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Can Remote Sensing Products Detect the Air Quality Signal due to Aviation Emissions?

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Abstract

Regional air quality model predictions attributable to aircraft for total column aerosol optical depth (AOD) and vertically resolved aerosol extinctions/NO₂ concentrations are compared against MODIS AOD, CALIPSO aerosol extinctions, and SAGE aerosol extinctions/NO₂ concentrations. The goal of this work is to determine if an aircraft-specific signal is present in these metrics and how it compares to remote sensing products. In general, the modeled aircraft signal to aerosol based metrics (optical depth and extinctions) were relatively low (0.03-0.07% of the total modeled signal) limiting comparisons while the NO₂ signal at cruise levels (58% of the total modeled signal) provided a better basis for comparison.

Introduction

To evaluate air quality model performance, results are traditionally compared against ground based observation networks such as the Chemical Speciation Network (CSN), the Interagency Monitoring of Protected Visual Environments (IMPROVE) network, and the SouthEastern Aerosol Research and Characterization (SEARCH) network. These ambient monitoring networks, located at fixed locations throughout the U.S., directly measure ground based concentrations. In turn, these ground based measurements are compared against first layer model based predictions. Given that the intended use of regional air quality model results often include regulatory decision support or assessing health impacts, these ground based evaluations are considered adequate in determining general model performance for these intended applications. However, this approach is not without limitations as ground based observation networks provide relatively sparse coverage and no measurements above ground level.

An alternative approach currently being employed to evaluate model results is through the use of remote sensing products obtained via satellites. These satellites, which typically retrieve various forms of radiation (IR, visible, etc.), can potentially provide more widespread coverage as well as vertical profiles of measured quantities, depending on the satellite, sensor, and retrieval techniques used to obtain the measurement. Sensors are categorized as either active or passive. Active sensors (e.g. RADAR and

LiDAR) generate their own signal and retrieve the reflectance of that signal off objects such as aerosols and clouds. Conversely, passive sensors retrieve radiation typically originating from the sun which is reflected off or emitted by objects. In this study, retrievals from two passive sensors, the Moderate Resolution Imaging Spectroradiometer (MODIS) flying onboard the Aqua and Terra satellites and the Stratospheric Aerosol and Gas Experiment III (SAGE) which flew onboard a Russian Meteor-3M(1) platform, and a combination active sensor and passive sensor onboard the Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) satellite were used to compare against model results.

Regarding aircraft, emissions contain CO, NO_x, SO₂, VOCs, particulate matter, and a number of other hazardous air pollutants which all negatively impact air quality. However, one of the issues with quantifying the impacts from aircraft emissions to air quality is that the signal of these impacts is low (~1% of the total) compared to the signal from other sources in ground based measurements. Remote sensing provides an alternative dataset to determine if an aircraft related signal is present in total column and vertically resolved retrievals and to compare against aircraft modeled air quality impacts.

MODIS is a passive sensor, retrieving radiation originating from the sun and after it has been reflected off the Earth's surface (Figure 1). Since it is a passive sensor and retrieves radiation reflected by the Earth, only information regarding the total column of the atmosphere that the retrieved radiation passed through can be determined. An example of the type of retrievals made by MODIS, and the one used in this study, is aerosol optical depth (AOD), an inferred value commonly used to compare against air quality models. AOD is a total column measurement of the atmosphere's transparency and is a function of the amount of light either scattered or absorbed due to aerosols in the atmosphere. Since AOD is a total column measurement, no information regarding the vertical distribution of the aerosols contributing to AOD is available from the measurement. Considering contributions of aircraft to aerosols that impact AOD are relatively small compared to other emission sources, this type of measurement is limited in its ability to separate the aircraft signal from the noise. However, satellite based retrievals have

wide coverage areas. Therefore, it may be possible to find retrievals made in remote locations where the signal from aircraft is a higher percentage of the total signal. Additionally, MODIS AOD is a commonly used metric to compare regional air quality models against and therefore a good starting point (Roy et al., 2007, Zhang et al., 2009).

