Atmos. Chem. Phys. Discuss., 13, 1089–1132, 2013 www.atmos-chem-phys-discuss.net/13/1089/2013/ doi:10.5194/acpd-13-1089-2013 © Author(s) 2013. CC Attribution 3.0 License.



This discussion paper is/has been under review for the journal Atmospheric Chemistry and Physics (ACP). Please refer to the corresponding final paper in ACP if available.

A plume-in-grid approach to characterize air quality impacts of aircraft emissions at the Hartsfield-Jackson Atlanta International Airport

J. Rissman¹, S. Arunachalam², M. Woody³, J. J. West³, T. BenDor⁴, and F. S. Binkowski²

¹Energy Innovation: Policy and Technology LLC, 98 Battery St. Ste. 202, San Francisco, CA 94111, USA

²Institute for the Environment, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

³Department of Environmental Science and Engineering, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

⁴Department of City and Regional Planning, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA





Received: 13 November 2012 – Accepted: 21 December 2012 – Published: 9 January 2013

Correspondence to: S. Arunachalam (sarav@email.unc.edu)

Published by Copernicus Publications on behalf of the European Geosciences Union.





Abstract

This study examined the impacts of aircraft emissions during the landing and takeoff cycle on PM_{2.5} concentrations during the months of June 2002 and July 2002 at the Hartsfield-Jackson Atlanta International Airport. Primary and secondary pollutants were modeled using the Advanced Modeling System for Transport, Emissions, Reactions, and Deposition of Atmospheric Matter (AMSTERDAM). AMSTERDAM is a modified version of the Community Multiscale Air Quality (CMAQ) model that incorporates a plume-in-grid process to simulate emissions sources of interest at a finer scale than can be achieved using CMAQ's model grid. Three fundamental issues were investigated: the effects of aircraft on PM_{2.5} concentrations throughout northern Georgia, the differences resulting from use of AMSTERDAM's plume-in-grid process rather than a traditional CMAQ simulation, and the concentrations observed in aircraft plumes at sub-grid scales. Comparison of model results with an air quality monitor located in the vicinity of the airport found that normalized mean bias ranges from -77.5 % to

- ¹⁵ 6.2% and normalized mean error ranges from 40.4% to 77.5%, varying by species. Aircraft influence average $PM_{2.5}$ concentrations by up to 0.232 µg m⁻³ near the airport and by 0.001–0.007 µg m⁻³ throughout the Atlanta metro area. The plume-in-grid process increases concentrations of secondary PM pollutants by 0.005–0.020 µg m⁻³ (compared to the traditional grid-based treatment) but reduces the concentration of
- ²⁰ non-reactive primary PM pollutants by up to 0.010 µg m⁻³, with changes concentrated near the airport. Examination of sub-grid scale results indicates that puffs within 20 km of the airport often have average PM_{2.5} concentrations one order of magnitude higher than aircraft contribution to the grid cells containing those puffs, and within 1–4 km of emitters, puffs may have PM_{2.5} concentrations 3 orders of magnitude greater than the aircraft contribution to their grid cells. 21 % of all aircraft-related puffs from the Atlanta airport have at least 0.1 µg m⁻³ PM_{2.5} concentrations. Median daily puff concentrations
- tions vary between 0.017 and 0.134 μ g m⁻³, while maximum daily puff concentrations vary between 6.1 and 42.1 μ g m⁻³ during the 2-month period. In contrast, median daily





grid concentrations vary between 0.015 and 0.091 μ g m⁻³, while maximum daily grid concentrations vary between 0.751 and 2.55 μ g m⁻³. Future researchers may consider using AMSTERDAM to understand the impacts of aircraft emissions at other airports, for proposed future airports, for airport expansion projects under various future scenarios, and for other national-scale studies specifically when the maximum impacts at fine scales are of interest.

1 Introduction

The Hartsfield-Jackson Atlanta International Airport is the busiest airport in the world in terms of passenger traffic (Airports Council International, 2010). Major airports such as Atlanta Hartsfield can be important economic drivers in their regions and key transit hubs for people worldwide. However, a large airport produces emissions that have the potential to adversely affect air quality in communities near the airport and throughout the wider region. Aircraft engines emit nitrogen oxides (NO_x), sulfur dioxide, black carbon (soot), and other compounds that are primary air pollutants or contribute to formation of secondary pollutants through chemical reactions in the atmosphere.

In the past, numerical modeling of emissions along with atmospheric physical and chemical processes has been used to understand the air quality impacts of aircraft emissions. Fixed-grid (Eulerian) models are used to represent the effects of dispersed pollutant sources on air quality, but they lack the resolution to distinguish impacts near

- a major point source. Plume (Lagrangian) models represent pollutants as moving puffs to allow for better representation of impacts near a large point source and for chemical processing within a highly polluted plume. To gain the benefits of both techniques, plume-in-grid models have been developed, which represent large point sources such as a single power plant or collection of power plants in their regional context (Karam-
- chandani et al., 2002). Here we apply an Eulerian model with plume-in-grid capabilities to assess the effects of aircraft emissions on air quality near the airport and over a larger region. We represent airplane traffic from landing and takeoff as a series of





emitters near the airport, the first application that we are aware of to use a plume-ingrid model to represent moving, elevated sources.

We used the Advanced Modeling System for Transport, Emissions, Reactions, and Deposition of Atmospheric Matter, or AMSTERDAM (Karamchandani et al., 2010),
 to evaluate impacts of aircraft emissions during landing and takeoff (LTO) cycles (< 1000 m) on ground-level pollutant concentrations during June and July 2002 at the Atlanta Hartsfield airport. Our study had three objectives. First, we aimed to characterize the effect of aircraft emissions at Hartsfield-Jackson airport on ground-level fine particulate matter (PM_{2.5}) concentrations in Atlanta and surrounding areas. Second, we set out to understand the differences in modeled PM_{2.5} concentrations resulting from the use of the AMSTERDAM model, which incorporates a plume-in-grid process for

aviation emissions, relative to the use of a traditional gridded air quality model. Third, we compared the concentrations in aircraft plumes to the impacts of aircraft on grid cell concentrations, to better understand whether localized very high concentrations may be obscured in an analysis that does not characterize sub-grid scale variability.

We examine total PM_{2.5} and its components (black carbon, sulfate, nitrate, ammonia, organic, and uncategorized PM_{2.5}), because of the significant potential health impacts of fine particulate matter due to aviation (Levy et al., 2008, 2012; Arunachalam et al., 2011). Exposure to PM_{2.5} has been linked to increased rates of lung cancer and cardiopulmonary mortality (Pope et al., 2002).

Knowledge of aircraft contribution to pollutant concentrations is an important step in understanding the human and economic costs associated with aircraft-related pollution. Such analysis may also provide a useful baseline for comparison with scenarios that consider the efficacy of mitigation measures, such as use of biofuels, fuel-efficient

engine technologies, altering airline flight schedules, and re-balancing load between different regional airports. Results may also be of interest to local governments siting new airports and planning land use near airports, and to regulators setting emissions standards for jet engines.





Literature review 2

Model history and development 2.1

Numerical modeling has been used to evaluate air quality impacts from aircraft activity at airports for decades. Two models commonly used to quantify aircraft emissions in the United States are the Emissions Dispersion and Modeling System (EDMS) (Federal Aviation Administration, 1998) and its successor, the Aviation Environmental Design Tool (AEDT) (Aviation Environmental Design Tool, 2010).

EDMS is the most commonly used aircraft emissions model in the US because the Federal Aviation Administration (FAA) designated it in 1998 as the required model for

- air quality analyses of aviation emissions sources. EDMS calculates aviation emissions during the LTO cycle within the mixing height. Researchers have used EDMS to address topics that relate to local air quality impacts, such as the effects of a reduction in aircraft thrust at takeoff on annual NO, emissions (Hall, 2003) and the air quality impact of new construction projects at airports (Moss, 1994).
- The FAA is currently developing the Aviation Environmental Design Tool (AEDT), a model that estimates aircraft emissions, noise, and other impacts. Similar to EDMS, AEDT calculates aircraft flight performance and uses this information to generate emissions. Preliminary versions of this model have been used by researchers (Noel, 2009; Wilkerson, 2010). EDMS generates outputs at an airport level, while AEDT generates outputs from airport-level to national to global scales. EDMS and AEDT outputs can be 20
- used in dispersion models, such as the American Meteorological Society/US EPA Regulatory Model (AERMOD) (Cimorelli et al., 2005) and other chemistry transport models as discussed below.

AMSTERDAM takes emissions and meteorological information as inputs, and simulates chemistry and physical processes associated with emissions sources at subgrid-25 scales to determine the resulting environmental concentrations. As AMSTERDAM was built from a combination of two earlier models, we first discuss each component model. The first component is the Community Multiscale Air Quality modeling system (CMAQ)





15

5

(Byun and Schere 2006; Foley et al., 2010). CMAQ is an Eulerian model based on a 3-D grid. It accepts meteorology and emissions inputs, models chemical and microphysical processes, and determines the resulting chemical concentrations in each grid cell. CMAQ has been used in the past to model the impacts of aviation emissions (Unal

- et al., 2005; Ratliff et al., 2009; Arunachalam et al., 2008, 2011; Woody et al., 2011). However, CMAQ is limited by its reliance on grid cells that are relatively large in size and may not accurately represent the chemical processes in concentrated emissions plumes, such as those emitted by aircraft. Understanding these processes is critical for local-scale air quality assessment in and around an airport. Large grid cells may
 result in an artificial dilution of emissions, which can alter the chemical reactions that
- form pollutants and can result in the under-prediction of pollutant concentrations near emissions sources (Arunachalam et al., 2008).

