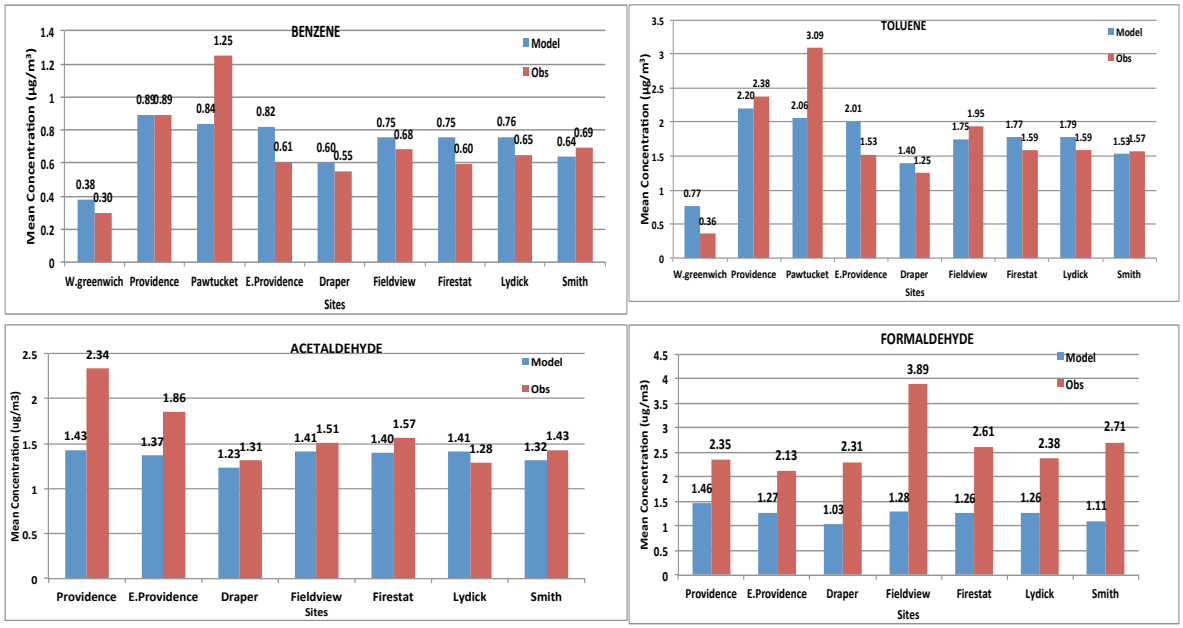


Figure 4: Bar plots representing mean annual concentration of model and observational values at all the monitoring sites for certain HAPs species

From Figure 4, one sees that the model underestimated the peak values, but was able to show the spatial variation among the sites by predicting higher concentrations at urban sites compared to airport sites. One other limitation involved with the model prediction is grid resolution, since all 3 airport sites (Fieldview, Firestation, Lydick) are located in same 4-km grid cell, CMAQ model predicts constant

concentration at all these sites. In this case, model was unable to account for the variability among the major airport sites, which may not cause significant uncertainty for certain species that do not exhibit large differences in concentrations between these 3 sites. But in the case of species such as formaldehyde that have larger magnitudes of emissions, not accounting the peak value and variability near runway site (Fieldview) may cause uncertainty in model prediction values. In such a situation, going to finer grid resolution (such as 1-km or less) might improve model predictions.

Overall Model Evaluation

In addition to the spatial comparison present in before section, we also provided overall model evaluation in this section. Since the model predictability varies with pollutant and spatial location. Therefore, in this section we presented overall Normalized Mean Error (NME) and Normalized Mean Bias (NMB) (Table 3) for each HAPs pollutant. And a scatter plot (Figure 5) that represents comparison of observed and predicted site-specific concentrations for each pollutant species (except for Naphthalene as observational data were not available).

HAPs Species	Overall	Overall	Airport Sites		AQS Sites	
	NMB(%)	NME(%)	NMB (%)	NME (%)	NMB(%)	NME(%)
Benzene	**7.3**	**52.7**	10.9	51.1	7.15	51.2
1,3-Butadiene	**-12.3**	**59.8**	-7.8	55.2	-33.8	53.7
Toluene	**-10.5**	**45.5**	4.82	50.7	26.9	65.7
Xylene	**-15.4**	**52.8**	-3.7	48.7	71.1	13.4
Formaldehyde	**-69.0**	**69.0**	-55.9	56.1	-39.0	45.8
Acetaldehyde	**-8.8**	**31.1**	-4.37	34.8	-32.6	39.2
Acrolein	**-91.6**	**91.6**	-92.4	92.40	-91.7	92

Table 3: Overall average normalized mean bias (NMB) and normalized mean error (NME) at all sites