CALIPSO retrievals, which are obtained by an active LiDAR sensor coupled with passive inferred and visible imagers, provide vertically resolved aerosol extinctions (removal of radiation due to aerosol scattering and/or absorption) for various altitudes in the atmosphere (Figure 1). CALIPSO is able to obtain vertical profiles due to its ability to retrieve both passive and active signals. For this application, CALIPSO retrievals have the advantage over MODIS in providing retrievals at various altitudes and of being examined at aircraft cruise altitudes.

Finally, SAGE is a passive instrument that provides vertically resolved retrievals of NO₂ and aerosol extinctions in the upper troposphere and lower stratosphere. SAGE obtains these retrievals during sunsets as sunlight traveling tangential to the Earth's surface passes through the atmosphere and is observed by the sensor (Figure 1). Disadvantages of this instrument include that there are only a limited number of years of data are available (2002-2005), retrievals below 10 km are limited and sometimes less reliable (dependent on the parameter being retrieved), and that spatial coverage is generally confined to latitudes above 45° N in the Northern Hemisphere.

The primary goals of this work are twofold: 1) to attempt to identify an aircraft-specific signal within various types of remote sensing data and 2) to evaluate how this signal compares against a regional air quality model which considers aircraft emissions at both the surface and at cruise altitudes. Previous regional air quality modeling studies examining the impacts of aviation emissions from landing and takeoff to surface level air quality have indicated that aircraft contributions are small (< 1%) compared to contributions from all other sources (Woody et al., 2011). If one attempted to compare the aircraft signal against ambient ground based measurements from monitoring networks, the aircraft signal would quickly

be lost in the noise of the total signal. This is where remote sensing retrievals may have the advantage, as increased spatial coverage provides opportunities to determine if an aircraft signal is present in more remote areas either in the vertical or horizontal directions.

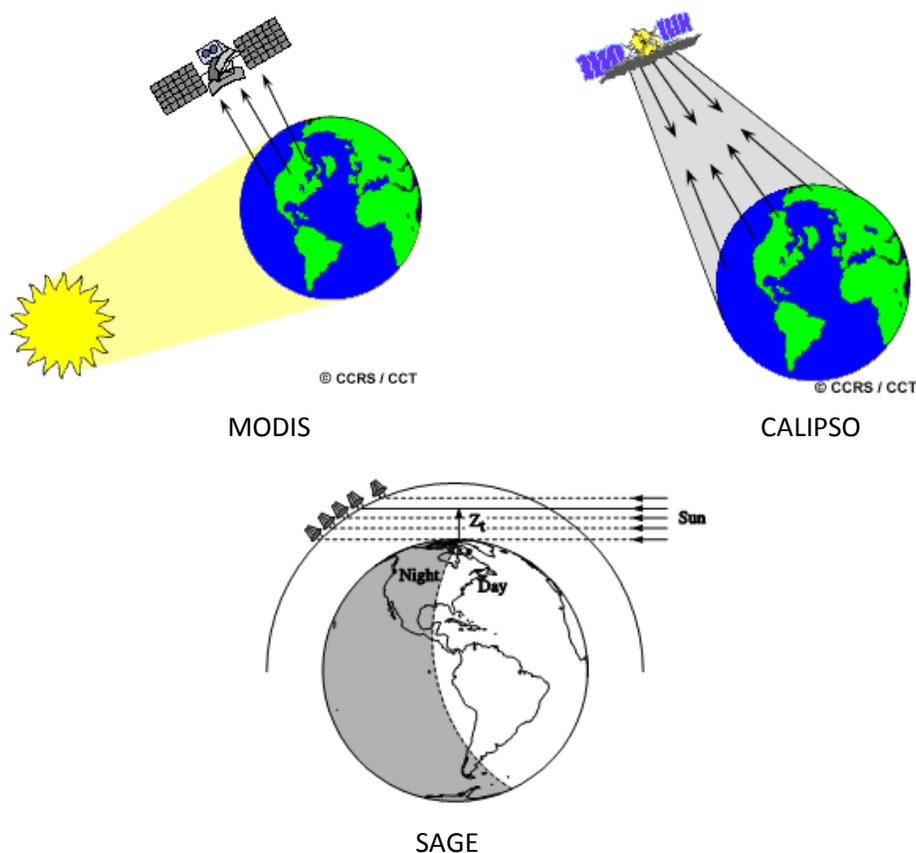


Figure 1. Schematics of MODIS (passive, total column) (Natural Resources Canada, 2012), CALIPSO (active, vertically resolved) (Natural Resources Canada, 2012), and SAGE (passive, vertically resolved) (NASA, 2004) retrievals.

