Development of an Interface for the Emissions and Dispersion Modeling System (EDMS) with the SMOKE Modeling System

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ABSTRACT

Currently, within the National Emissions Inventory (NEI), airport, including aircraft, emissions are estimated at the county level as area sources and are represented only in the surface layer of air quality models. In reality, however, aircraft release their emissions both on the surface and while airborne. Therefore, in order to provide a realistic representation of all emissions from aircraft sources, we have developed an interface, called EDMS2Inv, in the Sparse Matrix Operator Kernel Emissions (SMOKE) emission modeling system, that enables processing of emissions inventories from the Federal Aviation Administration (FAA)'s Emissions and Dispersion Modeling System (EDMS) to create emissions inputs to the Community Multiscale Air Quality (CMAQ) modeling system. A research version of EDMS was developed for this project to support the hourly, spatially-allocated, estimation of direct emissions for the criteria air pollutants (CAPs) (i.e., volatile organic compounds, CO, NO_x, SO_x, particulate matter of size less than 2.5 microns ($PM_{2.5}$) emitted by commercial aviation from the ground level up to 10,000 ft. EDMS provides a spatially and temporally allocated emissions inventory in an AERMOD-ready format. These emissions, when processed through the new EDMS2Inv interface in SMOKE, allow for an enhanced representation of hourly emissions from aviation sources, specifically in the layers aloft, to more accurately account for emissions from aircraft during takeoff and landing. In this study, we present case studies using EDMS2Inv with hourly EDMS outputs for modeling criteria air pollutants from commercial aircraft operations from three U.S. airports: Atlanta Hartsfield, Chicago O'Hare, and Providence T.F. Green. The EDMS2Inv interface is being used to process emissions from these airports for a nested CMAQ application over the Eastern United States. The improved representation of aviation emissions in all layers of the model facilitates developing new sensitivity scenarios that can subsequently be used to assess the impacts of the rapid growth of aviation in the United States on local-to-regional air quality and public health.

BACKGROUND AND MOTIVATION

About 150 airports in the United States are located in nonattainment areas for one or more criteria. Areas that are designated as nonattainment are mandated to develop State Implementation Plans (SIPs) that identify specific emissions control measures that, when implemented in the future, will improve air quality and thus bring the area into attainment. Current estimates of aircraft emissions that affect local air quality indicate that these emissions are relatively small when compared to emissions from other sources[1] and are small contributors to the overall atmospheric budget of air pollutants. However, it is estimated that passenger-miles traveled in the U.S. will be double or triple the 2006 levels within the next two decades[2]. It is thus imperative that we accurately understand, evaluate, and quantify the relative contribution of aviation emissions to ambient air quality.

Currently, aircraft emissions are treated as nonroad sources in regional emissions processing systems and are typically estimated at the county level. However, air quality models require that county-level emissions be more precisely spatially allocated. As an example, the Emissions Modeling System for Hazardous Pollutants (EMS-HAP)[3] and the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system[4,5] require that county-level emissions be disaggregated to a sub-county level. Grid models such as the Community Multiscale Air Quality (CMAQ) modeling system[6,7] require the allocation of emissions to grid cells. The existing paradigms for processing airport emissions have some limitations, such as:

- All emissions are allocated only to the air quality model's surface layer. This means that aircraft emissions due to take-off and landing activities are misrepresented spatially.

- If a county has two or more airports, all aircraft emissions are lumped into a single estimate making it difficult to identify the specific airports represented by a given Federal Information Processing Standards (FIPS) code and difficult to isolate the impact of a single airport on local-to-regional air quality.

- If a given airport straddles two counties, as is frequently the case, there is the potential for emissions to be allocated to the wrong county. Furthermore, aircraft leaving airports that are located in close proximity to a county border will release emissions in the adjacent county, which may not be accounted for in a county-level allocation.

- Most often, annual or seasonal estimates are used with uniform daily, weekly, and monthly temporal profiles being applied to allocate them to hourly estimates.

Strum et. al.[8] developed an approach for allocating aircraft and other airport-related emissions inventoried at the county level that utilizes information on airport location and activity data. Specifically, this approach was applied to spatially allocate airport-related emissions for air quality modeling in EMS-HAP and SMOKE. However, this study had limitations, and the authors recommended that airport-related emissions be inventoried and submitted at the local level with the specific location coordinates (latitude and longitude) and airport names with which they are associated.

Unal et al.[9] used CMAQ to model a summer 2000 episode at a 4 km grid resolution to assess the impacts of emissions from the Atlanta airport on air quality. They also compared air quality impacts from airports in general by processing emissions in two different ways: first, by allocating all emissions to the airport itself and second, by accounting for flight paths, aircraft operating mode, and plume-rise within the landing-takeoff (LTO) cycle. The differences in impacts between these two methodologies on predicted O_3 and particulate matter of size less than 2.5 microns ($PM_{2.5}$) were quite significant. However, the study was limited by the short time period studied and it did not include treatment of hazardous air pollutants (HAPs).

Air quality model outputs are often used for exposure and human health risk assessment. Therefore, it is important that aircraft and airport emissions are properly represented in air quality analysis.

INTRODUCTION

Since 1998, the Federal Aviation Administration (FAA)'s Emissions and Dispersion Modeling System (EDMS)[10] has been the required model for assessing the air quality impacts of airport emission sources, which consist of aircraft, auxiliary power units (APUs), ground support equipment (GSE), ground access vehicles, and stationary sources. EDMS interfaces with the American Meteorological Society/EPA Regulatory Model (AERMOD) Version 04300 [11] and its supporting weather and terrain processors, AERMET and AERMAP. EDMS can be used as part of an air quality assessment conducted using AERMOD, or it can be applied to simply generate emission inventories. Currently, EDMS

estimates emissions of total hydrocarbons (THC), non-methane hydrocarbons (NMHC), volatile organic compounds (VOC), CO, oxides of nitrogen (NO$_x$), particulate matter of size less than 2.5 microns (PM$_{2.5}$) in aerodynamic diameter. EDMS also includes GSE emission factor data from EPA's NONROAD model, and an interface to EPA's MOBILE version 6.2 for obtaining on-road vehicle emission factors. Aircraft activity in EDMS is expressed in terms of LTO cycles, which include taxiing, queuing, takeoff, climb out, approach, and landing.