The second component is the Second-Order Closure Integrated Puff Model with CHEMistry (SCICHEM), which evolved from a model called "SCIPUFF". SCIPUFF is

- ¹⁵ a Lagrangian dispersion model originally developed to model the fate and transport of hazardous materials (Sykes and Gabruk, 1997; Sykes et al., 1998). It tracks emissions as a series of individual "puffs" in three-dimensional space. SCIPUFF focuses on modeling the locations and sizes of emitted puffs, accounting for physical factors such as winds and buoyancy. It is capable of dividing puffs that become too large into smaller
- ²⁰ puffs and merging overlapping puffs together (Karamchandani, 2010). SCIPUFF was later extended with the capability to utilize chemistry routines to account for reactions occurring inside the puffs and renamed "SCICHEM" (Santos et al., 2000). SCICHEM supports both intra-plume and inter-plume interactions by treating both splitting and merging of puffs to account for wind shear effects and varying chemistry across the
- plume. SCIPUFF and SCICHEM have been used in numerous research studies of plume dispersion, specifically from major point sources such as power plants, but they have seldom if ever been used to model aviation emissions.

Finally, we review the development history behind AMSTERDAM. Karamchandani et al. (2002) created an air quality model by combining CMAQ and SCICHEM.





Karamchandani et al. (2002) named their model "CMAQ-APT" wherein "APT" stands for "Advanced Plume Treatment," referring to the capabilities added by SCICHEM. In this model, emissions that are not of direct interest are added directly to the grid, as in a traditional CMAQ model simulation. Emissions from sources of interest are rep-

- resented as Gaussian puffs, which are tracked separately in three-dimensional space within the CMAQ grid. The combination of these two approaches is called Plume-in-Grid (PinG). In CMAQ-APT, the same chemistry routines are used to model reactions within the puffs as well as within each grid cell. As puffs age, they grow larger and more dilute due to infiltration of background air. When puffs are sufficiently large or dilute, it
- ¹⁰ is no longer worthwhile to track them separately from the surrounding air. At that point, the puffs' contents are added to the grid cells where the puffs are located (based upon the centroid of the puffs), and the puffs themselves are removed from the model. Thus, in each timestep, new puffs are added to the simulation while old puffs are "merged" into the grid.
- ¹⁵ Karamchandani et al. (2006) then enabled their model to utilize a different mechanism for simulation of particulate matter: the Model of Aerosol Dynamics, Reaction, Ionization, and Dissolution (MADRID), whose most important changes related to the model's particle size distribution and secondary organic aerosol formation. By 2008, they produced a version with new mercury- and aerosol-related processes called the
- "Advanced Modeling System for Transport Emissions, Reactions and Deposition of Atmospheric Matter" (AMSTERDAM), whose impacts on mercury results were examined by Vijayaraghavan et al. (2008). In a later paper, the same team describes AMSTER-DAM as a "suite" of three models: CMAQ-AERO3-APT (which uses the original CMAQ particulate matter treatment plus SCICHEM PinG), CMAQ-MADRID (which uses the
- MADRID particulate matter treatment without PinG), and CMAQ-MADRID-APT (which uses both the MADRID PM treatment and SCICHEM PinG) (Karamchandani et al., 2010). In our study, we used only the first of these model configurations, i.e. the version that combines CMAQ and APT. Additional details about this model and its configuration options are available in Karamchandani et al. (2010).





2.2 Prior model applications for Hartsfield-Jackson International Airport

This study extends prior modeling work that has been conducted to understand the impacts of aircraft emissions at the Hartsfield-Jackson Atlanta International Airport. Unal et al. (2005) modeled aircraft emissions during a high-pollution episode from 11–20 August 2000 using CMAQ. For PM_{2.5} emissions, they relied on a first-order approximation by Wayson et al. (2003), which is a predecessor to the method used in this study (Wayson et al., 2009). Using emissions differentiated by flight mode and added to the model in 3-D space based on aircraft flight paths, they found the airport had a maximum impact on PM_{2.5} levels of 4.4 µg m⁻³ and impacts of about 1 µg m⁻³ in a radius of 16 km around the airport.

In order to enable the airport to be efficiently examined with the CMAQ model, Baek et al. (2007) developed a tool, "EDMS2Inv", which is capable of converting the emissions files created by EDMS (intended for use in AERMOD) into a format that allows them to be used in CMAQ. This tool was used to conduct an analysis of the impacts of

LTO emissions at three airports: Providence T. F. Green (PVD), Chicago O'Hare (ORD) and Atlanta Hartsfield-Jackson (ATL) (Arunachalam et al., 2008). In that study, annual and monthly average aircraft contribution to PM_{2.5} and its components were modeled at CMAQ grid resolutions of 12 km and 36 km. Arunachalam et al. 2008 found that in the grid cell with the maximum impact due to aircraft at the 12 km resolution, annual average PM_{2.5} concentrations increased by over 0.2 µg m⁻³.

A study estimating mortality due to PM_{2.5} exposure from LTO emissions at three airports (ATL, ORD, and PVD) used emissions derived from EDMS in CMAQ simulations (Arunachalam et al., 2011). ATL was investigated at 36 km, 12 km, and 4 km grid resolutions. The run with 4 km resolution included June and July 2002 and used the same background (i.e., non-aviation) emissions as the present study. They reported that the monthly average PM_{2.5} contribution due to ATL airport emissions at the grid cell containing the airport ranged from slightly below 0.1 to 0.65 μg m⁻³ depending on modeled grid resolution. The study concluded that a lower-resolution model with large





domain is suitable for understanding population-average exposure, but an assessment of maximum individual risk would require high-resolution modeling near the airport.

Woody and Arunachalam (2012) investigated the effects of aircraft on secondary organic aerosol (SOA) formation near Hartsfield-Jackson International Airport. That

- s study used EDMS emissions processed through the EDMS2Inv tool as input data for CMAQ model runs at 36 km, 12 km, and 4 km grid resolutions. Woody and Arunachalam found that in the grid cell containing the airport at the 36 km and 12 km resolutions, aircraft reduced SOA concentrations because of the reaction of aircraft NO_x emissions with NO₃ radicals, leaving fewer nitrate radicals to oxidize SOA precursors. However,
- at the 4 km grid resolution, aircraft increased SOA concentrations by providing a higher concentration of primary organic aerosol (POA) to serve as seed particles onto which SOA could partition. The use of larger grid cells diluted POA concentrations, lowering SOA production in those model runs.

2.3 Notable related modeling work

- Plume modeling of aircraft impacts is an area of active research, and a number of scientists are using related approaches to understand the environmental consequences of aviation emissions. For example, Naiman et al. (2010) developed a subgrid plume model (SPM) and used it to track aircraft emissions by modeling linear aircraft contrails. Naiman et al. (2010) suggest that their model is computationally efficient and, in the
- future, could be used as a subgrid process in a large-scale atmospheric simulation. Meilinger et al. (2005) note the difficulty of accounting for the chemistry and microphysics of aircraft exhaust in Chemistry Transport Models due to their coarse grids. They present a model in which background photochemistry and chemical and physical plume processes are handled in separate "boxes", with mixing between the two. Wong
- et al. (2008) are also developing a model, the Aerosol Dynamics Simulation Code (ADSC), to calculate plume chemistry, dilution, and microphysics of aircraft plumes. Their inputs are based on several measurement campaigns (Herndon et al., 2008; Timko et al., 2010). Although Wong's model is not yet ready to be employed as a





subgrid process within a gridded air quality model due to long computational times, we are aware of ongoing work to parameterize those outputs and use them as inputs to CMAQ.

3 Modeling approach

- ⁵ We completed three model simulations, or "test cases", using a modified version of the CMAQ-AERO3-APT model from AMSTERDAM. This configuration uses the Carbon Bond IV chemical mechanism for gas-phase chemistry and the AERO3 module for aerosol treatment. All test cases used a 504 × 408 km domain with 4 km grid cell resolution centered on the Atlanta airport. The model used 19 vertical layers from the surface to 100 mb (about 15 km) whose thickness increased with altitude. Air quality was modeled for June and July 2002 (plus an 11-day spin-up period in May). The ini
 - tial and boundary conditions were extracted from another regional-scale simulation at 12 km resolution for the same period.

Meteorology inputs for 2002 were based upon the Pennsylvania State Univer-¹⁵ sity/NCAR Mesoscale Model (MM5) (Grell et al., 1994). Each test case used background (non-aviation) emissions based on the National Emissions Inventory (NEI) for 2002 produced by the US Environmental Protection Agency (US EPA, 2010) and processed through the Sparse Matrix Operator Kernel Emissions (SMOKE) model (Houyoux et al., 2000).