Previous studies attempting to find an aircraft-specific NO_2 signal from total column remote sensing data have largely been unsuccessful to date (Beirle, 2004; Pujadas et al., 2011; Van der Veen, 2011). Pujadas et al. (2011) examined the aircraft NO_2 signal in the Canary Islands and North Atlantic Flight Corridors. In both corridors, Pujadas et al. (2011) concluded that the aircraft-specific signal was lower than the detection limit of the retrieval instruments (SCIAMACHY and OMI) and therefore undetectable. Van der Veen (2011) reported similar results when examining NO_2 column retrievals over clouds, where the clouds were meant to act as a filter for ground level NO_2 . Given that efforts to identify aircraft-specific signals to total column NO_2 have not produced optimal results, this work searches for an

aircraft-specific signal to aerosols (both total column and vertically resolved) as well as a vertically resolved NO₂ signal.

Methodology

MODIS, CALIPSO, and SAGE data were obtained with the goal of identifying an aircraft-specific signal and comparing this signal against modeled results of aircraft contributions. AOD (total column) from MODIS and vertically resolved aerosol extinctions from CALIPSO were obtained and regridded to the model domain (36-km resolution Continental U.S. domain) using the EPA's Remote Sensing Information Gateway (RSIG) (EPA, 2012). Vertically resolved concentrations of NO₂ as well as vertically resolved aerosol extinctions retrieved by SAGE were obtained via NASA's Reverb-ECHO web interface (NASA, 2012) and regridded to the model domain using MATLAB. Regridding of the satellite data was performed to allow it to be paired (in space and time) with and compared against the model results.

Contributions from aircraft were estimated using the Community Multiscale Air Quality (CMAQ) model v5.0.1 (Byun and Ching, 1999; Byun and Schere, 2006) at a 36-km horizontal grid resolution with 34 vertical layers. Simulations were performed for July over the Continental U.S. Meteorological inputs were based on 2005 conditions and generated using the Weather Research and Forecasting (WRF) model. Base case emissions (emissions from all sources with the exception of aircraft) for 2005 were estimated using the EPA's 2005 National Emissions Inventory (NEI) (EPA, 2007) and excluding NEI reported commercial aircraft emissions. Aviation emission estimates were based on a 2006 global aircraft emission inventory (Wilkerson et al., 2010) generated using the Aviation Environmental Design Tool (AEDT) and include full flight (both landing/takeoff and cruise level) emissions. AEDT emissions were gridded into CMAQ ready emission inputs using the AEDTproc utility (Baek et al., 2012). For the sake of this analysis, the intra-year variability in aircraft emissions between 2005 and 2006 is assumed to be negligible. Two simulations were run in CMAQ, a base case with all emissions except aircraft and a sensitivity (sens) case where aircraft emissions were added to the base case. By taking the difference

between the two cases (sens minus base), the incremental contribution attributable to aircraft can be calculated.

CMAQ calculates aerosol extinction coefficients using an empirical approach known as the “reconstructed mass extinction” (Binkowski and Roselle, 2003). The aerosol extinction coefficient β_{sp} , is given by

$$\begin{aligned} \beta_{sp}(km^{-1}) = & 0.003 \times f(RH) \times \{[ammonium\ sulfate] + [ammonium\ nitrate]\} \\ & + 0.004 \times [organic\ mass] + 0.01 \times [elemental\ carbon] + 0.001 \times [fine\ soil] \\ & + 0.0006 \times [coarse\ mass] \end{aligned}$$

where terms in brackets indicate mass concentrations and $f(RH)$ is a relative humidity correction factor obtained from a look-up table given in Malm et al. (1994). Modeled aerosol optical depth can be estimated as the summation of the product of aerosol extinction coefficients and layer heights (ΔZ) over all layers, written as