A research version of EDMS was developed for this study to estimate criteria pollutants from commercial aviation activities from the ground level upto 10,000 feet. This version differs from the publicly available release of EDMS which models emissions up to the mixing height, typically 3,000 ft., and uses a variable fidelity grid that is dense below 1,000 ft., and sparse above. The research version of EDMS uses a grid that is consistent with the chosen CMAQ application from the surface to 10,000 ft. EDMS uses the AERMOD model for air pollutant dispersion; however, the dispersion modeling component within EDMS was not used for this study.

This study is intended to improve the assessment of aviation emission impacts on local-to-regional air quality using CMAQ, a state-of-the-art, comprehensive, one-atmosphere air quality modeling system that treats gas-phase chemistry, particulate matter (PM), and Hazardous Air Pollutants (HAPs) or Air Toxics. To provide realistic representations of all emissions from aviation and airport-related sources, we developed an interface to the SMOKE modeling system to process hourly emission inventory outputs from the FAA EDMS to create emissions inputs to CMAQ. Three airports are the focus of this study: Atlanta Hartsfield (ATL), Chicago O'Hare (ORD), and Providence T.F. Green (PVD). These were chosen based upon the availability of existing Environmental Impacts Statements (EISs). Figure 1 shows an overview schematic of this research project. EDMS estimated criteria air pollutants (CAPs) from commercial aircraft sources at these three airports will be processed through the SMOKE model and then merged with the baseline emissions (which does not contain aviation emissions) for subsequent modeling in CMAQ. The focus of this paper is on the EDMS-SMOKE interface; in addition, the outputs from the air quality model will be fed into a health impacts assessment project. The analysis of those results is beyond the scope of this report.

EDMS2Inv, the newly developed interface in the SMOKE emissions model allows the incorporation and processing of the emissions estimates from EDMS. This interface allows enhanced representation of emission inputs from aviation sources in air quality models and can help in designing new sensitivity scenarios to assess the impacts of the rapid growth of aviation in the United States. The primary objectives of this interface are to convert the EDMS output that has historically only been used by AERMOD to an inventory format for SMOKE and ensuring that aviation emissions are processed correctly. We also enhanced SMOKE to compute emissions layer fractions to allow these aircraft emissions to be distributed into the appropriate model layers aloft.

Figure 1. Overview of data flow between EDMS, CMAQ, and AERMOD.
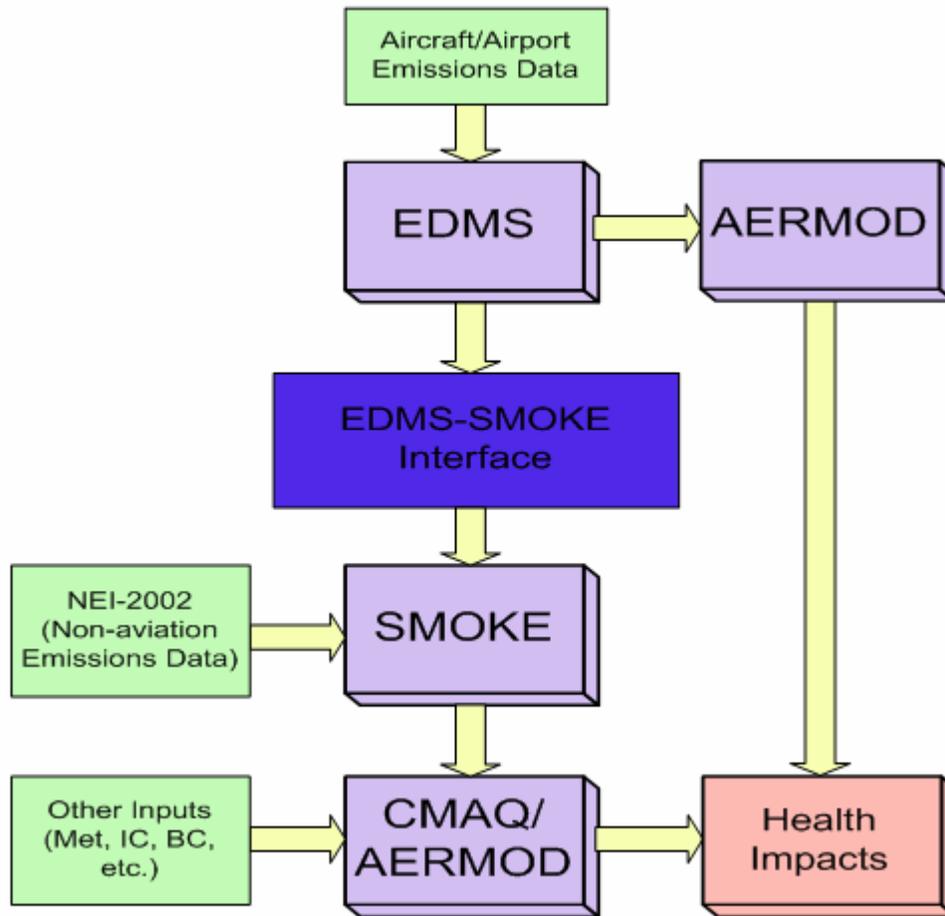
EMISSIONS AND DISPERSION MODELING SYSTEM (EDMS)

For this study, EDMS emissions were generated for the three airports. The airport layout was defined using the information provided by the FAA's National Aeronautical Charting Office (NACO), and the commercial aircraft operations were obtained from previous EIS studies. The aircraft activity information reflects the analysis year selected for the EIS. Table 1 lists the year assumed for the commercial aircraft activity for each of the airports. Although EDMS can estimate emissions for all of the source types that can be found at airports, this analysis included only the emissions from the main engines of commercial aircraft.

Table 1. Commercial aircraft activity year by airport.

No.	Airport	Activity Year
1	Atlanta Hartsfield – ATL	2005
2	Chicago O'Hare – ORD	2002
3	Providence T.F. Green – PVD	2004

While the operations reflect different analysis years, meteorological data for year 2002 was used consistently for the analysis. For EDMS, TD-3505 surface weather observations and TD-6201 upper air soundings were obtained from the National Climatic Data Center (NCDC). These data were used by

EDMS to estimate the runway that each aircraft would likely have used. In addition, the aircraft performance and emissions computations also use the meteorological data for their calculations. Specifically, the emissions indices (from the International Civil Aviation Organization's (ICAO) Engine Exhaust Emissions Databank which were based upon standard atmospheric conditions) are adjusted for the airport-specific conditions of ambient temperature, pressure and humidity.