From table 3, we can observe that the overall model error involved with all the pollutants except for acrolein is in between 36-60%, which is statistically acceptable quantitative range for normalized error in the air quality modeling community. But in the case of acrolein, the model has higher underprediction and we suspect this could be due to uncertainty in emissions, chemistry and observational data. Previous studies (Leucken et al., 2006) indicated that the underprediction of acrolein in CMAQ is mainly attributed to the emissions and observational data uncertainty. Seaman et al., 2006 mentioned acrolein sampling to be highly challenging due to the high degradation of acrolein and its derivatives. To address high underprediction of acrolein, further investigation of sampling detection limits and error involved in the

monitoring data are required, but that are outside the scope of this paper. From emission analysis, we also observed acrolein as second highly emitted air toxic from airports after formaldehyde. Thus, it is important to carry out HAPs monitoring studies at some of the major airports at an even finer spatial-temporal resolution (than performed by RIDEM) to address this modeling issue and for better characterization of acrolein emissions near airport.

Secondly, NMB in the case of formaldehyde is high when compared to the other pollutants. It is one of the highly reactive and mainly produced from secondary formation in the atmosphere. Prior studies (Leucken et al., 2006) clearly stated that 90% of formaldehyde (FORM) concentrations in the atmosphere occur due to secondary formation from VOC (volatile organic compound) and 10% occurs due to primary emission sources. Therefore in other words we can say that FORM concentration levels are dependent on VOC concentrations. So the uncertainty in VOC model predictions will definitely have an impact on secondary formed pollutants like FORM. We suspect that all the model uncertainties involved in VOC predictions could be one of the causes for high bias in FORM predictions (total concentrations). On the other hand, we observed the concentrations of FORM to be relatively high near runway site (Fieldview) and the models are usually unable to predict the peak concentrations since in the Eulerian grid model like CMAQ the concentrations are diluted in the considered grid volume.

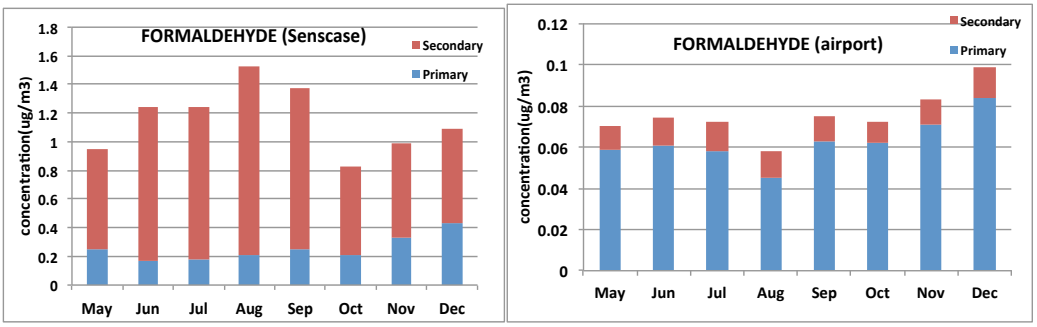


Figure 5: Secondary and Primary Formaldehyde Monthly Concentrations for senscase (left) and airport (right)

In figure 5 we can observe that the major proportion of senscase concentrations are due to secondary formaldehyde and airport concentrations are mainly due to the primary formaldehyde. Therefore it is necessary to represent chemistry (secondary) accurately in order to predict the total concentrations and emissions (primary) to accurately predict the local sources like airport.

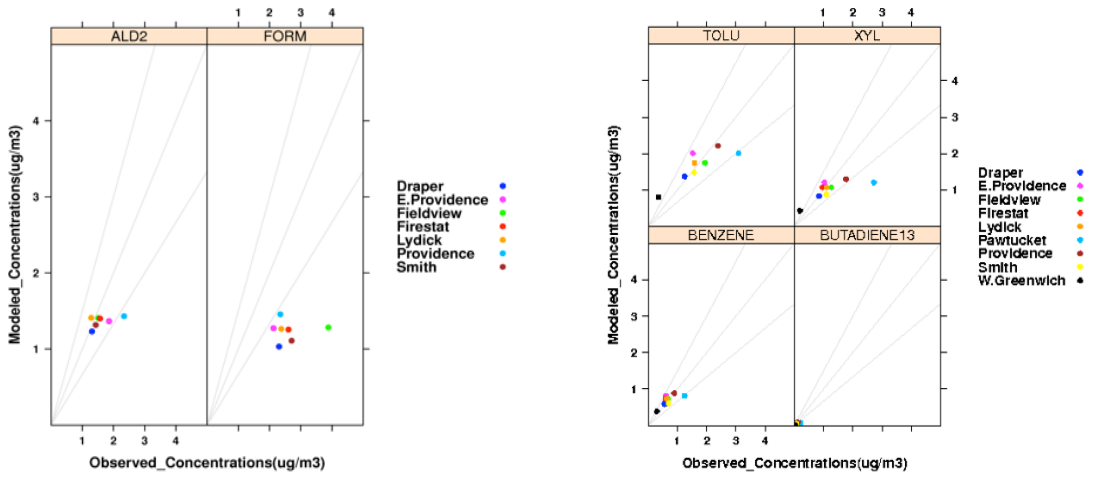


Figure 6: Scatter plots representing the site wise comparison of observed and modeled values.