$$Model_{AOD} = \sum_{i=1}^N \beta_{sp,i} \times \Delta Z_i$$

Of the three satellite data products, note that only MODIS data was available for 2005, the year the base case emissions and meteorological inputs are based. For CALIPSO, retrievals were available for 2006, the year the aircraft emission estimates were based. To prevent the difference in years impacting results, two separate comparisons of CALIPSO and CMAQ results were performed. The first comparison paired the 2006 CALIPSO data in space and time. The second paired seasonally averaged (June-August) CALIPSO results from 2006 to 2008 in space with monthly average 2005 CMAQ results. For SAGE, retrievals range from 2002 to 2005. Given that these retrievals occur at cruise levels, it would be preferable to compare against 2006 retrievals. However, since data is not available for 2006, seasonally averaged (June-August) retrievals for 2002 through 2005 are compared against July CMAQ monthly average results paired in space. Table 1 summarizes the remote sensing datasets used and the CMAQ

results they were compared against. In each instance, CMAQ results were averaged across the hours the instrument retrieves values over the U.S. (15-20 UTC for MODIS and CALIPSO and 0-4 UTC for SAGE) to reduce noise associated with the model results and following the methodologies of other comparison studies of model results to remote sensing data (Roy et al., 2007; Zhang et al., 2009).

Table 1. Summary of remote sensing data and the relevant model results used to compare against.

Sensor/Satellite	Retrieved Parameter(s)	Retrieval Time Period	CMAQ Time Period
MODIS (total column)	AOD	Jul 2005	Jul 2005 (15-20 UTC)
CALIPSO (vertically resolved)	Aerosol Extinction	Jul 2006 Jun-Aug 2006-2008	Jul 2005 (15-20 UTC) Jul 2005 (15-20 UTC)
SAGE (vertically resolved)	NO ₂ Aerosol Extinction	Jun-Aug 2002-2005	Jul 2005 (0-4 UTC)

Results and Discussion

MODIS

Comparisons of total column AOD indicate that CMAQ generally overpredicts AOD in July with a domain average of 0.2458 (unitless) in the sens case compared to a MODIS average retrieval of 0.2044 (Table 2). This overprediction corresponds to a normalized mean bias (severity of over/underprediction) of 20.3% and a normalized mean error of 61.3%. Considering only results in the Eastern U.S., normalized mean bias and error improve to 11.7% and 57.3%, respectively. This improved performance is reflected in spatial trends of July monthly average AOD values, where MODIS AOD retrievals compare more favorable to CMAQ predictions in the Eastern U.S. (Figure 2). The improved performance is partially attributable to more accurate AOD retrievals from MODIS in the Eastern U.S. due to heavier vegetative cover (Hoff and Christopher, 2009). The MODIS AOD vs. CMAQ results are comparable to those reported by Roy et al. (2007) and Zhang et al. (2009) who reported normalized mean biases ranging from -37.1 to -17.6% and normalized mean errors ranging from 48.1-88.2%. Note that in this work the bias indicates an overprediction by CMAQ whereas these previous studies indicated an underprediction. One possible cause for the shift in bias is that the previous 2 studies compared 2001 whereas here the

comparison is for 2005 with results derived from different inputs (e.g. meteorological conditions, emissions, etc.).

Table 2. July MODIS and CMAQ AOD values.

Mean MODIS AOD	Model Scenario	Mean CMAQ AOD	Normalized Mean Bias (%)	Normalized Mean Error (%)	Coefficient of determination (R ²)
CMAQ Domain					
0.2044	base	0.2457	20.2	61.3	0.1227
	sens	0.2458	20.3	61.3	0.1228
Eastern U.S.					
0.2714	base	0.3028	11.6	57.3	0.2138
	sens	0.3030	11.7	57.3	0.2140

Comparisons of total column AOD values in CMAQ with and without aircraft indicate that the aircraft emissions signal to modeled AOD is relatively low ($1-2 \times 10^{-4}$ or approximately 0.03-0.04% of total AOD) both throughout the domain and in the Eastern U.S. In comparison, aircraft predicted contributions to surface level PM_{2.5} are on average $0.0034 \mu\text{g}/\text{m}^3$ throughout the entire domain (0.12% of total PM_{2.5}) and $0.0109 \mu\text{g}/\text{m}^3$ in the Eastern U.S. (0.14% of total PM_{2.5}). These results indicate the aircraft-specific signal to AOD is similarly low as compared to the aircraft surface level PM_{2.5} signal on a percent basis.