- Test case 1 (TC1) included aviation emissions within the LTO cycle modeled using the plume-in-grid (PinG) process built into the AMSTERDAM model. Test case 2 (TC2) omitted aviation emissions. Test case 3 (TC3) included aviation emissions but avoided use of PinG by adding those emissions to the CMAQ grid directly. The emissions are identical in quantity and chemical composition to those in TC1.
- ²⁵ In TC1 and TC3, we use engine data from the International Civil Aviation Organization (ICAO, 2010) and a methodology developed by Wayson et al. (2009) to estimate sulfate, organic PM_{2.5}, and black carbon aviation emissions. This methodology, known





as FOA3.0 (version 3.0 of a first-order approximation), is also used in the EDMS and AEDT models. It is based on a statistical correlation between smoke number (a metric based on the coloration of soot from a particular engine) and available data on PM emissions by engine. The process used to calculate aviation emissions at each time step is detailed in the next section.

Our study attempts to build on prior work in a number of ways. This is the first time that a plume-in-grid model has been used to characterize airport-related aviation emissions in the context of a regional air quality model with chemistry (CMAQ). EDMS and AERMOD, the most commonly used models in the past, do not adequately represent the chemical processes occurring in the aircraft plume and have not been as effective as a detailed chemistry-transport model such as CMAQ at predicting aircraft impacts on primary and secondary pollutants at large distances from the airport.

10

In addition, this is the first use of AMSTERDAM in which multiple emitters have been used to represent emissions from a large number of individual points (aircraft engines)

- that vary in space and time. In the past, AMSTERDAM has primarily been used to study emissions from power plants (Karamchandani et al., 2006; Vijayaraghavan et al., 2008). These large sources were widely spread across the country, and a single Gaussian puff emitter represented each source. More recently, AMSTERDAM was also used to study toxic air pollutants from highway mobile sources in New York City (Karamchandani
- et al., 2009). In this study, we used 51 distinct emitters to represent activity in the immediate geographic vicinity of the airport, and emitters were divided into four types based on the mode of flight they represented (taxi, takeoff, climb out, and approach). By using many emitters in close proximity to one another with differing emissions profiles, we gain finer control over the location and characteristics of the emissions input to the model.

Third, this work does not use a preexisting emissions inventory for Hartsfield-Jackson generated by EDMS. Rather, we calculate aircraft emissions in each timestep using a detailed understanding of the characteristics of the individual aircraft engines used at Hartsfield-Jackson Airport, as well as the number of flights that occurred in each





hour of the modeling period. This method is described in detail below, and the resulting emissions totals are compared to the EDMS-derived values used in prior work (Arunachalam et al., 2008, 2011).

4 Calculating aviation emissions

⁵ In order to model air quality impacts from the Atlanta International Airport, it was necessary to represent aircraft emissions during LTO activity as a number of point source emitters. This involves two steps: determining the quantities of different pollutants that are emitted at each timestep and positioning the emitters in 3-D space. These steps are discussed in the next two subsections.

10 4.1 Quantifying emissions by timestep

25

In this project, we model LTO emissions up to 1000 m above the ground. Emissions in this altitude range are the result of four activities: taxi (or idle) emissions which occur on the ground, take off emissions which occur from zero to 304 m for departing planes, climb out emissions which occur from 304 to 1000 m for departing planes, and approach emissions from 1000 to zero meters for arriving planes (Rice, 2003).

Emissions above 1000 m, including all cruise emissions, are omitted from the model runs to focus on the effect of LTO emissions at ATL on surface air quality. Furthermore, cruise emissions would be associated with aircraft from many airports. Omitting emissions above this altitude may lead to an under-estimation of overall aircraft impacts on

²⁰ surface air quality, particularly in grid cells that are not near the airport and along flight corridors. Two recent studies have quantified this impact using global scale models (Barrett et al., 2010; Whitt et al., 2011).

We performed our own emissions calculation based on the physical characteristics of each engine model when operating in each mode of flight. We use 2005 arrival and departure data to represent the number of flights using each engine at Hartsfield-Jackson





in 2002 (the year represented by our other inputs, such as meteorology and background emissions) because a detailed breakdown of how many flights used each model of engine was not available for 2002.

Aircraft engines have different emissions characteristics depending on their power
setting. Key properties that change with power setting include fuel flow rate, smoke number (a metric based on the coloration of emitted soot), and emissions indices (mass ratios of pollutant emitted to fuel burned) for various pollutants. Therefore, in order to determine the total amount of each pollutant emitted by aircraft during 2005, it is necessary to total the emissions from each model of engine from each phase of the LTO cycle. This was done according to Eq. (1) for each chemical species:

$$\sum_{1}^{N_{\text{models}}} 2F_{\text{engine}}((T_{\text{takeoff}} \cdot E_{\text{takeoff}}) + (T_{\text{climbout}} \cdot E_{\text{climbout}}) + (T_{\text{approach}} \cdot E_{\text{approach}}) + (T_{\text{taxi}} \cdot E_{\text{taxi}}))$$
(1)

In Eq. (1), F_{engine} refers to the number of flights using that engine model in 2005. N_{models} is the number of engine models used to generate emissions inputs. T_{mode} is time-inmode, the average time aircraft spend in that particular mode of flight. E_{mode} refers to 15 the emissions rate of a pollutant (in g or mol s⁻¹) for that particular engine model in that flight mode. The coefficient 2 is present because we assume that there are two engines per aircraft. Thus, we sum the emissions from every engine in each mode to estimate the total emissions for each pollutant.

The values of *F*_{engine} for each engine model are the same as those used in Arunachalam et al. (2011) and were based upon previous environmental impact studies. For time-in-mode values, we chose to use the reference values recommended for gaseous emissions calculations by the International Civil Aviation Organization (ICAO, 1993): 0.7 min for takeoff, 2.2 min for climb out, and 4.0 min for the approach. Although the accuracy of these values for modern jet aircraft has been questioned (Rice, 2003), we felt there were no more accurate, authoritative values available. We chose to use an average value for taxi mode specific to the Atlanta International Airport in 2005





of 27.22 min (consistent with the approach used in Arunachalam et al., 2008, 2011), rather than ICAO's reference value of 26.0 min.

Key engine characteristics necessary to calculate emissions rates were obtained from ICAO's engine databank (2010). The engine databank provided fuel flow rates (kg s⁻¹), engine type (single or multiple turbofan), bypass ratio (ratio of air drawn through the periphery of the engine to air drawn through the core), smoke numbers, and emissions indices for hydrocarbons, carbon monoxide, and NO_x. When an engine did not have mode-specific smoke number data available in the ICAO databank, a revised version of the Calvert method (Eyers, 2007) (which provides factors by which take off smoke numbers may be multiplied to obtain mode-specific smoke numbers for various engine classes) was used to calculate mode-specific smoke numbers.

Emission indices for SO₂, H₂SO₄, organic PM, and elemental carbon (also called black carbon or soot) were obtained via the methodologies described by Wayson et al. (2009). However, for values related to sulfur, we used numbers suggested by the FAA for use in the AEDT model. In particular, we assume that 2% of emitted sulfur is S(VI) rather than S(IV), and we use a sulfur fuel content of 600 ppm. The ICAO engine databank provides a hydrocarbon emissions index, which we multiply by 1.16 to obtain the total organic gas (TOG) emissions index. The engine databank also provides a total NO_x emissions index, which we speciate as 76% NO, 23% NO₂, and 1% HONO

²⁰ (Wood et al., 2008).

15

To be represented in the model, TOG must be further speciated into its component parts. We used a breakdown of TOG components from a joint FAA/EPA document describing best practices for quantifying organic gas emissions from aircraft engines (FAA and EPA, 2009). This document is based upon a series of recent aircraft mea-²⁵ surement campaigns and is a substantial update to the previous approach developed by Spicer et al. (1994), which has been used in the literature for speciating aircraftemitted TOG to date. The new approach divided TOG into 77 explicit organic compounds and 4 categories of unknown compounds. These species were then mapped onto the 8 compounds that represent TOG in AMSTERDAM's chemical mechanism (a





modified version of Carbon Bond IV), using ratios provided by the US EPA's SPECIATE tool (US EPA, 2011).

Emissions were calculated for the 17 most commonly used engines at Hartsfield-Jackson. This encompassed 96.5% of the total aircraft activity at the airport. The re-⁵ maining 3.5% of activity was represented as a weighted average of the top 17 engines. Using this process, we obtained total annual emissions values for CO, NO, NO₂, HONO, H₂SO₄, SO₂, organic PM, elemental carbon, and eight Volatile Organic Compound (VOC) species in each of the four flight modes.

We assumed that the relative use of different engine models was constant throughout
the year, so the emissions in each one-hour timestep were directly proportional to
total aircraft activity in that timestep. Information on the relative frequency of flights in
each month of the year, day of the week, and hour of the day at Atlanta International
Airport was based upon previously generated emission inventories for Atlanta used by
Arunachalam et al. (2008, 2011). We used these activity ratios and the total annual
emissions for each flight mode to calculate timestep-specific emissions for each flight
mode. Each mode's emissions were divided evenly among the emitters we defined for
that mode in every timestep.