In the publicly released version of EDMS, the model is able to estimate the following criteria air pollutants (CAPs) for commercial aircraft: CO, THC, NMHC, VOC, NO_x, primary PM_{10}, and primary $PM_{2.5}$. The research version was augmented to incorporate additional CAPs such as NO, NO_2, and three components of primary PM: nonvolatile, SO_4, and organics. The $PM_{2.5}$ speciation is based upon the First Order Approximation (FOA) Version 3.0 (FOA3)[12]. FOA3 was developed by the ICAO Committee for Aviation Environmental Protection (CAEP) Working Group 3 to predict PM from commercial aircraft engines. FOA3 represents the most current and advanced approach to quantifying PM emissions from aircraft. THC needs to be converted to VOC or total organic gases (TOG) for later speciation process in SMOKE.

EDMS outputs are provided in the form of two files for each pollutant. These outputs can be used by AERMOD in conjunction with meteorological data for modeling concentrations or can be processed into input for CMAQ through SMOKE. In the first file (*.INP), the definition of the emission source locations is provided, and in the second (*.HRE) the hourly emission rates for each of those sources are defined. While EDMS is typically used to model aircraft activity within the LTO cycle, it includes an aircraft performance module that can modeling an entire flight from gate-to-gate. Also, while EDMS is able to estimate ground delays due to runway congestion, this module requires that the complete airport demand profile be provided. Since only commercial aircraft were modeled for this project, the taxiway speed limit was adjusted to reflect the recorded taxi times in the FAA's Aviation System Performance Metrics (ASPM) database.

Typical LTO-cycle modeling limits the output to those emissions below the mixing height, which is nominally 3,000 ft above the ground. For our analysis, a more detailed representation of the emissions up to 10,000 ft was included to examine the potential impacts of high altitude emissions on surface air quality. Flight paths of airborne aircraft in the publicly-released version of EDMS are represented as area sources that are 200 m × 20 m in 20 m vertical increments; this would have resulted in an unmanageable output file size for this project. For compatibility with the CMAQ application to be used later in this study, the emissions from EDMS were output at the air quality model's vertical heights listed in Table 2. Figure 2 shows the vertical resolution of the air quality model (CMAQ), and the lowest 15 layers where aviation emissions are represented. Since the data were going to be assigned to a significantly coarser grid within CMAQ, the emissions sources were represented as 800 m × 20 m areas located at the release height of each layer. Increasing the area size of airborne sources also increased the horizontal threshold for active sources from 60 km to 80 km, which allowed for all emissions to be captured. This increase was necessary, as Enhanced Traffic Management System (ETMS) data showed that commercial aircraft travel 60-80 km to climb to and descend from 10,000 ft. In addition, aircraft were assumed to depart and arrive along straight paths to the runway. While it is possible that aircraft may not have been consistently represented in the most accurate grid cell, incorporating radar or similar data to precisely model the aircraft trajectories is beyond the scope of this analysis.

Table 2. Emissions layers output by EDMS.

Layer	Floor Height (m)	Ceiling Height (m)	Release Height (m)
15	2560	3048	2810.0
14	2110	2560	2335.0
13	1720	2110	1915.0
12	1380	1720	1550.0
11	1090	1380	1235.0
10	844	1090	967.0
9	637	844	740.5
8	468	637	552.5
7	334	468	401.0
6	227	334	280.5
5	145	227	186.0
4	89	185	117.0
3	48	89	68.5
2	21	48	34.5
1	0	21	16.5

Figure 2. Vertical resolution used in CMAQ (left), and the lowest 15 layers where aviation emissions are modeled up to 10,000 ft (right).
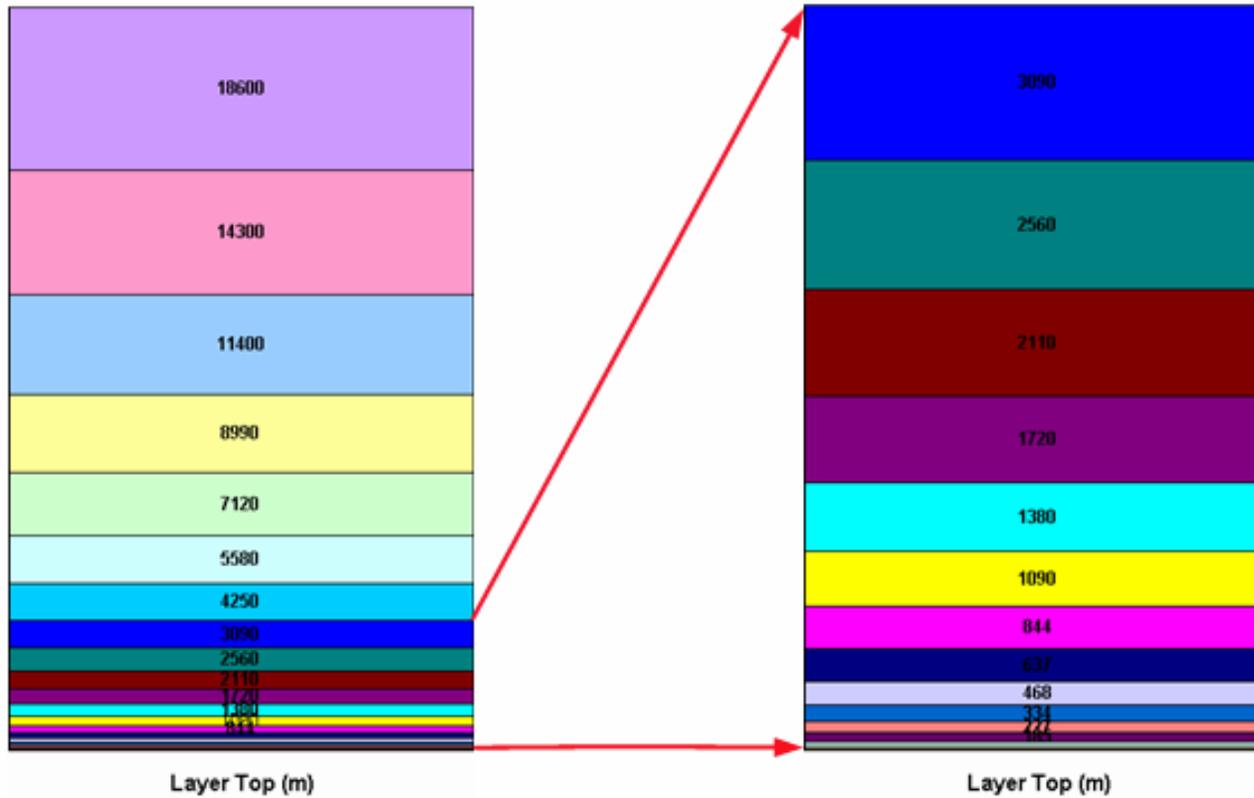
THE EDMS-SMOKE INTERFACE