Limiting the comparison to a 396 km^2 area off the coast of New England and over the Atlantic Ocean does little to strengthen the aircraft AOD signal. Within this area, aircraft contribute 2×10^{-4} to total AOD or 0.07% of the total. It may be that this area, located just off the coast, is impacted by transport from the Northeastern U.S. Future considerations might instead examine areas within the North Atlantic Flight Corridor further away from land masses, where the aircraft signal to AOD and PM_{2.5} should be higher relative to the signal from other sources.

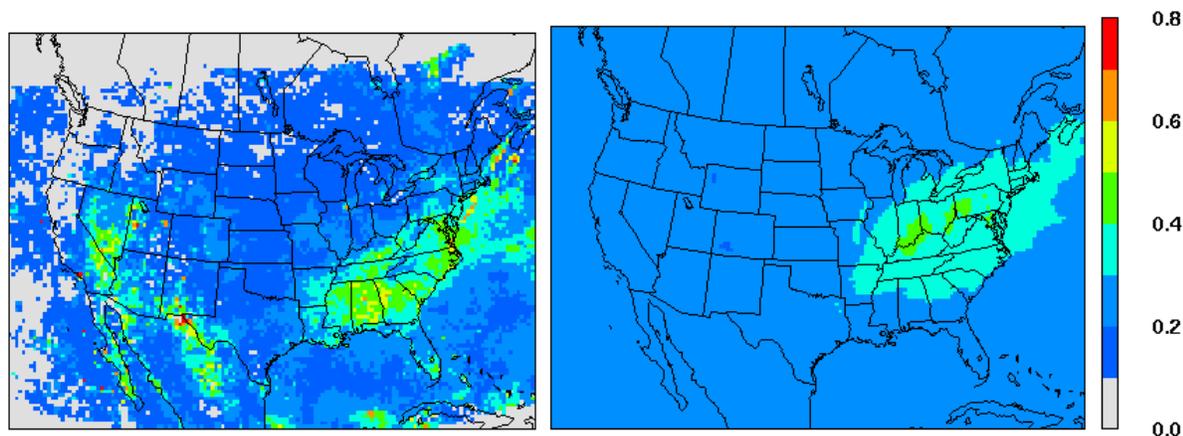


Figure 2. July monthly average AOD as retrieved by MODIS (left) and predicted by the CMAQ sens case (right).

CALIPSO

July 2006 CALIPSO aerosol extinction retrievals range from 0.1 km^{-1} near the surface to 0.02 km^{-1} near 14 km (Figure 3). When compared against CMAQ values, CALIPSO retrievals are higher at all altitudes and neither CMAQ nor CALIPSO appear to exhibit an increase in aerosol extinctions at aircraft cruise altitudes. Averages of CALIPSO retrievals from Jun-Aug 2006-2008 were also examined and used to determine if the higher July 2006 CALIPSO retrievals were outliers or part of the general trend (Figure 3). Based on these longer term results, the CALIPSO values still range from approximately 2 to 10 times higher than the CMAQ aerosol extinctions. One possibility as to why CALIPSO aerosol extinctions are much higher than CMAQ predictions is that the detection limit of the sensor ranges from approximately $1-2 \times 10^{-2} \text{ km}^{-1}$ (Ye et al., 2010). These detection limits correspond to the range of average values as predicted by CMAQ at aircraft cruise altitudes and, assuming CMAQ does not underpredict aerosol extinctions, indicate that CALIPSO data may not be suitable for higher altitudes (above 5,000 m). The limitation of the detection limit is also reflected in the number of CALIPSO retrievals at cruise altitudes. For Jul 2006, only 38 retrievals were available at an altitude of 10 km compared to 1,401 retrievals at 1 km. Finally, the CALIPSO retrievals are also much higher than SAGE retrievals presented in the subsequent section and the Global Ozone Monitoring by Occultation of the Stars (GOMOS), which report

aerosol extinction coefficients at 10 km ranging from approximately $1-4 \times 10^{-3} \text{ km}^{-1}$ (Vanhellemont et al., 2010).