4.2 Placing emitters to represent air traffic

In AMSTERDAM, the number and locations of emitters in 3-D space cannot be
 changed over the course of a model run. Therefore, it was necessary to determine a static arrangement of emitters that would best represent the totality of aviation emissions from the airport. Hartsfield-Jackson Atlanta Airport has five runways, all oriented in the East-West direction and ranging from 2740–3624 m in length. However, in the model year (2002), the southernmost runway was not yet operational. Of the remaining four runways, the outer two are used for arriving planes, while the inner two are used for departures. At any given time, landings and takeoffs are either conducted from West to East or from East to West depending on the prevailing winds. A study an-





approximately equal frequency (Gladstone, 2000). We assume both directions of operation were equally frequent during our modeling period, so emissions are divided evenly between the two directions.

- A total of 51 emitters were used in the model. These emitters were divided into four ⁵ modes: takeoff, climb out, approach, and taxi. For each departure runway and each direction, two emitters were used to produce takeoff mode emissions and five emitters for the climb out mode emissions. For each arrival runway, five emitters were used to produce approach emissions in each direction. Three emitters were used to produce taxi emissions: one near the taxiways for each pair of runways and one near the gates 10 (Fig. 1). Please see the Supplement for a file ("ATL_Emitters_GoogleEarth.kmz") that
- ¹⁰ (Fig. 1). Please see the Supplement for a file ("AIL_Emitters_GoogleEarth.kmz") that allows the emitters to be explored interactively in 3-D space using the Google Earth software program. The emitters along the westbound departure path from the northern runway are connected with green lines to assist in visualizing how emitters are positioned to follow a flight path.
- ¹⁵ Within each flight mode, each emitter receives an equal share of that mode's emissions in each timestep, so we place emitters so as to most evenly cover the space in which aircraft operate in each mode, taking into account the fact that accelerating or decelerating aircraft spend more time in one part of that space than another. Aircraft were assumed to have constant acceleration and deceleration during each mode of
- flight, with planes in take-off mode going from 0 to 225 ft s⁻¹, climb out from 225 to 422 ft s⁻¹, and approach mode decelerating from 422 to 250 ft s⁻¹. These speeds were used in conjunction with ICAO's time-in-mode estimates to determine the linear distance traveled by aircraft in each mode (ICAO, 1993). Aircraft were assumed not to turn or change heading within the lowest 1000 m of altitude, the region included in this
- study. The distance covered by aircraft in each flight mode was divided into segments that represent equal time intervals rather than equal lengths (so that mode-specific emissions would be equal in each segment). An emitter was positioned at the timebased center of each segment (i.e., the location a plane would be once half of the time that plane spent in a segment had elapsed). The path of travel in each flight mode was





assumed to be linear, except for the takeoff mode, wherein the first segment was assumed to be along the runway and the entire altitude gain was included in the second segment.

Using these assumptions, the horizontal and vertical position of each emitter was calculated. Google Earth was used to position emitters relative to the airport runways and to obtain latitude and longitude coordinates for each emitter. Ultimately, climb out emitters spanned six grid cells (24 km) in the East–West direction and approach emitters spanned twelve grid cells (48 km) in the East–West direction. Vertically, emitters spanned the lowest 11 layers (up to about 1 km) of the 19-layer modeling domain.

10 4.3 Comparison of aviation emissions

Table 1 compares the total annual emissions of several species used in TC1, and the emissions totals below 1000 m produced by EDMS, which was used in past work such as that by Arunachalam et al. (2008, 2011). The emissions used in this study were less than the emissions calculated by EDMS for all species except NO_2 .

15 5 Results and analysis

5.1 Model performance

Model performance was evaluated by comparing our results to measurements from the Chemical Speciation Network (CSN), which reports results as a 24 h average every third day. Within our modeling domain, there were 11 CSN monitors. Results from TC1 were compared with all of these CSN monitors. Concentrations, normalized mean error and normalized mean bias averaged across the model run are reported in Table 2. Since most of these monitors are far from the airport, results in Table 2 reflect the performance of the model as a whole, rather than the error and bias of airport-specific impacts.





Table 3 shows results from all three test cases compared with the single monitor closest to the airport in Decatur (monitor number 130890002), located 11.2 km northeast of the airport's edge. All four test cases produced mean results that match to within a few hundredths of a µg m⁻³, and normalized mean error and bias typically vary by no more than 1 % between the test cases. Notably, the differences between TC1 (the base case) and TC3 (the case without the PinG process) are too small to draw meaningful conclusions about whether the PinG process increases or decreases model accuracy or precision. The two pollutants with the most underprediction are secondary organic aerosol and sulfate aerosol. Small improvements in model performance among the test cases do not necessarily imply more accurate methods of modeling aircraft, as the uncertainty in all model simulations is relatively large. However, the PinG approach helps us with an enhanced characterization of sub-grid scale variability, as we will illustrate

later. For the base test case (TC1), the model predicted two-month average $PM_{2.5}$ concentrations from 10, 10, 0 mm r^{-3} in when contact with concentrations on law on 4.7 mm r^{-3}

¹⁵ trations from 10–12.2 μ g m⁻³ in urban centers, with concentrations as low as 4.7 μ g m⁻³ in rural regions (Fig. 2). The airport does not stand out in this figure because aircraft contribution to average surface PM_{2.5} was only 0.23 μ g m⁻³ in the airport's grid cell.

5.2 Aircraft impacts

Aircraft increased the average concentration of total $PM_{2.5}$ in June and July 2002 near the airport and throughout the Atlanta metro area (Fig. 3). Concentrations in the grid cell containing the airport were elevated by an average of 0.232 µg m⁻³. In the airport's grid cell, the contributions of species to aircraft impact on average $PM_{2.5}$ were: sulfate (54 %), elemental carbon (28 %), primary organic aerosol (9 %), ammonium (8 %), and nitrate (1 %). These results are comparable to those presented in Arunachalam et al. (2011).

Near the airport, aircraft raised sulfate concentrations by up to $0.130 \,\mu g \,m^{-3}$ (Fig. 3). In some areas far from Hartsfield-Jackson, aircraft caused small reductions in sulfate aerosol concentrations (< $0.0005 \,\mu g \,m^{-3}$). Tsai et al. (2001) observed a similar result



CC I

when using a Lagrangian plume model to investigate aircraft impacts on sulfate pollution over Taiwan (2001). They attributed the reduction to the fact that aircraft plumes are rich in SO₂ emissions. The SO₂ initially reacts with OH radicals to form sulfate aerosol. However, in aged plumes, OH radicals become depleted, slowing sulfate formation from both the aircraft-derived SO₂ and background SO₂.

Aircraft increased elemental carbon concentrations near the airport by $0.036 \,\mu g \,m^{-3}$ (Fig. 3). As elemental carbon is non-reactive in the AMSTERDAM model, the increase is due to direct elemental carbon emissions, and concentrations decrease with distance due to dilution and deposition. Aircraft also had a small positive effect on total organic PM concentrations (Fig. 3), almost all of which was due to primary organic aerosol (POA). Like elemental carbon, POA is treated as a non-reactive species in AMSTERDAM, so the spatial impacts for elemental carbon and total organic PM look similar.

5.3 Effects of the Plume-in-Grid process

5

Figure 4 shows the results when TC3 (CMAQ without PinG) is subtracted from TC1 (the base case with PinG). Positive values indicate that the plume-in-grid process resulted in higher concentrations. In most grid cells, the use of PinG increased total PM_{2.5} concentrations by 0.0005–0.020 µg m⁻³. This may be due to a higher concentration of reactants in the puffs, which are more likely to collide with each other when they are not diluted in a 4 km grid cell. Similarly, coagulation processes, which rely on collisions between particles, should proceed faster when the same emissions are confined to a smaller volume.

Except in the two cells nearest the airport, the entire east-west line of cells containing the aircraft approach and departure paths exhibited a smaller increase in total

PM_{2.5} due to the PinG process than rows immediately above and below, indicating that there is a countervailing phenomenon operating in these cells. It is possible that the high altitude of emitters in these cells causes PM to remain above the ground layer





in TC1, whereas downward movement of pollutants may be more rapid in TC3 when pollutants are not confined to puffs. One possible explanation for this difference is that puffs are added to the model at a higher temperature than the surrounding air and experience heat-driven "plume rise" which carries them upward. Pollutants added directly

⁵ to the 4 km grid cell do not experience heat-driven plume rise, given their instantaneous dilution.

The PinG process increased concentrations of sulfate, nitrate, and ammonium aerosol in almost every cell. Sulfate experienced the largest increases, while the effects on nitrate were the smallest.