Details of the design of the new EDMS-SMOKE interface, EDMS2Inv, are provided in a separate document[13]. Table 3 lists the source categories typically provided from EDMS, such as aircraft (categorized into modes), GSE, APU, fire stationary sources, and vehicular sources (including roadways and parking facilities). The attributes of each source included in EDMS outputs are: location (in x, y coordinates), elevation height (meters above the ground), source dimension, and several other parameters.

Table 3. Source categories mapped to AERMOD source ID in EDMS.

Source Category	Operation Mode	AERMOD Source ID	Common parameters
Commercial Aircraft	Landing Takeoff Landing-runway Takeoff-runway Taxiway	L##X#### T##X#### RL##[C|T]#### RT##[C|T]#### TW#######	
Ground Support Equipment	GSE for aircraft GSE populations (EPA NONROAD)	GATE_###	
Auxiliary Power Units	On-board Taxiing	GATE_###	• Location (x,y,z) • Dimension (width, length, angle) • Elevation height (m)
Roadways	Vehicle moving (EPA MOBILE6)	RD######	
Parking Facilities	Vehicle idling Vehicle moving	PARKA###	
Stationary Sources	Generators Incinerators Fuel tanks Aircraft deicing etc.	STAT_###	
Fires	Training fires	FIRE_###	

EDMS2Inv Interface

To process emissions from EDMS, SMOKE requires a Federal Information Processing Standards (FIPS) code to identify the state and county, a source classification code (SCC), the time zone for each airport source, and other source-specific information including location coordinates and elevation. SMOKE can import hourly inventory data using a combination of annual and hourly inventory files. The annual file provides describes each source along with its annual emissions values. The hourly inventory file contains the hourly emissions data and a source identifier that is used to match the sources to the annual inventory.

To process the emissions from EDMS, we have developed the EDMS2Inv interface program. Based upon information from EDMS outputs listed in Table 3, EDMS2Inv creates two entries for SMOKE, one for the "master" aviation file, which includes source characteristics (FIPS, SCC, aviation ID, location ID, and location coordinate), and the other for the hourly emissions from the EDMS output

files. To import hourly emissions from EDMS, all EDMS aviation sources (including aircraft activity, GSE/APU, roadway, parking facilities, stationary sources, and training fires) were treated as point sources during SMOKE processing. The annual point-source inventory format for SMOKE treats many fields that are not available from aviation EDMS inventories as either missing or zero values. For example, aircraft sources do not have defined stack parameters.

The overall updated processing logic of the EDMS-to-SMOKE interface is as follows:

- Specify the pollutants to be processed through SMOKE for input to CMAQ.

- Assign FIPS codes to the EDMS outputs based on the airport modeled.

- Convert coordinates of all aviation sources defined by EDMS in local (x, y) coordinates to latitude and longitude coordinates using the airport reference point.

- Assign SCCs and descriptions for all aviation sources that will be provided by EDMS (e.g. SCC 27750200000: Commercial Aircraft).

- Treat all aviation sources, including aircraft activity, GSE/APU, roadway, training fires, and parking facilities, as point sources in SMOKE using the computed latitude and longitude coordinates, elevation, and source dimension information.

- Using a complete list of AERMOD source IDs that begin with the keyword "LOCATION" in the EDMS output file, create a "master" aviation file (PTINV) that includes FIPS code, SCC, latitude, longitude, elevation height, source dimension, and aviation ID (a combination of ICAO airport code and AERMOD source ID) (e.g., KJFK-L01X001 refers to AERMOD source ID L01X001 for the John F. Kennedy Airport, New York).

- Convert EDMS hourly emissions (which are in $g/s/m^2$) to short tons/h by a conversion factor.

- Create an hour-specific aviation emission inventory file (PTHOUR) for SMOKE using EDMS hourly emissions (created for AERMOD) with FIPS code, SCC, and aviation ID. These source characteristics are used to match aviation sources from a master aviation file (PTINV), and import EDMS hourly emissions to SMOKE.

EDMS2Inv can process multiple pollutants and multiple airports at the same time. The user can create an index file that contains the list of all pollutants and all airports that is read by the interface to simultaneously process them all.

Units Conversion

We processed CAPs (CO, THCs, speciated NO_x [NO and NO_2], and speciated $PM_{2.5}$ [particulate organic carbon (POA), particulate elemental carbon (PEC), and particulate sulfate (PSO4)] from commercial aircraft sources (SCC: 2275020000) as emission modeling input for SMOKE. To process EDMS emissions through SMOKE, various EDMS output units need to be converted to the hourly emission units that SMOKE needs (short tons/h). Figure 3 shows the detailed procedure we developed to process CAPs and HAPs estimates together through SMOKE to create CMAQ-ready outputs.

Since commercial aircraft show different partitionings of NO_x emissions into NO and NO_2 according to operation mode, the research version of EDMS was modified to estimate NO and NO_2 emissions separately in NO_2 equivalency. We subsequently converted NO emissions from NO_2 equivalency to NO equivalency.

The conversion factor from THC to VOC for a commercial aircraft [14] is set to 1.0947, assuming a mass per carbon for THC in the effluent as measured by the flame ionization detector (FID) of 13.8758. However, if the EDMS THC is estimated as CH_4 equivalency (molecular weight of 16.04), the mass of THC is overestimated. To correct THC in CH_4 equivalent to VOC as carbon (C) equivalency, we applied the following correction:

$$VOC = THC \times 1.0947 \times (13.8758/16.04), \text{ or}$$

$$VOC = THC \times 0.947$$

Thus, THC estimates from EDMS (in grams in $CH_4/s/m^2$) are appropriately converted to grams $C/s/m^2$ by multiplying by a factor of 0.947.