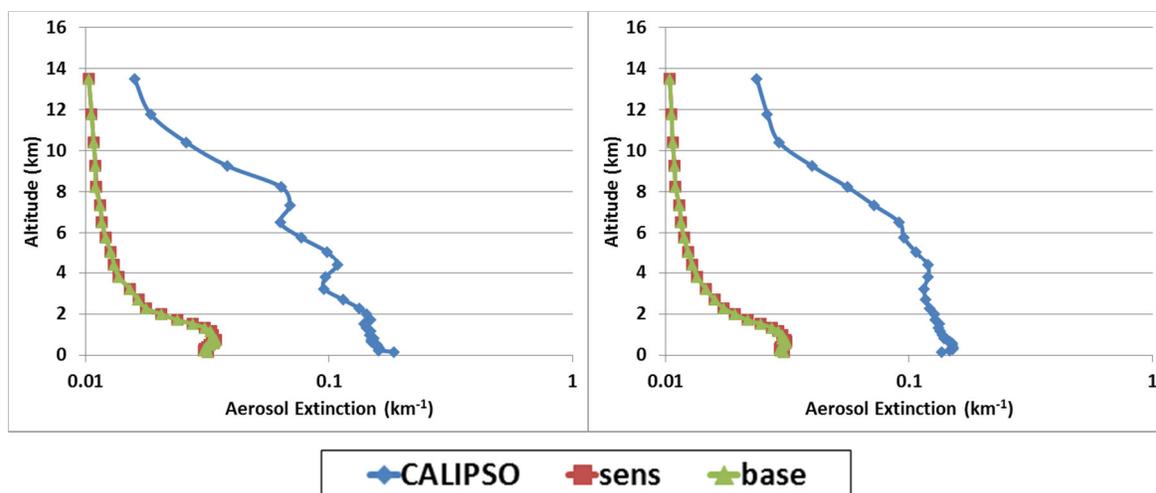


Figure 3. CALIPSO vs. CMAQ aerosol extinction profiles in Jul 2006 (left) and CALIPSO Jun-Aug 2006-2008 average vs. CMAQ Jul monthly average aerosol extinctions (right).

Contributions of aircraft in CMAQ increase average aerosol extinctions at 10 km by approximately $4.4 \times 10^{-6} \text{ km}^{-1}$ (0.04% of the total aerosol extinction at cruise altitudes) with a maximum 1 hour contribution of $7 \times 10^{-4} \text{ km}^{-1}$ (5% of the extinction coefficient value at that hour). This value is well below the detection limit of CALIPSO, suggesting it may not a viable option to use to assess contributions from aircraft emissions at cruise altitudes.

SAGE

Summer averaged vertical profiles of NO_2 and aerosol extinctions as retrieved by SAGE indicate an increase in both at typical aircraft cruise altitudes of approximately 10 km (Figure 4). When compared against CMAQ vertical profiles to those as retrieved by SAGE for NO_2 , the CMAQ profile with aircraft emissions (sens) does appear to better represent the profile of the SAGE retrievals (Figure 4). CMAQ concentrations increase by 59% between 8-10 km compared to a 21% increase in SAGE retrievals between 8-11.5 km (or 41% increase between 9-11.5 km). While the maximum impacts occur at different

altitudes, this may, in part, be due to the regridding of SAGE data to the more coarse CMAQ vertical resolution.