From figure 6 we can conclude that model performed better at all airport sites for all species except formaldehyde. We suspect that this could be due to emissions since we are unable to see significant differences between winter and summer months. Therefore we believe that with better characterization of emissions, model performance can be improved further.

Comparison with NATA

National Air Toxics Assessment (NATA, 2005) is a state-of–the-science screening tool developed by U.S EPA to evaluate the health risks involved with air toxics both at regional (state) and local (counties, census tract) level in U.S. EPA recently released latest NATA-2005 assessment based on same NEI 2005 emissions inventory. NATA uses AERMOD dispersion model to predict the air toxics concentrations for primary pollutants and most of the health assessment studies rely on dispersion model predictions to emphasize the toxic exposure levels. The recent NATA-2005 assessment included about 20,000 airports in their emissions inventory. They also considered secondary formation of acetaldehyde, formaldehyde, acrolein and decay of 1,3-butadiene to acrolein from CMAQ modeling at 12-km resolution, which eliminated the major inability of not predicting secondary formed pollutants in dispersion models to certain extent. The latest NATA report also mentioned that pollutants like formaldehyde and Polycyclic Aromatic Hydrocarbons (PAHs) from aircraft were observed to increase in 2005 NATA assessment (NATA, 2005). So we compared NATA results with our CMAQ predictions in order to illustrate difference between local-scale dispersion (AERMOD) and detailed chemical transport model (CMAQ)-based HAPs predictions. Since NATA is a screening level assessment tool that provides estimations at very finer scale (census tract),

comparison and evaluating with other detailed models (like CMAQ) gives us a better understanding of the model performance and future developments that need to be addressed.

In Figure 7, we compared NATA census tracts with CMAQ total concentrations (all sources, senscase) and observational data to understand model performance at local scales near the airport. In understanding this comparison, a key distinction to be noted is that NATA does not report data for the airport's census tract block as no population are present in that particular census block. One can observe this clearly in figure 7, formaldehyde overlay plot (circled location, no small circle (NATA census tract) between stars (observed)).