The VOC-to-TOG conversion is essential, since all speciation profiles are on a total organic gases (TOG) basis. Based upon the latest SPECIATE database,[14, 16] the speciation profile 1098 is used to speciate TOG estimates into the individual model species. The VOC emissions are first converted to TOG using a factor of 1.148106 estimated based on speciation profile 1098. For each pollutant, Table 4 lists the original units from EDMS and the units that SMOKE uses.

Table 4. Pollutant units used in the EDMS and SMOKE models.

No.	Pollutant Name	EMDS Unit	NEI (SMOKE) Unit
1	CO	grams in $CO/s/m^2$	short tons in CO/h
2	NO	grams in $NO_2/s/m^2$	short tons in NO/h
3	NO2	grams in $NO_2/s/m^2$	short tons in NO_2/h
4	SO2	grams in $SO_2/s/m^2$	short tons in SO_2/h
5	TOG	grams in $CH_4/s/m^2$	short tons in C/h
6	POA	grams/s/m^2	short tons/h
7	PEC	grams/s/m^2	short tons/h
8	PSO4	grams/s/m^2	short tons/h

Integrated CAPs and HAPs Processing

The chemical mechanism chosen for this study is the Carbon Bond 2005 (CB05) mechanism with updates for chlorine chemistry and toxics[17]. If both CAPs and explicit HAPs estimates are made on a consistent basis for the airport sources by EDMS, it is possible that there can be an integrated processing of the CAPs and HAPs estimates, i.e., combine explicit toxics estimates and the aggregated TOG (=1.148106 *VOC) estimates without double counting certain organic species. There are two options in SMOKE for processing CAPs and HAPs: the "integrate" and "no-integrate" options. The "integrate" option involves computing no-HAPs TOG named as NONHAPTOG by subtracting toxics TOG emissions from the criteria TOG emissions to avoid double counting of TOG when the emissions are speciated. The "no-integrate" option does not compute NONHAPTOG but drops toxics emissions for toxics TOG pollutants if they are not part of the chemical mechanism or if they are not air quality model species. However, to choose the "integrate" option, it is essential that TOG and HAPs estimates were made on a consistent basis for the given emission source(s), and that all of the gaseous HAPs estimates that are expected are available for later NONHAPTOG computation.

Once both of these criteria are satisfied for the EDMS estimates in this study, the project could choose the "integrate" option to process hourly EDMS HAPs and CAPs together. However, we would perform the NONHAPTOG computation in EDMS2Inv, since the "integrate" option is not applicable for hourly or day-specific inventories. Because the chemical speciation step in SMOKE involves converting the inventory pollutants to the model species, the input files to this step must include the NONHAPTOG

pollutant and revised conversion factors that have been adjusted for the reduced mass in NONHAPTOG instead of TOG (Figure 3). The toxics-CB05 "integrate" option handles the situation in which the user wants to use the toxics inventory for modeling toxics pollutant species in CMAQ; these species could be either explicitly part of the chemical mechanism (e.g., formaldehyde), or simply added on as a model species but not part of the chemistry (e.g., benzene and naphthalene). In these cases, the non-toxics part of the TOG mass is retained as NONHAPTOG and mapped to the toxics-CB05 species. The toxic TOG mass will then be mapped to one of the following:
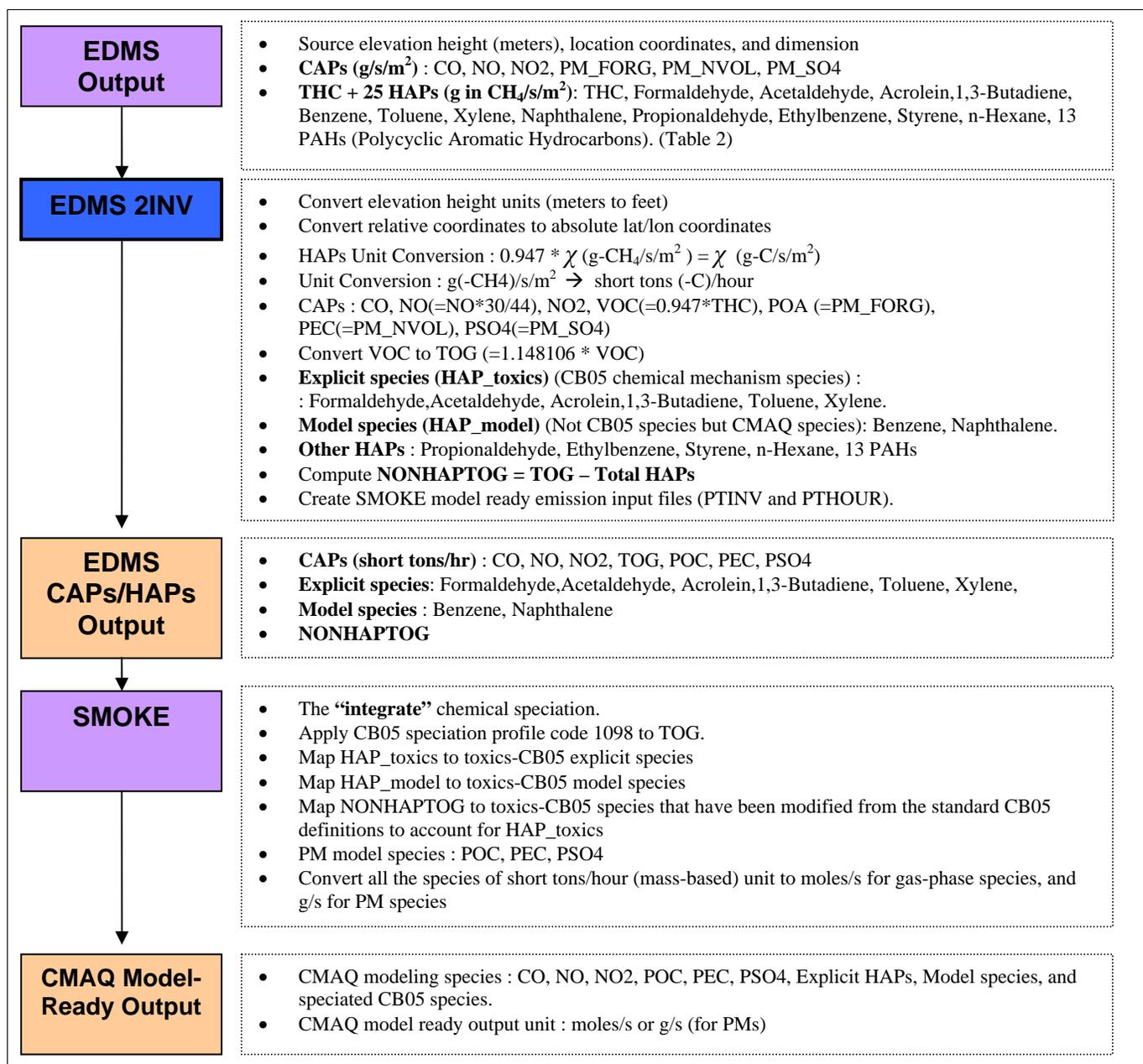
- the explicit toxic species that are part of the chemistry (formaldehyde, acetaldehyde, acrolein, and 1,3-butadiene) and the explicit toxics species for the extended chemical mechanism (toluene, and xylene), or