- In most areas, particularly at the airport and along the approach and departure flight paths, use of the PinG process lowered elemental carbon concentrations by 0.0006– $0.010 \,\mu g \,m^{-3}$. One possible explanation stems from the fact that elemental carbon is non-reactive while sulfate (as well as nitrate and ammonium) are formed in the atmosphere through secondary reactions. By concentrating sulfate precursors, the PinG
- process enables sulfate aerosol to be generated more rapidly. In contrast, elemental carbon particles are emitted directly and concentrating them does not influence formation. However, increasing EC concentration can increase their rate of coagulation into larger particles that deposit more rapidly. (While sulfate would also be deposited more rapidly in the PinG scenario, this is outweighed by the faster rate of formation.)
- ²⁰ Increases in elemental carbon concentrations likely relate to differences in transport between grid cells when the chemicals are confined to puffs. This may lead to slightly higher values in some grid cells and slightly lower values in others.

The results for organic PM are mixed. In most of the grid cells where emitters are located, the PinG process reduced organic PM concentrations. Aircraft influence on

organic PM is overwhelmingly due to POA, which is considered non-reactive in AM-STERDAM and therefore may undergo increased deposition as for elemental carbon. However, 12 cells exhibit increased concentrations due to the PinG process. This may be due to differences in movement between cells when chemicals are confined to puffs, as well as the small contribution of secondary organic aerosol, which is formed in the







ACPD

13, 1089–1132, 2013

A plume-in-grid

approach to

characterize air

quality impacts

J. Rissman et al.

Title Page

Introduction

References

Figures

Abstract

Conclusions

Tables

Discussion Paper

Discussion Paper

Discussion Paper

Discussion Paper

atmosphere and may be increased by the PinG process due to more concentrated precursors.

5.4 Examination of aircraft impacts at subgrid scale

We instrumented AMSTERDAM to output the concentrations and centroid locations of all puffs in each timestep, and we compared the concentrations found within puffs to the aircraft contribution to the concentrations in underlying grid cells. Figure 5 shows the puffs that exist in one particular hour of the simulation graphed on top of the aircraft contribution to grid cell concentrations in that same hour. The puffs originate along two east-west lines that follow the approach and departure paths for each pair of runways at Hartsfield-Jackson. Puffs emitted in earlier model timesteps have been blown

- northward by prevailing winds, forming strands emerging from each emitter. Newlygenerated puffs frequently have concentrations much higher than the aircraft contribution to the grid cells they contain. While some puffs have a concentration higher than $1.5 \,\mu g \,m^{-3}$ in this hour, no grid cells report an aircraft contribution higher than
- 0.314 µg m⁻³. Individual puffs may have aircraft-contributed PM_{2.5} up to 3 orders of magnitude larger than that modeled with coarse grid cells. However, it is important to remember that each emitter consolidates the emissions from aircraft along a short flight segment into a single point source emitter. Therefore, while the 4-km grid cells may artificially dilute emissions, point source emitters using our methodology may artificially concentrate emissions, and the true contributions of aircraft emissions near an airport
- concentrate emissions, and the true contributions of aircraft emissions hear an airport may lie somewhere in between.

Figure 5 also shows that the largest aircraft influences are due to sulfate, which is only positive at close distances to the airport. The next most important species are elemental carbon and organic aerosols (overwhelmingly POA).

Next, we obtained puff concentrations of each species from each hour in June and July, and we analysed the distribution of concentrations in comparison with the underlying grid cells, paired in space and time (i.e. grid cells that do not contain puffs are not included in this analysis). Up to 99 % of all the aircraft-related puffs remain chemically active in the subgrid-scale phase at a distance of 60 km from the airport, with a few puffs active even at a distance of 145 km, before they are merged into the host grid in CMAQ based upon physical or chemical criteria for puff maturity. 21% of all aircraft-related puffs from the Atlanta airport have at least 0.1 μ g m⁻³ PM_{2.5} concentrations (mean of 0.14 μ g m⁻³ and max of 42.1 μ g m⁻³ from all puffs during the 2-month sim-

- f (mean of 0.14 µg m⁻³ and max of 42.1 µg m⁻³ from all puffs during the 2-month simulation). In order to better understand air quality impacts due to aircraft emissions as distance from the airport increases, we performed this comparison for six concentric rings (or domains) centered on the airport: a 68 × 68 km region, 52 × 52 km, 36 × 36 km, 20 × 20 km, 12 × 12 km, and 4 × 4 km (i.e., the airport's own grid cell), and shown in
- Fig. 6. In the 4 × 4 km and 12 × 12 km domains, concentrations in puffs are higher than the aircraft contribution to the grid cells for all statistics except the minimum values. For the minimum values, the puffs are at least 50 % more negative than the most negative aircraft contribution to a grid cell. (CMAQ-AMSTERDAM treats the aircraft sources in the subgrid-scale as perturbations, and hence a negative concentration in a puff im-
- plies that the total concentration near the puff is less than the background concentration in the grid cell.) This confirms that our finding that puffs generally have much higher concentrations than the underlying aircraft contribution to grid cells near the airport (Fig. 5) holds true across the entire two-month period. When we include the outliers from the distribution for each concentric ring (see Supplement), the maximum incre-
- ²⁰ mental concentrations due to aircraft emissions can be as high as 42.1 µg m⁻³ in the surface layer. Furthermore, when we include all layers in the analyses, the maximum concentrations can be as high as 38 µg m⁻³ within the airport's 4 km grid cell. However, the general pattern in grid averages at varying distances doesn't change much when we include only the surface layer versus all layers. The highest concentrations both within puffs and grid cells typically occur within the 12 × 12 km domain, indicating that
- at least some grid cells adjacent to the airport tend to receive more severe impacts than the airport's own grid cell.

We also examined the chemical composition of puffs and of aircraft impact on grid cells in these domains. In Fig. 7, we present the $PM_{2.5}$ composition in the puff or grid





cell with maximum concentrations in each concentric ring in the surface layer and in all layers. Note that the maximum puff concentration in the ground layer is 16.8 times that of the aircraft contribution to the underlying grid cell. We find that aircraft contribution to grid cells follows a similar pattern for all grid cell domains, with the highest magnitude

- ⁵ impacts in the 12 × 12 km domain, second-highest in the 4 × 4 km domain, and thirdhighest in the 20 × 20 km domain. Sulfate is the most important component of aircraft contribution to grid cells, followed by elemental carbon, primary organic matter, and ammonium. This confirms that our speciated findings for one timestep (Fig. 5) also hold true across the model run.
- ¹⁰ Speciated results for puffs, shown in Fig. 7 (for maximum puff/grid cell concentrations) and in Fig. S2 in the Supplement (median concentrations), indicate that the most important species in puffs are the same as those in grid cells, except ammonium in puffs is not significant in layers aloft. In contrast, ammonium is significant for puffs near the surface. Ammonium contributions are significant within grid cells at the sur-
- face but decrease aloft (Fig. S2), while sulfate contributions are significant both at the surface and aloft. This may be attributable to the fact that ammonia is primarily emitted from agricultural operations and other anthropogenic activities at the surface, while smokestacks (treated within the grid in this application) and aircraft emit sulfate and SO₂ aloft. Additional analysis presenting speciated values of median PM_{2.5} concentrations from puffs and grid cells is included in the Supplement.

Finally, we analyze variability in the maximum concentrations of puffs and maximum aircraft contribution to grid cells in several concentric rings near the airport for each day of the run (Fig. 8). The general trends in magnitudes of maximum concentrations in puffs in various rings do not change much with time, where the highest is seen in

the 12×12 km, followed by the 4×4 km and then the remaining rings. However, within the grid cells, the daily variability is quite high, where the maxima fluctuate between the first 4 domains that span up to 36×36 km. This is an indication of the variability in underlying transport patterns and in the times of puffs merging their concentrations with





the underlying grid cells. When including all layers, the maximum puff concentrations also seem to fluctuate between the various domains.

We also analysed the daily variability in median concentrations (Fig. S5 in the Supplement) in the puffs and grid cells. The daily variability in median puff concentrations 5 oscillates between the 4 × 4 km and 12 × 12 km domains, but the grid cells' median is always highest in the 4 × 4 km domain. Furthermore, the maximum concentrations for each day (Fig. 8) exceed the median (Fig. S5) by a factor of up to 100 in the case of puffs, and by a factor of up to 6 in the case of grid cells. Also, while the general ranges of median concentrations in puffs are comparable to those in the grid cells, the daily maximum concentrations in puffs are usually 10-20 times higher than the underlying grid cells. These results emphasize the value of subgrid-scale treatment of the physical and chemical processes related to aircraft emissions, particularly for understanding their potential maximum air quality impacts.

Conclusions 6

We have successfully implemented a novel approach for modeling aircraft emissions 15 at a major US airport using a plume-in-grid modeling technique to assess the subgridscale variability of aircraft impacts.