CMAQ predictions of NO_2 at 10 km with aircraft emissions are approximately twice that of predictions without aircraft emissions (1.34×10^8 vs. 5.68×10^7 molecules cm^{-3}). However, CMAQ predictions of NO_2 in both the base and sens cases are approximately an order of magnitude lower compared to SAGE retrievals (4.25×10^9 molecules cm^{-3} at 10 km). It is unclear as to why CMAQ predictions are lower, but possibilities include the aircraft emissions in the model being too low or issues with the modeled chemistry or transport processes at higher modeled altitudes. Future investigations into this issue may prove useful in determining why this might be the case and the accuracy of CMAQ NO_2 predictions aloft. It should also be noted that these simulations did not include NO_x emissions from lightning, another major source of NO_2 at aircraft cruise altitudes, which could also lead to an underprediction of NO_2 .

Aerosol extinctions are approximately 2 to 3 times higher in CMAQ when compared to SAGE retrievals. Additionally, CMAQ does not appear to capture the profile of increasing aerosol extinction values near aircraft cruise altitudes indicated by SAGE. In fact, the CMAQ sens and base case results predict nearly identical aerosol extinction values, differing by 0.03% at locations of SAGE retrievals. CMAQ predicted aerosol extinctions also change minimally (~1%) between the altitudes plotted in Figure 4. SAGE, on the other hand, indicates an increase of 26.4% between 8-9 km. However, when only considering the SAGE data, it is difficult to determine to what extent aircraft are responsible for the increase in aerosol extinctions at 9 km. Also, it is difficult to determine the reasons behind the differences in CMAQ predictions and SAGE retrievals. This issue is compounded by the weak signal of aircraft emissions to CMAQ aerosol extinctions, due possibly to the assumptions used to calculate aerosol extinctions, underestimates of particulate matter aircraft emissions at cruise altitudes, or transport processes. Given that aircraft are the only emission source aloft currently considered in the model, one

would expect them to comprise a larger percentage of extinctions and future considerations are needed to determine to what extent aircraft actually contribute at cruise altitudes.

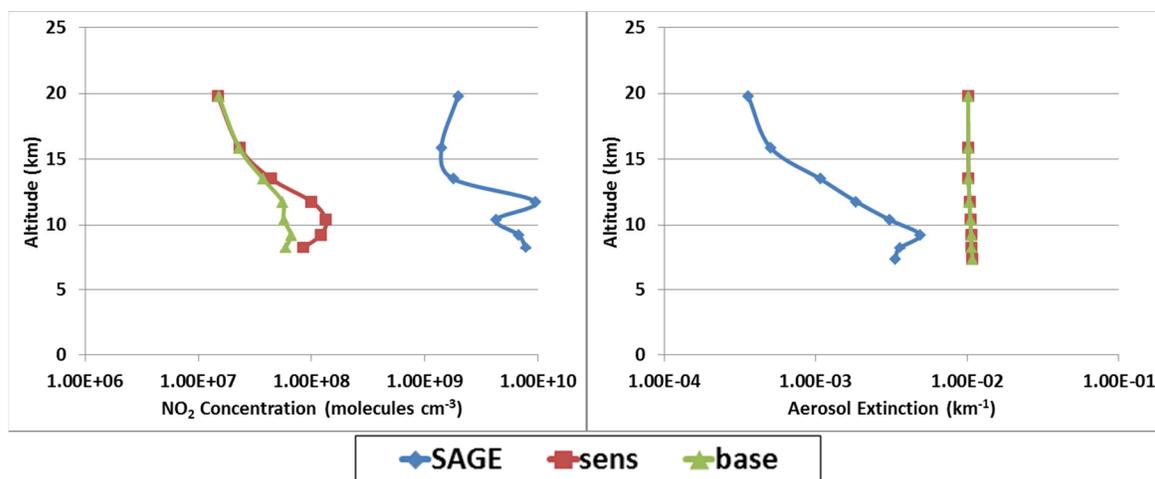


Figure 4. SAGE Jun-Aug 2002-2005 vs. CMAQ Jul vertical profiles of NO₂ and aerosol extinctions.