- other toxic species (e.g., benzene and naphthalene), or

- altered CB05 species whose definitions have been altered to account for the four new mechanism species (formaldehyde, acetaldehyde, acrolein, and 1,3-butadiene).

RESULTS

Figures 4a through 4c show the vertical allocation of the EDMS emissions of CO, NOx, THC, and total PM$_{2.5}$ [sum of the three PM$_{2.5}$ species (POA, PEC and PSO4)] in the CMAQ model for a typical day. While the maximum emissions (by layer) are in the surface layer for all three airports, there is a distinct vertical profile of the emissions distribution in layers aloft. These emissions are shown in units of short tons per day.

To improve the representation of EDMS emissions estimates temporally and spatially for use by air quality models, we processed the EDMS emissions for the three airports through the EDMS2Inv interface program and through SMOKE. EDMS2Inv allows for a spatially enhanced vertical representation of emission inputs by allocating the aircraft emissions into the appropriate CMAQ modeling layers aloft and a temporally enhanced representation by allocating the hourly EDMS emissions into the air quality model instead of using uniform seasonal or monthly profiles. To ensure that aviation emissions are processed correctly, we performed several quality assurance checks including the following:

Figure 3. Flow chart showing combining toxics and criteria inventories from EDMS through SMOKE.

EDMS Output

- Source elevation height (meters), location coordinates, and dimension
- **CAPs (g/s/m^2)** : CO, NO, NO2, PM_FORG, PM_NVOL, PM_SO4
- **THC + 25 HAPs (g in CH$_4$/s/m^2)**: THC, Formaldehyde, Acetaldehyde, Acrolein,1,3-Butadiene, Benzene, Toluene, Xylene, Naphthalene, Propionaldehyde, Ethylbenzene, Styrene, n-Hexane, 13 PAHs (Polycyclic Aromatic Hydrocarbons). (Table 2)

EDMS 2INV

- Convert elevation height units (meters to feet)
- Convert relative coordinates to absolute lat/lon coordinates
- HAPs Unit Conversion : $0.947 * \chi$ (g-CH$_4$/s/m^2) $= \chi$ (g-C/s/m^2)
- Unit Conversion : g(-CH4)/s/m^2 → short tons (-C)/hour
- CAPs : CO, NO(=NO*30/44), NO2, VOC(=0.947*THC), POA (=PM_FORG), PEC(=PM_NVOL), PSO4(=PM_SO4)
- Convert VOC to TOG (=1.148106 * VOC)
- **Explicit species (HAP_toxics)** (CB05 chemical mechanism species) :
  : Formaldehyde,Acetaldehyde, Acrolein,1,3-Butadiene, Toluene, Xylene.
- **Model species (HAP_model)** (Not CB05 species but CMAQ species): Benzene, Naphthalene.
- **Other HAPs** : Propionaldehyde, Ethylbenzene, Styrene, n-Hexane, 13 PAHs
- Compute **NONHAPTOG = TOG – Total HAPs**
- Create SMOKE model ready emission input files (PTINV and PTHOUR).

EDMS CAPs/HAPs Output

- **CAPs (short tons/hr)** : CO, NO, NO2, TOG, POC, PEC, PSO4
- **Explicit species**: Formaldehyde,Acetaldehyde, Acrolein,1,3-Butadiene, Toluene, Xylene,
- **Model species** : Benzene, Naphthalene
- **NONHAPTOG**

SMOKE

- The **"integrate"** chemical speciation.
- Apply CB05 speciation profile code 1098 to TOG.
- Map HAP_toxics to toxics-CB05 explicit species
- Map HAP_model to toxics-CB05 model species
- Map NONHAPTOG to toxics-CB05 species that have been modified from the standard CB05 definitions to account for HAP_toxics
- PM model species : POC, PEC, PSO4
- Convert all the species of short tons/hour (mass-based) unit to moles/s for gas-phase species, and g/s for PM species

CMAQ Model-Ready Output

- CMAQ modeling species : CO, NO, NO2, POC, PEC, PSO4, Explicit HAPs, Model species, and speciated CB05 species.
- CMAQ model ready output unit : moles/s or g/s (for PMs)

- Correct spatial allocation of the aviation emissions within the modeling grid
- Correct vertical allocation of the emissions aloft in the model's vertical layers
- Mass conservation of the emissions as we process them through the interface.

To investigate the improvement of temporal allocations by using EDMS emissions, we compared hourly EDMS estimates with the temporally allocated national emissions inventory 2002 (NEI-2002) through the SMOKE model. The diurnal variations of these emissions for CO and NO are shown in Figure 5. While NEI-2002 uses the standard day of the week, and hour of the day hourly temporal profiles, the EDMS emissions vary for each hour based upon actual activity data, thus illustrating the significant differences in the diurnal profiles. This illustrates the significant temporal allocation enhancement of providing hourly emission estimates to air quality models.