Impact of Aircraft: In June and July 2002, aircraft emissions during LTO contributed $0.232 \,\mu g \,m^{-3}$ to average $PM_{2.5}$ concentrations in the airport's grid cell and between 0.001 and $0.007 \,\mu g \,m^{-3}$ in a multi-county region covering more than 15000 square

- 20 kilometers. At the airport, aircraft contribute 54 % of total PM_{2.5} as sulfate aerosol, 28% as elemental carbon, 9% as primary organic aerosol, and 8% as ammonium. Far from the airport, aircraft decrease sulfate concentrations by up to $0.0005 \,\mu g \,m^{-3}$ due to depletion of OH radicals required for sulfate formation.
- Effects of PinG process: Use of a plume-in-grid process for modeling aircraft 25 emissions tends to increase the concentrations of secondary PM pollutants by $0.0005-0.020 \,\mu g m^{-3}$ in a multi-county area surrounding the airport, likely due to





10

increased concentration of reactants when consolidated into puffs. For non-reactive primary pollutants, such as POA and EC, the PinG process tends to lower concentrations in grid cells where emitters are located by up to $0.010 \,\mu g \,m^{-3}$ possibly due to increased coagulation and resulting deposition. However, concentrations are some-

times increased in nearby areas by up to 0.003 µg m⁻³, likely due to differences in pollutant transport when pollutants are confined to puffs, and hence transported further downwind from the source regions. Model performance analysis did not find significant differences in error and bias between a model run that utilized the PinG process and one that did not, so it is unclear if the PinG process improves model performance based upon monitoring data available in the region.

Subgrid Scale Analysis: Puffs generally have maximum concentrations at least an order of magnitude higher (a factor of 16-20) than the maximum aircraft contribution to model grid cells, whereas the median concentrations are somewhat comparable between puffs and grid cells at all distances (except in a 12×12 km ring around the

airport, where the puffs can have concentrations over an order of magnitude higher than the grid cells). Maximum puff impacts are seen within the 12 × 12 km ring, not in the airport's own grid cell, while maximum grid cell impacts do occur within the airport's grid cell. 21 % of all aircraft-related puffs from the Atlanta airport have at least 0.1 µg m⁻³ PM_{2.5} concentrations. Median daily puff concentrations vary between 0.017 and 0.134 µg m⁻³, while maximum daily puff concentrations vary between 6.1 and 42.1 µg m⁻³ during the 2-month period. Except for ammonium aloft, the component species in puffs are the same species that compose aircraft contribution to grid

cells, in roughly the same ratios.
 Sources of Uncertainty: There are many sources of uncertainty affecting our re sults in ways that are difficult to characterize numerically. These include imperfections and assumptions inherent in gridded meteorological input data, a lack of knowledge of precise aircraft timing and trajectories, uncertainty in engine emissions estimates, the need to use a finite number of emitters to represent moving aircraft, simplifications





in the model's chemical mechanism which reduce hundreds of real-world species to a smaller number of model species, and potential undiscovered errors in the model.

There are a number of areas future researchers might consider to extend this work. Many airports in the US have existing emissions inventories, which were produced

via the EDMS model. A program could be developed which reads EDMS emission outputs and generates a set of PinG input files for AMSTERDAM on the basis of those emissions (for instance, by placing an emitter in the center of each EDMS grid cell). This would allow AMSTERDAM to be used efficiently to model the impacts from many airports using existing EDMS-based emissions inventories. Similarly, a program could
 be developed to adapt the new AEDT global inventories for use in AMSTERDAM.

Although this study examined only a past year (2002), a similar technique could be used to model emissions in a future year, assuming changes in background emissions (due to new or improved control technologies, regulations, changes in GDP, etc.) and differences in aircraft emissions (due to changes in fleet composition, air travel demand, engine technology, etc.).

15

20

25

Additional work is ongoing to improve ADSC to model organics and volatile PM. Recent work by Miracolo et al. (2011) show that aircraft emissions can form much higher levels of SOA when non-traditional precursors are considered. Incorporating these updates will likely improve CMAQ's SOA performance, enhance our understanding, and increase the magnitude of the aircraft contribution to total PM_{2.5}.

This work only included LTO cycle emissions due to our focus on assessing their impacts on surface air quality near the airport, and thus excluded the impacts of aircraft emission during cruise mode at higher altitudes. Researchers may consider including cruise mode emissions in future simulations, particularly when studying emissions impacts in a larger region.

Finally, this work modeled the airport with a set of 51 static emitters. Future researchers may consider using a greater number of emitters to determine influences on model accuracy and the increased computational resources necessary to perform





a simulation with more emitters. They may also consider extending AMSTERDAM to enable the use of moving, elevated emitters.

Supplementary material related to this article is available online at: http://www.atmos-chem-phys-discuss.net/13/1089/2013/ acpd-13-1089-2013-supplement.zip.

Acknowledgements. This work was funded by the FAA, NASA, EPA, DOD and Transport Canada under FAA Grant No. 07-C-NE-UNC, Amendment Nos. 001 to 005, and 09-C-NE-UNC Amendment Nos. 001 to 004 under the Partnership for AiR Transportation Noise & Emissions Reduction (PARTNER). The authors would like to acknowledge the Georgia Department of Natural Resources, CSSI, Inc., Prakash Karamchandani, Lawrence Rissman, Neil Davis, and Mark Reed for their support with this project. Any opinions, findings, conclusions, or recommendations are those of the authors and do not necessarily reflect the opinions of PARTNER or its sponsors.

References

Airports Council International: ACI releases World Airport Traffic Report 2009, available at: http: //www.aci.aero/Media/aci/file/Press%20Releases/2010/PR_WATR2009_050810_FINAL.pdf (last access: 4 January 2013), 2010.

Arunachalam, S., Baek, B. H., Holland, A., Adelman, Z., Binkowski, F. S., Hanna, A., Thrasher, T., and Soucacos, P.: An Improved Method to Represent Aviation Emissions in Air Quality

Modeling Systems and their Impacts on Air Quality, in: Proceedings of the 13th Conference on Aviation, Range and Aerospace Meteorology, New Orleans, LA, January 2008, 135626, available at: https://ams.confex.com/ams/pdfpapers/135626.pdf (last access: 30 November 2012), 2008.

 Arunachalam, S., Wang, B., Davis, N., Baek, B. H., and 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, Atmos. Environ., 45, 3294–3300, doi:10.1016/j.atmosenv.2011.03.029, 2011.





- Aviation Environmental Design Tool: http://www.faa.gov/about/office_org/headquarters_offices/ apl/research/models/aedt/ (last access: 25 October 2010), 2010.
- Baek, B. H., Arunachalam, S., Holland, A., Adelman, Z., Hanna, A., Thrasher, T., and Soucacos, P.: 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, Emissions Inventories: Integration, Analyses and Communication, Raleigh, NC, May 2007, available at: http://www.epa.gov/ttn/chief/conference/ei16/session1/baek.pdf (last access: 30 November 2012), 2007.

Barrett, S. R. H., Britter, R. E., and Waitz, I. A.: Global mortality attributable to aircraft cruise emissions, Environ. Sci. Technol., 44, 7736–7742, 2010.

10

Byun, D. W. and Schere, K. L.: Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System, J. Appl. Mech. Rev., 59, 51–77, doi:10.1115/1.2128636, 2006.

Cimorelli, A., Perry, S., Venkatram, A., Weil, J., Paine, R., Wilson, R., Lee, R., Peters, W., and

- Brode, R.: AERMOD: A dispersion Model for Industrial Source Applications, Part I: General Model Formulation and Boundary Layer Characterization, J. Appl. Meteorol., 44, 682–693, doi:10.1175/JAM2227.1, 2005.
 - Eyers, C. and Gilboy, M.: Revision of Calvert method for filling in missing smoke number data, QinetiQ, 2007.
- FAA and EPA: Recommended Best Practice for Quantifying Speciated Organic Gas Emissions from Aircraft Equipped with Turbofan, Turbojet, and Turboprop Engines, http://www.faa.gov/regulations_policies/policy_guidance/envir_policy/media/ FAA-EPA_RBP_Speciated%20OG_Aircraft_052709.pdf (last access: 28 February 2011), 2009.
- Federal Aviation Administration: Emissions and Dispersion Modeling System (EDMS) policy for airport air quality analysis: Interim guidance to FAA Orders 1050.1D and 5050.4A, Federal Register, 63, 18068, available at: http://www.faa.gov/about/office_org/headquarters_offices/ apl/research/models/edms_model/media/EDMS%20Requirement%20for%20Airport% 20Air%20Quality%20Analysis.pdf (last access: 20 November 2012), 1998.
- Foley, K. M., Roselle, S. J., Appel, K. W., Bhave, P. V., Pleim, J. E., Otte, T. L., Mathur, R., Sarwar, G., Young, J. O., Gilliam, R. C., Nolte, C. G., Kelly, J. T., Gilliland, A. B., and Bash, J. O.: Incremental testing of the Community Multiscale Air Quality (CMAQ) modeling system version 4.7, Geosci. Model Dev., 3, 205–226, doi:10.5194/gmd-3-205-2010, 2010.





- Gladstone, C., Glover, G., Massimini, P., Skiotsuki, C., and Simmons, B.: Analysis of Triple Arrivals to Hartsfield Atlanta International Airport, MITRE Technical Report, available at: http://www.caasd.org/library/tech_docs/2000/mtr00w0000023.pdf (last access: 6 March 2011), 2000.
- ⁵ Grell, G., Dudhia, J., and Stauffer, D.: A Description of the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5), NCAR Technical Note, available at: http://nldr.library.ucar.edu/ repository/assets/technotes/asset-000-000-214.pdf (last access: 30 December 2011), 1994.
- Hall, C., Mondoloni, S., and Thrasher, T.: Estimating the Impact of Reduced
 Thrust Takeoff on Annual NOx Emissions at Airports, CSSI, Inc., available at: http://www.cssiinc.com/public/technicalpapers/docs/13-Estimating%20the%20Impact%
 20of%20Reduced%20Thrust%20Takeoff%20on%20Annual%20NOx%20Emissions.pdf
 (last access: 16 February 2011), 2003.