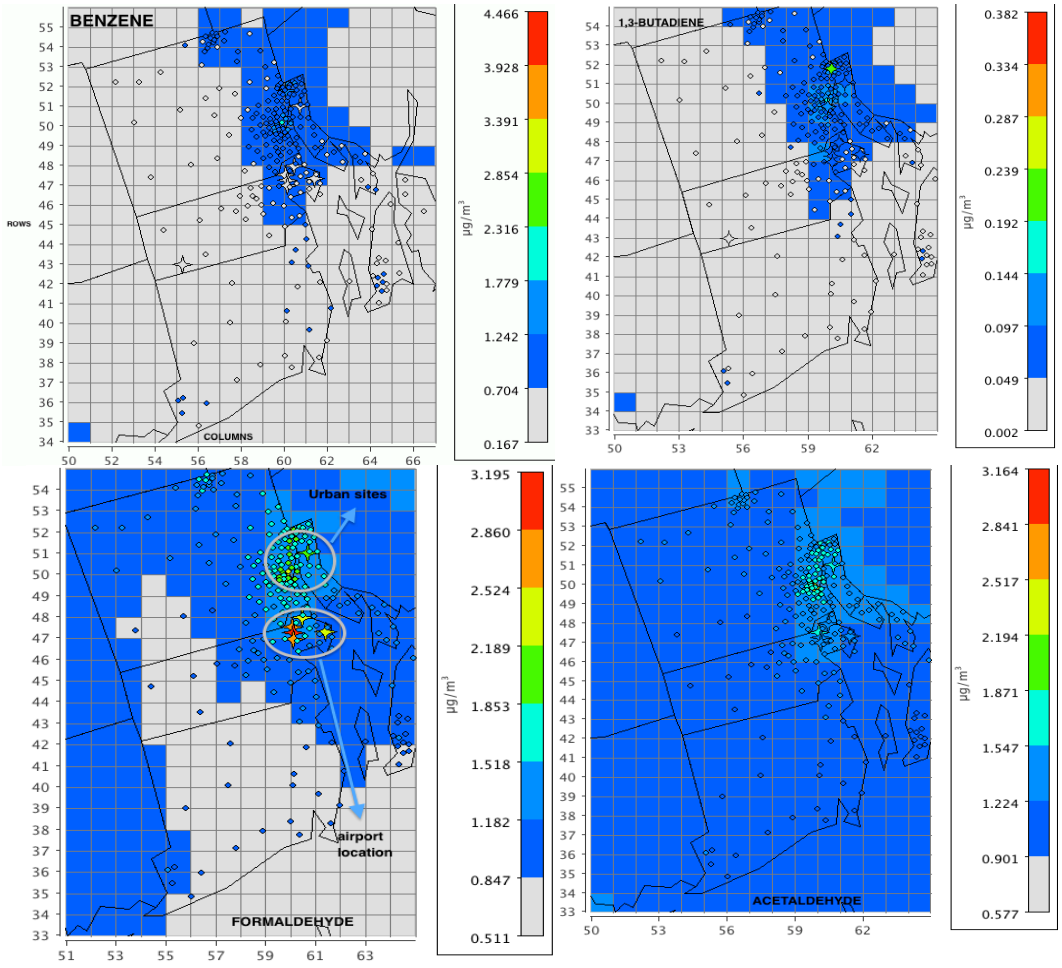


Figure 7: CMAQ concentration spatial plots with overlay of NATA census tract data (circles) and Observational data (stars) for few species (remaining species are also analyzed, but not presented here).

From Figure 7 we could observe that in the case of benzene, NATA census tract values in the vicinity of the airport are close to observational values while CMAQ concentrations are overestimated. But

in the case of 1,3-butadiene, NATA underestimated the values whereas CMAQ and observed values look comparable. The interesting observation in the case of formaldehyde is that both NATA and CMAQ underpredicted concentrations at airport sites, whereas NATA had good agreement with the observational data near urban sites. Therefore, we conclude that even highly resolved modeling such as at the census-tract scales reported by NATA was unable to predict the high concentration of formaldehyde near airport sites. Since this underprediction was not observed in acetaldehyde, this confirms it as a pollutant-specific uncertainty and can be improved with better emission characterization of formaldehyde. But overall NATA and CMAQ had good agreement with the observational data for other pollutants. NATA was able to predict the local scale values and CMAQ was able to capture the spatial trend.

Comparison of NATA airport and CMAQ airport concentrations: As this paper main focus is to study airport-based concentrations, we envisioned to compare HAPs concentrations due to airport emissions in CMAQ versus those from NATA. However, in NATA, airport concentrations were not reported separately, and instead combined with other non-road sources and collectively reported as non-road concentrations. Since there is no straightforward way to calculate the airport concentrations from NATA, we decided to calculate percent contribution of airport emissions in non–road NEI emissions and apply these numbers to NATA non-road concentrations in order to obtain NATA airport concentrations at county level. This approach might not give accurate values but provide us with approximate airport concentrations in non-road sector as reported by NATA.

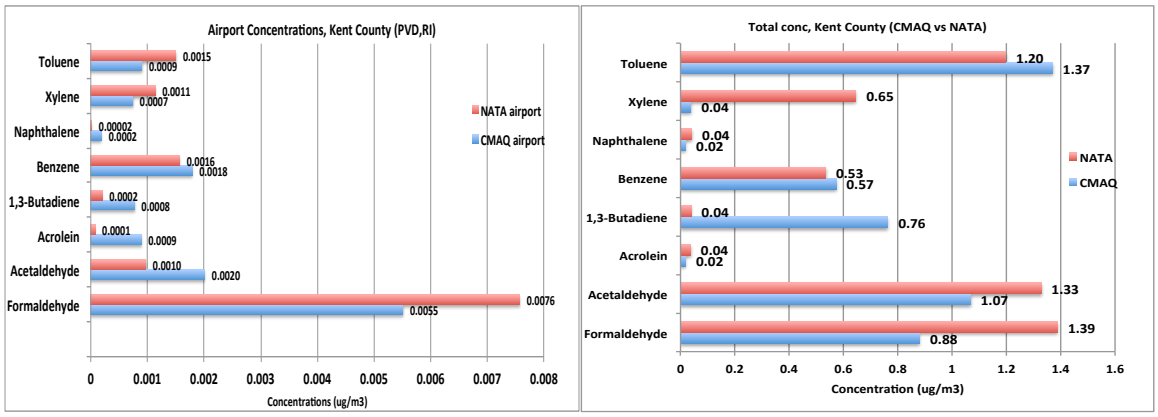


Figure 8: NATA and CMAQ Kent county total concentrations (all sources, right) and airport concentrations (left) of Kent county (where PVD airport is located)

In figure 8 (right) we compared airport concentrations of NATA and CMAQ to see the variation in the model predictions but we could not find any specific trend in their predictions. The differences

observed in total concentrations of two model values (figure 8, left) are reflected in the airport concentrations. The major differences appear in the case of acrolein, 1-3 butadiene where CMAQ concentrations are higher than NATA. But since some of the highly reactive and secondary formed HAPs pollutants have high temporal variability relying on annual concentrations reported by NATA may not be beneficial in all cases, therefore CMAQ which takes into account detailed photochemistry gives us better predictions.