Conclusions

Regional air quality predictions for aerosol optical depth, aerosol extinctions, and NO₂ concentrations attributable to aircraft were compared against remote sensing data from MODIS, CALIPSO, and SAGE satellite retrievals. In general, CMAQ AOD predictions were comparable to MODIS AOD retrievals, particularly in the Eastern U.S., where normalized mean bias and normalized mean error in the sens case were 11.7% and 57.3%, respectively. However, the aircraft-specific signal to AOD was relatively low (0.03-0.07%) and was in fact lower than contributions to PM_{2.5} concentrations (0.12-0.14%) on a percentage basis, suggesting that AOD does not provide an improvement over aircraft-specific PM_{2.5} contributions compared against ambient measurements.

Similarly, aerosol extinctions at cruise altitudes as predicted by CMAQ indicate a small aircraft-specific signal with an average contribution of $4.4 \times 10^{-6} \text{ km}^{-1}$ (0.04% of the total aerosol extinction at cruise altitudes). Assuming CMAQ does not underpredict aerosol extinctions at cruise levels (SAGE data suggests it overpredicts), this value is well below CALIPSO's detection limit of $1-2 \times 10^{-2} \text{ km}^{-1}$ and suggests it is not a viable option to compare aircraft contributions against.

SAGE does indicate an increase in both aerosol extinctions and NO₂ concentrations at aircraft cruise altitudes, although further analysis is required to determine to what extent aircraft contribute to these profiles. This could include identifying retrievals made within areas of higher known flight activity and comparing them against retrievals in areas with limited flight activity. It could also include obtaining NO₂ profiles from other data sources, such as the SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY (SCIAMACHY) remote sensing instrument. While on a percentage basis, the increase in NO₂ at cruise altitudes compares favorably between CMAQ and SAGE (59% compared to 21-41%), the SAGE measurements are an order of magnitude or more higher than CMAQ predictions. For aerosol extinctions, SAGE indicates an increase of 26.4% between 8-9 km whereas CMAQ predictions vary minimally with changing altitudes (~1%). Additionally, CMAQ predictions are 2 to 3 times higher at cruise altitudes and do not appear to indicate a strong aircraft signal.

There are a number of limitations associated with remote sensing retrievals that require mentioning. Some of these limitations have already been discussed, such as inaccurate AOD retrievals in the Western U.S. by MODIS, the detection limit of CALIPSO, and the limited spatial coverage of SAGE. Other limitations include that remote sensing retrievals are not direct measurements but inferred values based on measured optical properties (Hoff and Christopher, 2009). Assumptions are required to relate the retrieved optical property to a concentration or total column value and the methodologies are not always robust, particularly for aerosols which vary significantly in size, composition, and hydration (Christopher and Hoff, 2009). Also, clouds can prevent retrievals or cause inaccurate retrievals and though many instruments such as CALIPSO provide quality control measures to remove artifacts attributable to clouds, the quality control protocols are not foolproof. Finally, some information is lost when satellite data is regridded from its native retrieval grid to other grids, as is the case when spatial data is aggregated and averaged.

The results in this exploratory work are preliminary and require further evaluation and investigation. Possible future extensions could compare the results from other CMAQ domains, such as a

hemispheric CMAQ domain, to examine the signal for aircraft in other regions of the Northern Hemisphere. The hemispheric domain would provide more opportunities to examine regions where the aircraft signal is a larger percentage of the total signal, such as in the North Atlantic Flight Corridor. Also, retrievals from other remote sensors should be considered. Given that the aircraft signal to NO₂ was stronger compared to AOD and aerosol extinctions, it would seem comparisons against gas phase species would likely produce more desirable results. Possible remote sensors to consider include SCIAMACHY NO₂ profiles and Measurements of Pollutants in the Troposphere (MOPITT) CO profiles.

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Student Biography

Matt is a PhD candidate in the Department of Environmental Sciences and Engineering at the University of North Carolina at Chapel Hill. As a fifth year student, he is currently working under Dr. Saravanan Arunachalam with the UNC Center for Environmental Modeling for Policy Development and Dr. J. Jason West with the UNC Department of Environmental Sciences and Engineering on the PARTNER Project 16 - Investigation of Aviation Emissions Air Quality Impacts. His chief research interests include atmospheric air pollution, air quality modeling, and secondary organic aerosols.