Herndon, C., Jayne, J., Lobo, P., Onasch, T., Fleming, G., Hagen, D., Whitefield, P., and

¹⁵ Miake-Lye, R.: Commercial Aircraft Engine Emissions Characterization of in-Use Aircraft at Hartsfield-Jackson Atlanta International Airport, Environ. Sci. Technol., 42, 1877–1883, 2008.

Houyoux, M. R., Vukovich, J. M., Coats Jr., C. J., Wheeler, N. J. M., and Kasibhatla, P. S.: Emission inventory development and processing for the seasonal model for regional air quality (SMRAQ) project, J. Geophys. Res., 105, 9079–9090, 2000.

International Civil Aviation Organization (ICAO): International Standards and Recommended Practices – Environmental Protection Volume II, Second Edition, 1993.

20

International Civil Aviation Organization (ICAO): Emissions Databank Issue 17, http://www.caa. co.uk/default.aspx?catid=702 (last access: 28 February 2011), 2010.

- ²⁵ Karamchandani, P., Seigneur, C., Vijayaraghavan, K., and Wu, S. Y.: Development and application of a state-of-the-science plume-in-grid model, J. Geophys. Res.-Atmos., 107, 4403– 4415, doi:10.1029/2002JD002123, 2002.
- Karamchandani, P., Vijayaraghavan, K., Chen, S., Seigneur, C., and Edgerton, E.: Plume-in-grid modeling for particulate matter, Atmos. Environ., 40, 7280–7297, doi:10.1016/j.atmosenv.2006.06.033, 2006.
 - Karamchandani, P., Lohman, K., and Seigneur, C.: Using a sub-grid scale modeling approach to simulate the transport and fate of toxic air pollutants, Environ. Fluid Mech., 9, 59–71, 2009.





- Karamchandani, P., Vijayaraghavan, K., Chen, S., Balmori-Bronson, R., and Knipping, E.: Development and application of a parallelized version of the advanced modeling system for transport, emissions, reactions and deposition of atmospheric matter (AMSTERDAM): 1. Model performance evaluation and impacts of plume-in-grid treatment, Atmospheric Pollu-
- tion Research, 1, 260-270, doi:10.5094/APR.2010.033, 2010. 5
 - Levy, J., Hsu, H., and Melly, S.: High Priority Compounds Associated with Aircraft Emissions: PARTNER 11 final report on subtask: Health Risk Prioritization of Aircraft Emissions Related Air Pollutants, Partnership for AiR Transportation Noise and Emissions Reduction, available at: http://web.mit.edu/aeroastro/partner/reports/proj11/p11compndsemiss.pdf (last access: 10 April 2011), 2008.
- 10

15

20

25

- Levy, J. I., Woody, M., Baek, B. H., Shankar, U., and Arunachalam, S.: Current and Future Particulate Matter-related Mortality Risks from Aviation Emissions in the United States, Risk Anal., 32, 237–249, doi:10.1111/i.1539-6924.2011.01660.x. 2012.
- Meilinger, S. K., Kärcher, B., and Peter, Th.: Microphysics and heterogeneous chemistry in aircraft plumes - high sensitivity on local meteorology and atmospheric composition. Atmos.
 - Chem. Phys., 5, 533-545, doi:10.5194/acp-5-533-2005, 2005.
- Miracolo, M. A., Hennigan, C. J., Ranjan, M., Nguyen, N. T., Gordon, T. D., Lipsky, E. M., Presto, A. A., Donahue, N. M., and Robinson, A. L.: Secondary aerosol formation from photochemical aging of aircraft exhaust in a smog chamber, Atmos. Chem. Phys., 11, 4135-4147, doi:10.5194/acp-11-4135-2011, 2011.
- Moss, M. and Segal, H.: Emissions and Dispersion Modeling System: Its Development and Application at Airports and Airbases, J. Air Waste Manage., 44, 787–790, 1994.
- Naiman, A. D., Lele, S. K., Wilkerson, J. T., and Jacobson, M. Z.: Parameterization of subgrid plume dilution for use in large-scale atmospheric simulations, Atmos. Chem. Phys., 10, 2551-2560, doi:10.5194/acp-10-2551-2010, 2010.
- Noel, G., Cointin, R., Allaire, D., Jacobson, S., and Willcox, K.: Assessment of the Aviation Environmental Design Tool, 8th USA/Europe Air Traffic Management Research and Development Seminar, Napa, CA, 29 June-9 July 2009, 84, available at: http://www.atmseminarus. org/seminarContent/seminar8/papers/p_084_EI.pdf (last access: 30 November 2012), 2009.
- Pope, C., Burnett, R., Thun, M., Calle, E., Krewski, D., Ito, K., and Thurston, G.: Lung can-30 cer, cardiopulmonary mortality, and long-term exposure to fine particulate air pollution, JAMA-J. Am. Med. Assoc., 287, 1132–1141, doi:10-1001/pubs.JAMA-ISSN-0098-7484-287-9-joc11435, 2002.





- Ratliff, G., Sequeira, C., Waitz, I., Ohsfeldt, M., Thrasher, T., Graham, M., and Thompson, T.: Aircraft Impacts on Local and Regional Air Quality in the United States, Partnership for Air Transportation Noise and Emissions Reduction, available at: http://web.mit.edu/aeroastro/ partner/reports/proj15/proj15finalreport.pdf (last access: 24 March 2011), 2009.
- ⁵ Rice, C.: Validation of Approach and Climbout Times-in-Mode for Aircraft Emissions Computation, 2003 Transportation Research Board Annual Meeting, Washington, DC, 12 January 2003, available at: http://www.ltrc.lsu.edu/TRB_82/TRB2003-001446.pdf (last access: 30 November 2012), 2003.

Santos, L. Sykes, R., Karamchandani, P., Seigneur, C., Lurmann, F., Arndt, R., and Kumar,

N.: Second-order Closure Integrated Puff (SCIPUFF) model with gas and aqueous phase chemistry and aerosols, 11th Joint Conference on the Applications of Air Pollution Meteorology with the Air and Waste Management Association, Long Beach, CA, 9–14 January 2000, 10436, 2000.

Spicer, C. W., Holdren, M. W., Riggin, R. M., and Lyon, T. F.: Chemical composition and pho-

- tochemical reactivity of exhaust from aircraft turbine engines, Ann. Geophys., 12, 944–955, doi:10.1007/s00585-994-0944-0, 1994.
 - Sykes, R. I. and Gabruk, R. S.: A Second-Order Closure Model for the Effect of Averaging Time on Turbulent Plume Dispersion, J. Appl. Meteorol., 36, 1038–1045, doi:10.1175/1520-0450(1997)036<1038:ASOCMF>2.0.CO;2, 1997.
- Sykes, R. I., Parker, S. F., Henn, D. S., Cerasoli, C. P., and Santos, L. P.: PC-SCIPUFF Version 1.1PD.1 Technical Documentation, ARAP Report No. 718, Titan Corporation, Titan Research & Technology Division, ARAP Group, P.O. Box 2229, Princeton, NJ, 08543–2229, 1998.
 - Timko, M., Onasch, T., Northway, M., Jayne, J., Canagaratna, M., Herndon, S., Wood, E., and Miake-Lye, R.: Gas Turbine Engine Emissions–Part II: Chemical Properties of Particulate Matter, J. Eng. Gas Turb. Power, 132, 061505–061519, doi:10.1115/1.4000132, 2010.
 - Tsai, F., Sun, W., and Chen, J.: A Composite Modeling Study of Civil Aircraft Impacts on Ozone and Sulfate over the Taiwan Area, Journal of Terrestrial, Atmospheric, and Oceanic Sciences, 12, 109–135, 2001.

25

 Vijayaraghavan, K., Karamchandani, P., Seigneur, C., Balmori, R., and Chen, S.: Plumein-grid modeling of atmospheric mercury, J. Geophys. Res.-Atmos., 113, D24305, doi:10.1029/2008JD010580. 2008.