Comparison with BME

When there is a dearth of monitoring data over a study region, one relies on modeling approaches to obtain increased spatial coverage for characterizing air quality (Eberly et al., 2004; Wong et al., 2004). Linear Interpolation, Kriging, Bayesian Maximum Entropy (BME) are some of the statistical model techniques commonly employed to predict concentrations at locations with no monitoring data. As mentioned before most of the airports are deficit of the monitoring data. Hence we made efforts to study the performance of the statistical model near airport region**.** BME is extensively used in many epidemiology health assessment studies and air quality studies to predict background concentrations (Akita et al., 2012). It is a spatiotemporal epistemic knowledge-processing framework that can capture both spatial and temporal trends (Christakos et al., 1990, Christakos et al., 2001). It can also integrate nonlinear and non-gaussian knowledge unlike other interpolation techniques (Audrey et al., 2011). BME uses the available observational data and integrates modeled data based on model performance that makes the integration robust. Here we account only on the application of BME, to get detailed theoretical knowledge readers are recommended to refer some other resources (Christakos et al., 1990, Christakos et al., 2001). Having said that, in this section we considered observational data set (RIDEM, AQS) and combined modeled (CMAQ)-observed data set as inputs to BME tool to study if the predictions can be improved in case of highly emitted reactive pollutants like formaldehyde.

We first considered the complete CMAQ domain and provided the available formaldehyde observational data in the domain (Figure 9, left) as input to BME and the output was compared with CMAQ model predictions (Figure 9, right). The CMAQ predicted spatial concentration plot with an overlay of the BME estimates (values are estimated in the domain present on the left) indicates that at certain locations other than the observational data locations BME overestimates than CMAQ and the error

variance is observed to be higher at these locations. Therefore BME is exaggerating the variability away from the monitoring locations and predicting some higher concentrations even in remote places. So in order to reduce this shortcoming, techniques are developed in prior studies (Audrey et al., 2011) to include the model data along with observation to account for the chemistry and transport of pollutants. Furthermore, due to availability of sufficient observational data near PVD airport (Figure 9), BME shows comparable values as CMAQ due to the ability of BME to consider some of the physical, spatial, temporal terms in the calculation.

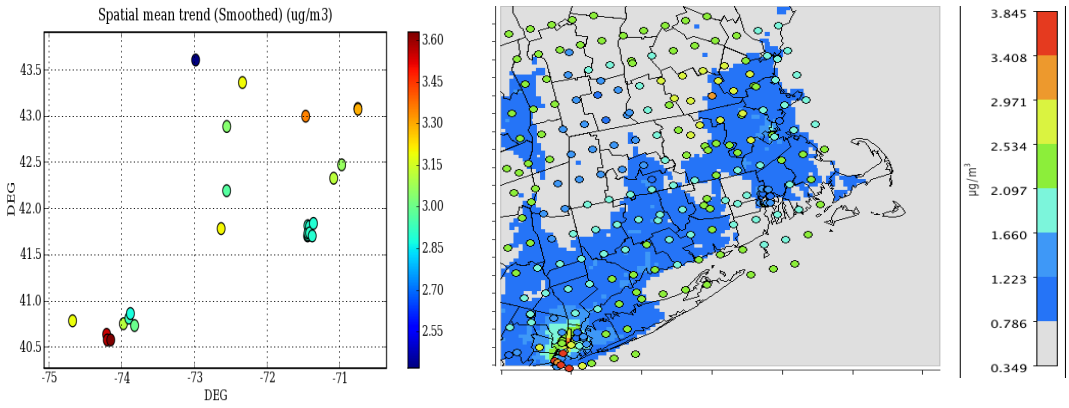


Figure 9: BME spatial mean trend and location of considered observational data (left) and BME estimates overlay on CMAQ concentrations for winter day (right).

Since the complete 4k CMAQ modeling domain did not provide us with more details of BME predictions near airport, thus we focused on PVD airport region to see how predictions are improved with observed data and combined modeled-observed data. Figure 10 represents the PVD region in Rhode Island state and the observed sites (airport and urban) present in the region.