- Wayson, R. L., Fleming, G. G., and Kim, B.: Status report on proposed methodology to characterize jet/gas turbine engine particulate matter emissions, Federal Aviation Administration, 2003.
- Wayson, R., Fleming, G., and Iovinelli, R.: Methodology to Estimate Particulate Matter Emis-
- sions from Certified Commercial Aircraft Engines, J. Air Waste Manage., 59, 91–100, doi:10.3155/1047-3289.59.1.91, 2009.
 - Whitt, D., Jacobson, M. Z., Wilkerson, J. T., Naiman, A. D., and Lele, S. K.: Vertical mixing of commercial aviation emissions from cruise altitude to the surface, J. Geophys. Res-Atmos., 116, D14109, doi:10.1029/2010JD015532, 2011.
- Wilkerson, J. T., Jacobson, M. Z., Malwitz, A., Balasubramanian, S., Wayson, R., Fleming, G., Naiman, A. D., and Lele, S. K.: Analysis of emission data from global commercial aviation: 2004 and 2006, Atmos. Chem. Phys., 10, 6391–6408, doi:10.5194/acp-10-6391-2010, 2010.
 Wong, H., Yelvington, P., Timko, M., Onasch, T., and Miake-Lye, R.: Microphysical Modeling of Ground-Level Aircraft-Emitted Aerosol Formation: Roles of Sulfur-Containing Species, J.
- ¹⁵ Propul. Power, 24, 590–602, doi:10.2514/1.32293, 2008.
- Wood, E., Herndon, S., Timko, M., Yelvington, P., and Miake-Lye, R.: Speciation and chemical evolution of nitrogen oxides in aircraft exhaust near airports, Environ. Sci. Technol., 43, 1884– 1891, doi:10.1021/es072050a, 2008.

Woody, M. and Arunachalam, S.: Secondary Organic Aerosol Produced from Aircraft Emissions

- ²⁰ at the Atlanta Airport: An Advanced Diagnostic Investigation Using Process Analysis, Under Review, 2012.
 - Woody, M., Baek, B. H., Adelman, Z., Omary, M., Lam, Y. F., West, J., and Arunachalam, S.: An Assessment of Aviation Contribution to Current and Future Fine Particulate Matter in the United States, Atmos. Environ., 45, 3424–3433, doi:10.1016/j.atmosenv.2011.03.041, 2011.
- ²⁵ Unal A., Hu Y., Chang M. E., Odman M. T., and Russell A. G.: Airport related emissions and impacts on air quality: Application to the Atlanta International Airport, Atmos. Environ., 39, 5787–5798, doi:10.1016/j.atmosenv.2005.051, 2005.
 - US EPA: 2002 National Emissions Inventory Data and Documentation, http://www.epa.gov/ttn/ chief/net/2002inventory.html (last access: 1 November 2010), 2013.
- ³⁰ US EPA: SPECIATE Version 4.3, http://www.epa.gov/ttn/chief/software/speciate/index.html (last access: 10 March 2011), 2013.





Table 1. Comparison of total annual aircraft emissions (in kg) from the Atlanta airport at altitudes below 1000 m for TC1 and EDMS-derived emissions used in Arunachalam et al. (2008, 2011).

Species	TC1	EDMS	EDMS/TC1
CO	3923571	4 963 366	127 %
NO	2214591	3664692	165 %
NO ₂	1 027 648	558514	54 %
SO ₂	454 324	515342	113%
TOG	351 081	1 101 578	314 %
Sulfate PM (PSO4)	14 198	39 456	278 %
Org PM (POA)	3318	19271	581 %
EC (PEC)	11340	14931	132 %

Discussion Pa		AC 13, 1089–	PD 1132, 2013		
per Discussion		A plum appro charact quality J. Rissn	e-in-grid ach to erize air impacts nan et al.		
Paper		Title	Page		
—		Abstract	Introduction		
Disc		Conclusions	References		
ussion		Tables	Figures		
Pap		14	►I.		
θŗ		•	Þ		
		Back	Close		
)iscussi		Full Screen / Esc			
on Pa		Printer-frie	ndly Version		
aper		Interactive Discussion			



	TC1 mean	observed mean	norm mean error	norm mean bias
Nitrate Aerosol	0.291	0.581	78.2%	-49.8%
Sulfate Aerosol	3.083	6.000	49.4 %	-48.6%
Ammonium Aerosol	1.066	1.649	44.1%	-35.4%
EC	0.509	0.724	50.4 %	-29.7 %
OC	0.933	4.926	81.1 %	-81.1 %
TC	1.443	5.657	74.5%	-74.5%
PM _{2.5}	8.388	19.125	56.2%	-56.1 %

Table 2	Comparison	of TC1	model	results	(in	µg m⁻	^{.3}) to	monitor	observations	from	the	11
CSN mo	nitors in June	and Ju	y 2002									

AC	ACPD				
A plum appro charact quality J. Rissn	A plume-in-grid approach to characterize air quality impacts J. Rissman et al.				
Title	Title Page				
Abstract	Abstract Introduction				
Conclusions	Conclusions References				
Tables	Figures				
I4	۰				
•	•				
Back	Back Close				
Full Scr	Full Screen / Esc				
Printer-frie	Printer-friendly Version				
Interactive Discussion					

Discussion Paper

Discussion Paper

Discussion Paper

Discussion Paper



Table 3. Comparison of model results (in μ g m⁻³) for three test cases to observations from the Decatur monitor (#130890002) in June and July 2002. Normalized mean error and normalized mean bias are shown.

		TC1	TC2	TC3
NO ₃	test case mean	0.463	0.460	0.461
0	observed mean	0.436	0.436	0.436
	norm mean error	72.4 %	71.9%	72.1 %
	norm mean bias	6.1%	5.4%	5.7%
SO ₄	test case mean	2.426	2.415	2.420
	observed mean	5.696	5.696	5.696
	norm mean error	58.8%	59.0%	58.9%
	norm mean bias	-57.4%	-57.6%	-57.5%
NH ₄	test case mean	0.970	0.965	0.967
	observed mean	1.367	1.367	1.367
	norm mean error	40.4 %	40.7 %	40.6 %
	norm mean bias	-29.0%	-29.4%	-29.3%
EC	test case mean	0.763	0.759	0.762
	observed mean	0.763	0.763	0.763
	norm mean error	42.4 %	42.1 %	42.4 %
	norm mean bias	-0.1 %	-0.6%	-0.1 %
OC	test case mean	1.025	1.023	1.024
	observed mean	4.553	4.553	4.553
	norm mean error	77.5%	77.5%	77.5 %
	norm mean bias	-77.5%	-77.5%	-77.5%
тс	test case mean	1.787	1.782	1.787
	observed mean	5.316	5.316	5.316
	norm mean error	66.4 %	66.5%	66.4 %
	norm mean bias	-66.4%	-66.5%	-66.4%
PM _{2.5}	test case mean	8.508	8.482	8.496
	observed mean	18.418	18.418	18.418
	norm mean error	53.8%	53.9%	53.9%
	norm mean bias	-53.8%	-53.9%	-53.9%

ACPD 13, 1089–1132, 2013					
A plume-in-grid approach to characterize air quality impacts					
J. Rissr	nan et al.				
Title	Title Page				
Abstract	Abstract Introduction				
Conclusions	Conclusions References				
Tables	Tables Figures				
I	I4 FI				
•	A				
Back	Back Close				
Full Sci	Full Screen / Esc				
Printer-frie	Printer-friendly Version				
Interactive Discussion					

Discussion Paper

Discussion Paper

Discussion Paper

Discussion Paper





Fig. 1. Hartsfield-Jackson Atlanta International Airport with a subset of emitters as represented in Google Earth. Yellow = taxi mode emitter, pink = takeoff mode emitter, blue = climb out mode emitter, green = approach mode emitter. Red "E" and "W" markers are reference points at the ends of the runways relative to which emitters are placed.













Fig. 3. Aircraft impact on average surface concentrations $(ng m^{-3})$ of PM_{2.5} and five component species in June and July 2002 (i.e., base case TC1 minus no aircraft case TC2).







Fig. 4. Effects of plume-in-grid process on average surface concentrations $(ng m^{-3})$ of PM_{2.5} and five component species in June and July 2002 (i.e., base case TC1 minus no PinG case TC3). Each panel shows a 92 km by 112 km area centered on the airport.















Fig. 6. Box-and-whisker plots (excluding outliers and showing the 25th, 50th (red line), 75th percentiles, and 1.5 times the inter-quantile ranges) of hourly $PM_{2.5}$ concentrations in puffs and in aircraft contribution to grid cells at various distances in the modeled surface layer, and in all layers. All timesteps are included separately (i.e. not averaged), forming the distributions. The analysis includes only those grid cells in the outer-most ring as we go outward from the airport, and thus no overlap of grid cells between each box-and-whisker. Note that the vertical axis scale varies by graph.







Discussion Paper **ACPD** 13, 1089–1132, 2013 A plume-in-grid approach to characterize air **Discussion** Paper quality impacts J. Rissman et al. **Title Page** Introduction Abstract **Discussion** Paper Conclusions References **Tables Figures** 14 ► 4 Back Close **Discussion** Paper Full Screen / Esc **Printer-friendly Version** Interactive Discussion



Fig. 7. Maximum hourly concentration of $PM_{2.5}$ component species (during June–July 2002) in puffs and in aircraft contribution to grid cells at various distances in the surface layer and in all layers. The analysis includes only those grid cells in the outer-most ring as we go outward from the airport, and thus no overlap of grid cells in each bar. Note that the vertical axis scale varies by graph.



Fig. 8. Maximum hourly $PM_{2.5}$ concentrations for each day in puffs and in airport contribution to grid cells at various distances in modeled surface layer, and in all layers, during June and July 2002. The analysis includes only those grid cells in the outer-most ring as we go outward from the airport, and thus no overlap of grid cells in each bar. Note that the vertical axis scale varies by graph.