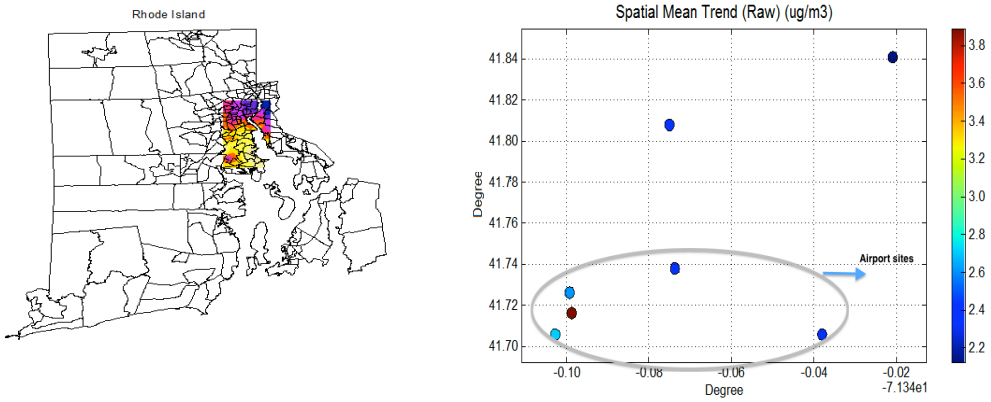


Figure 10: PVD airport region (colored part, left) and the location of the observed data sites in that region (right)

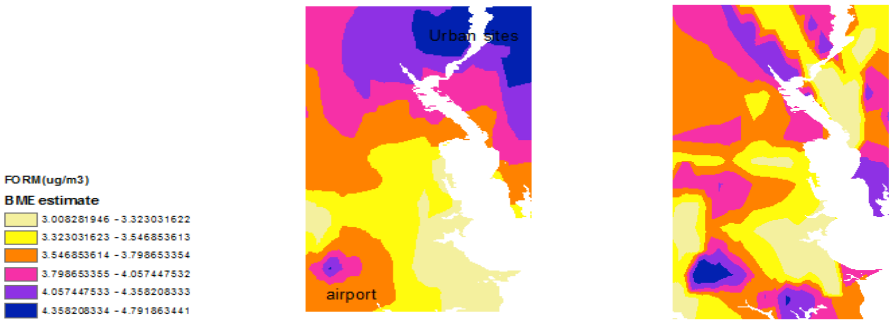


Figure 11: BME estimates obtained by using observational data as input (left) and model combined with observational data as input (right)

BME estimates are calculated for observed and modeled values in this region. BME mean estimate (Figure 11) for the two cases (observed, modeled+observed), we see that we are unable to predict some of the spatial variation with only observed case, whereas predictions other than at monitoring sites are over estimated. But in the case of modeled+observed, we could observe that BME is able to predict the spatial variation (Figure 11) even at other non-monitoring locations. Hence, we feel that considering both observed and monitoring improves the predictions at locations that lack monitoring data.

CONCLUSIONS

In this study, we performed observation and model-based characterization of HAPs near PVD, a mid-sized airport and investigated the performance of various types of models and ways to improve the predictions. This HAPs modeling knowledge near airport can have further implications on the modification of the emissions inventory, more monitoring data near the airports and finer scale modeling approach. Following are some of the major conclusions:

1) Variability: We studied model based temporal and spatial variability of HAPs whose results look comparable with observational data and earlier emission campaign studies. Temporal variability indicated that the concentrations in the winter months are slightly higher than the summer months. There is an absolute difference of 0.04 ug/m3 (relative percentage - 40%) between winter and summer month concentrations in the case of highly emitted pollutant like formaldehyde and lesser difference in remaining species. Our model results indicated airport contribution in the airport grid cell could vary from 7 % in the case of formaldehyde to 34 % in the case of acrolein. Comparing the mean concentration for both modeled and observed concentrations at different spatially located sites, our spatial analysis indicated that the urban

sites (Pawtucket, Providence) appear to have 40 % higher concentrations than airport sites (Field view, Fire station). Except for formaldehyde, we observed 60 % higher concentrations near runway site (Field view) than urban sites clearly indicating pollution from local source like airport.

2) Model Performance: CMAQ model was able to predict the general spatial and temporal trend but could not capture the peak formaldehyde value near runway site and greatly underpredicted acrolein at all sites. The high underprediction of acrolein observed in our modeling studies is similar to the previous studies (Leucken et al., 2006) findings even after considering fine-scale model resolution and highly resolved emissions near the airport in our model simulations. Therefore this issue of sampling detection limits and error involved with monitoring data needs further investigation. Overall model error for all HAPs species considered except for acrolein is within the statistically acceptable Normalized Mean Error range of 36 – 60 %. We also illustrated the need to represent accurately both chemistry to predict secondary contribution and emissions to predict primary contribution. The model evaluation results are based on the sparse dataset available during the simulation period with limited spatial and temporal variability. Hence these model trends and values are subjected to change with change in the size of the airport, location and background concentrations.

3) Model Comparison: We also observed that census tract recent 2005 NATA total model values are comparable with the CMAQ total concentrations (senscase). Both model values are in good agreement with observational data except for pollutants like formaldehyde, where the underestimation still exists. In the case of airport concentrations comparison based on airport contributions to non-road NEI emissions (though we approximated NATA airport concentrations from non-road annual concentrations), we observed significant difference between NATA and CMAQ.

We implemented BME technique on observed and modeled data to illustrate that spatio-temporal statistical model can be used to predict concentrations in the vicinity of the airport and near certain locations that lack monitoring data. Unlike normal kriging techniques, consideration of both observed and modeled data as input to BME accounts for peak values in observed data and variability in modeling data to predict concentrations.

FUTURE WORK

In future, we will perform analysis on other major pollutants to study the impact of highly reactive formaldehyde on other pollutants such as O_3, $PM_{2.5}$ near the airport due to photochemical chemistry. We would also like to improve BME analysis work by cross-validating the results and extend the analysis to other HAPs pollutants.

ACKNOWLEDGEMENTS

This work was funded by PARTNER, under Grant No. 07-C-NE-UNC and 09-C-NE-UNC, and a Fellowship from the UNC Institute for the Environment. The Local Air Quality project is managed by Christopher Sequeira. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of PARTNER and its sponsors. PARTNER is funded by FAA, NASA, and Transport Canada. I would like to acknowledge my advisors Saravanan Arunachalam and William Vizuete for their valuable advice and suggestions in this study.

REFERENCES

1) FAA 2010. FAA Aerospace Forecast Fiscal Years 2010-2030. Available at: http://www.faa.gov/about/office_org/headquarters_offices/apl/aviation_forecasts/aerospace_forecasts/2010-2030/media/FAA%20Aerospace%20Forecasts%20FY%202010-2030.pdf
2) FAA 2011. FAA National forecast FY 2011-2031 by Nan Shellabarger. Available at: http://www.faa.gov/news/conferences_events/aviation_forecast_2011/agenda/media/shellabarger.pdf
3) FAA 2012. FAA Aerospace Forecast Fiscal Years 2012-2032. Available at: http://www.faa.gov/about/office_org/headquarters_offices/apl/aviation_forecasts/aerospace_forecasts/2012-2032/media/FAA%20Aerospace%20Forecasts%20FY%202012-2032.pdf
4) Carslaw D,C., Ropkins K., Laxen Duncan., Moorcroft S., Marner B., Williams M,L., 2008. Near-Field Commercial Aircraft Contribution to Nitrogen Oxides by Engine, Aircraft Type and Airline by Individual Plume Sampling. Environ.Sci.Technol 42, 1871-1876.
5) E.C., Wood, S.C., Herndon, M.T., Timko, P.E., Yelvington and R.C., Miake-Lye., 2008. Speciation and Chemical Evolution of Nitrogen Oxides in Aircraft Exhaust near Airports. Environ. Sci. Technol. 2008, 42, 1884-1891.
6) Timko ,M,T., Herndon,S,C., Wood,E,C., Onasch,T,B., Northway,M,J., Jayne,J,T., Canagaratna,M,R., Miake-Lye,R,C., 2010. Gas Turbine Engine Emissions – Part I: Volatile Organic Compounds and Nitrogen Oxides. Journal of Engineering for Gas Turbines and Power, 2010, Vol.132.
7) M.Mazaheri, G.R., Johnson and L.Morawska, Particle and Gaseous Emissions from Commercial Aircraft at Each Stage of the Landing and Takeoff Cycle, Environ. Sci. Technol. 2009, 43, 441-446.
8) Arunachalam.S ., Wang, B., Baek,B.H., Levy, J.I. Effect of Chemistry – Transport Model Scale and Resolution on Population Exposure to $PM_{2.5}$ from Aircraft Emissions during Landing and Takeoff, Atmospheric Environment, 45 (2011) 1294 – 3300.
9) Woody.M ., B.H.Baek., Adelman Z., Omary M., Lam F.Y., West J.J., Arunachalam S., 2011. An Assessment of Aviation's contribution to Current and Future Fine Particulate Matter in United states, Atmospheric Environment, 45 , 3424-3433.
10) Unal A., Hu,Y., Chang, M.E., Odman, M.T., Russell, G.A., 2005. Airport related emissions and impacts on air quality: Application to the Atlanta International Airport, Atmospheric Environment, 39, 5787-5798.
11) ACRP 2008. Aircraft and Airport-Related Hazardous Air Pollutants: Research Needs and Analysis. FAA, Airport Cooperative Research Program, 2008.
12) Levy ,2008. High Priority Compounds Associated with Aircraft emissions, PARTNER Project 11, prepared by Jonathan I.Levy, Hsiao – Hsien Hsu, Steven Melly.
13) Herndon S,C., Rogers T., Dunlea E,J., Jayne J,T., Maike-Lye R., Knighton B., 2006. Hydrocarbon Emissions from In-Use Commercial Aircraft during Airport Operations. Environ.Sci.Technol 40, 4406-4413.

14) Anderson B,E., Chen Gao., Blake D.R., 2006. Hydrocarbon emissions from a modern commercial airliner. Atmospheric Environment 40, 3601-3612.
15) Schürmann, G., Schäfer, K., Jahn, C., Hoffmann, H., Bauerfeind, M., Fleuti, E., Rappenglück, B., 2007. The impact of NOx, CO and VOC emissions on the air quality of Zurich airport. Atmospheric Environment 41, 103e118.
16) APEX, 2009.Characterization of Emissions from Commercial Aircraft Engines during the Aircraft Particle Emissions eXperiment (APEX) 1 to 3, U.S EPA, October 2009
17) ASPM database. Available at: https://aspm.faa.gov/Default.asp
18) FAA, EDMS. Available at: http://www.faa.gov/about/office_org/headquarters_offices/apl/research/models/edms_model/
19) Baek, B.H., Arunachalam, S., Holland, A., Adelman, Z., Hanna, A., Thrasher, T., and Soucacos, P., 2007. Development of an Interface for the Emissions Dispersion and Modeling System (EDMS) with the SMOKE Modeling System. In: Proceedings of the 16th Annual Emissions Inventory Conference, Raleigh, NC, May 2007.
20) Grell, G.A., Dudhia, J., and Stauffer, D.R., 1994. A description of the fifth generation Penn State/NCAR mesoscale model (MM5). NCAR Technical note NCAR/TN- 398#STR.
21) Byun, D.W., Ching, J.K.S., 1999. Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. EPA/600/R-99/030. Office of Research and Development, U.S. EPA, Washington, D.C.
22) NATA 2005, An Overview of Methods for EPA's National-Scale Air Toxics Assessment, 2011,Available at: http://www.epa.gov/ttn/atw/nata2005/05pdf/nata_tmd.pdf
23) IRIS, EPA. Available at: http://www.epa.gov/IRIS/
24) D.J., Luecken, W.T., Hutzell, G.L., Gipson, 2006. Development and analysis of air quality modeling simulations for hazardous air pollutants. Atmospheric Environment 40, 5087- 5096.
25) Seaman V,Y., Bernett D,H., Cahill T,M., 2007. Origin, Occurrence, and Source Emission Rate of Acrolein in Residential Indoor Air. Environ. Sci. Technol, 2007, 41, 6940-6946.
26) Christakos et al., 1990. A Bayesian/Maximum Entropy View To the Spatial Estimation Problem. Mathematical Geology, Vol.22, No.7, 1990.
27) Akita Y., Chen J C., Serre M L., 2012. The moving-window Bayesian maximum entropy framework: estimation of $PM_{2.5}$ yearly average concentration across the contiguous United States. Journal of Exposure Science and Environmental Epidemiology (2012) 1-6.
28) Audrey D.N., Arunachalam S., and Marc L.S., 2010. Bayesian Maximum Entropy Integration of Ozone Observations and Model Predictions: An Application for Attainment Demonstration in North Carolina. Environ. Sci. Technol. 2010, 44, 5707-5713.
29) G. Christakos, P Bogaert , M L Serre, Temporal GIS: advanced functions for field-based applications, Springer, New York, c2001.
30) Eberly, S.; Swall, J.; Holland, D.; Cox, B.; Baldridge, E. (2004). Developing Spatially Interpolatied Surfaces and Estimating Uncertainty, United States Environmental Protection Agency
31) Wong, D,W., Yuan,L., Perlin,S., 2004. Comparison of spatial interpolation methods for estimation of air quality data. Journal of Exposure Analysis and Environmental Epidemiology (2004) 14, 404-415.
32) ACRP, 2012. Measurement of Gaseous HAP Emissions from Idling Aircraft as a Function of Engine and Ambient Conditions. Airport Cooperative Research Program, Report 23. 2012.

STUDENT BIOGRAPHY

Lakshmi Pradeepa Vennam is a second year PhD candidate in Department of Environmental Engineering at University of North Carolina, Chapel Hill. Presently, she is working under Saravanan Arunachalam investigating aviation impacts on air quality at multiple scales. Air quality modeling and atmospheric chemistry are her major research interests.