To show the significant spatial enhancement in the vertical representation of aviation emissions in the vicinity of the airports during the LTO cycle, we created vertical cross-section plots of CO, NOx, and PM$_{2.5}$ near the location of all three airports. As shown in Figure 6a for the Atlanta airport, while most of the emissions of all species are in the surface layer, there is a significant distribution of emissions in layers aloft. One can also see that in the top layers, emissions are at least 2 to 3 grid cells away from the grid cell where the airport is located, showing the path of aircraft as they approach or leave the airport during the LTO cycle. The individual components of PM$_{2.5}$ (i.e., PEC, POC and PSO4) are also shown in Figure 6a, to show the relatively higher contribution of PEC (or non-volatile PM) to total PM$_{2.5}$ emissions from aviation sources. Similar patterns are shown for the Chicago and Providence airports in Figures 6b and 6c, respectively.

Figure 4a: Atlanta Hartsfield airport emissions by CMAQ model layer and height.
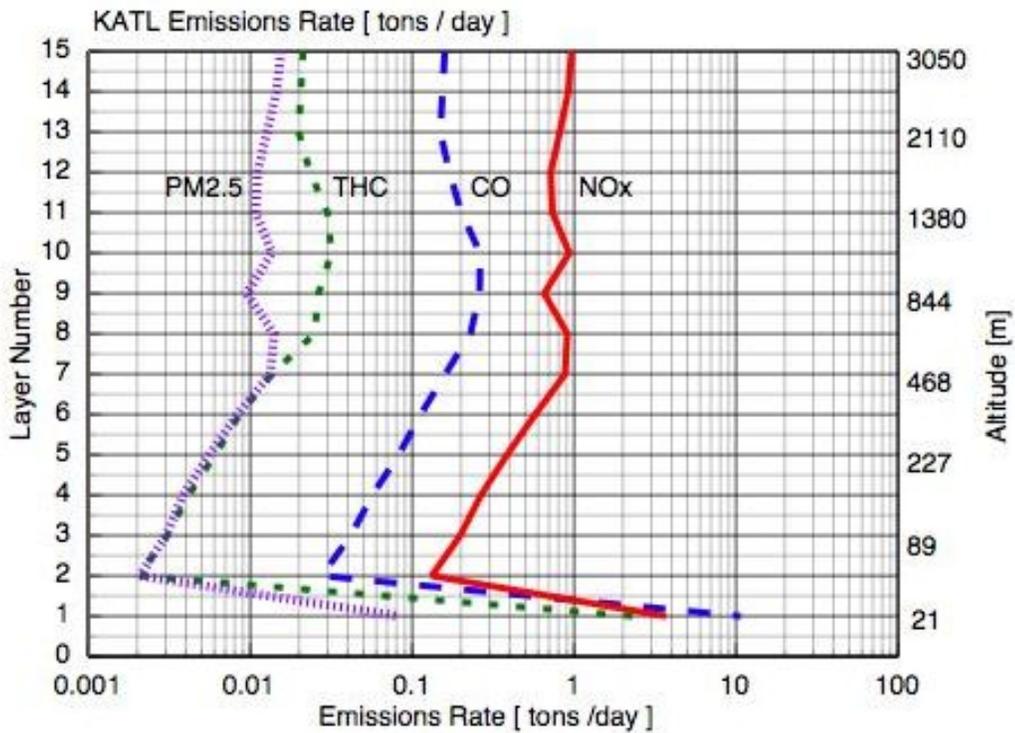
Figure 4b: Chicago O'Hare airport emissions by CMAQ model layer and height.
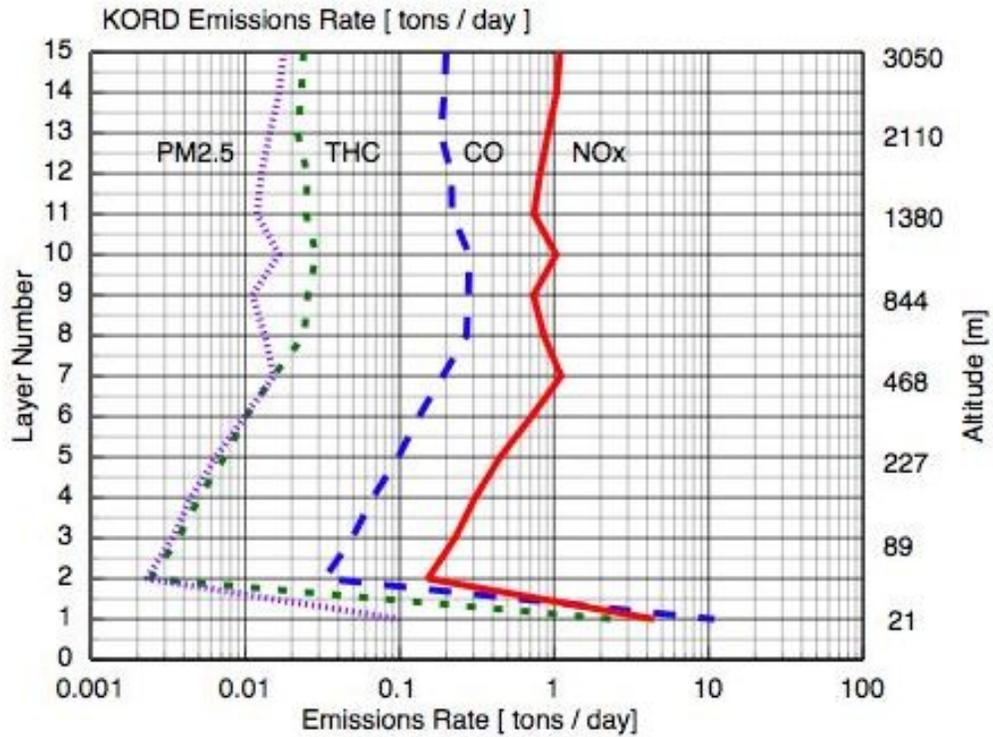
Figure 4c: Providence/TF Green airport emissions by CMAQ model layer and height.
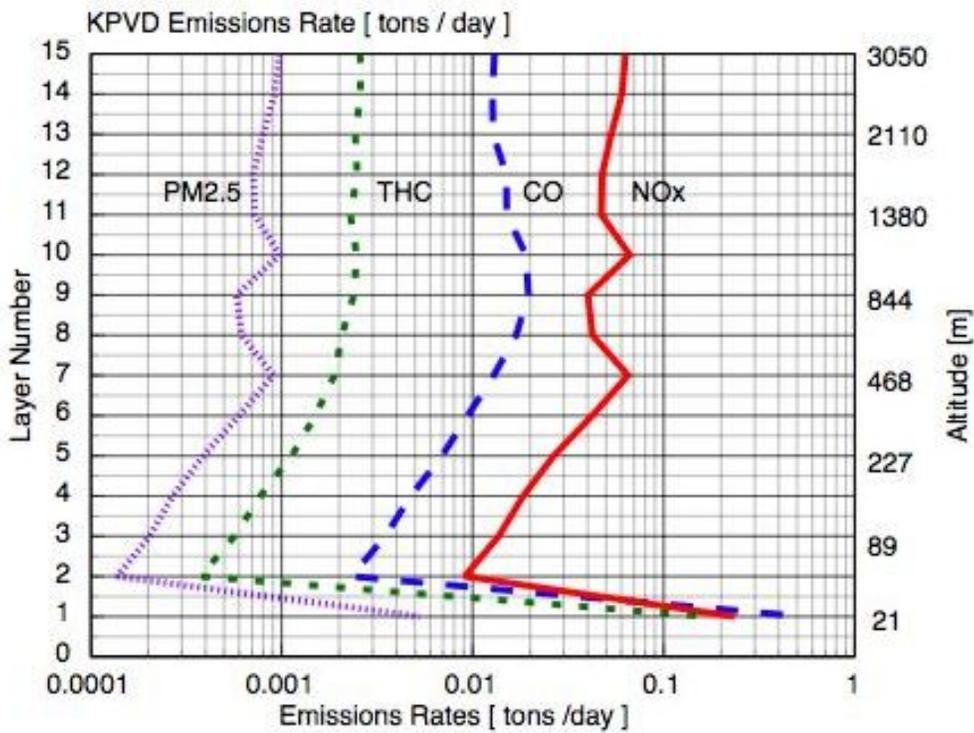
Figure 5. Comparison of EDMS and NEI-2002's diurnal variation of NO and CO from three airports on January 15, 2002.
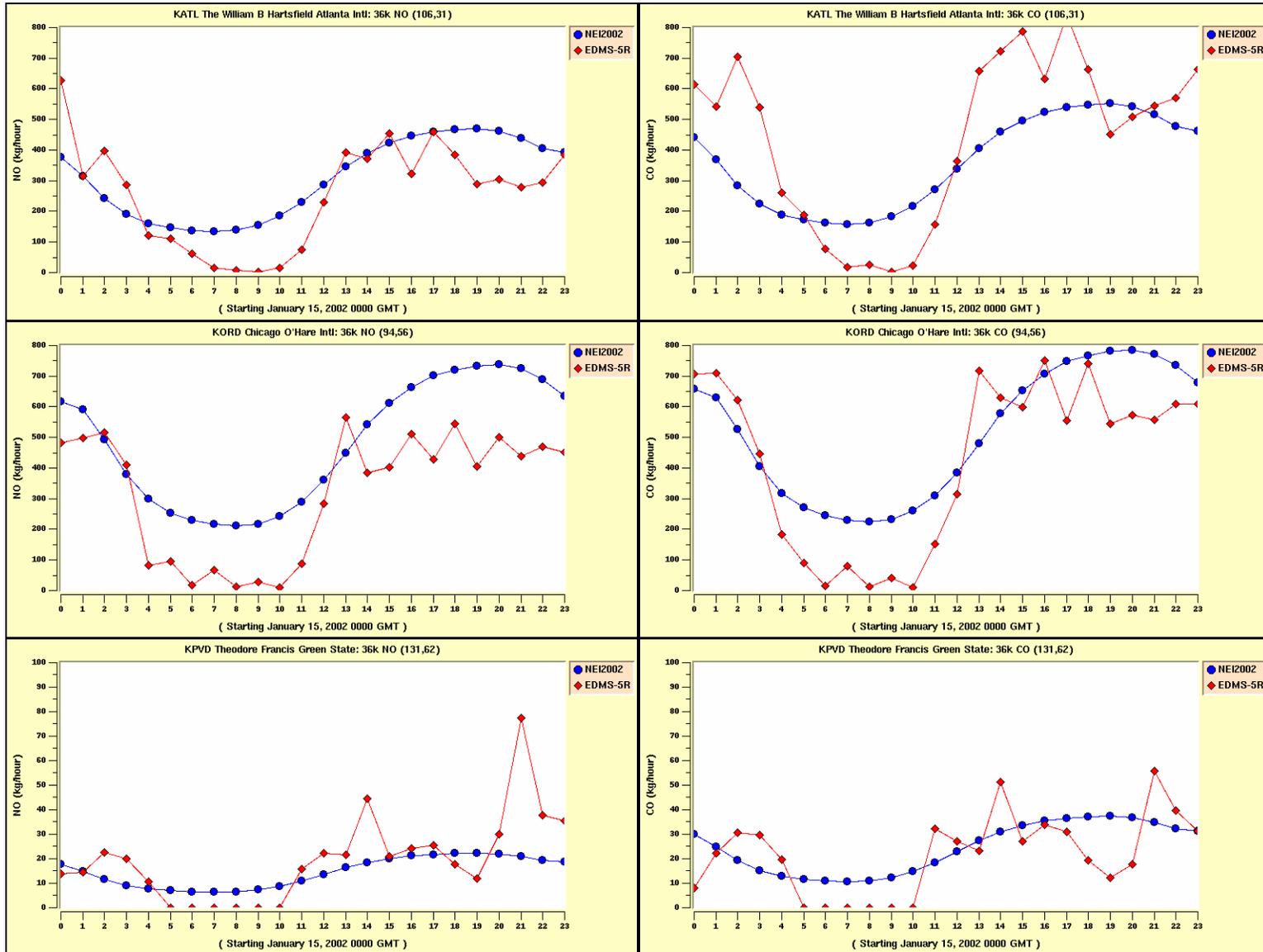
Note that input data (such as flight activity information) and version of EDMS used in NEI aircraft emission calculation may be different than what are used in our analysis. These differences could be potential causes of variations shown here. This relative comparison of emissions also indicates need to correctly account for and represent aviation emissions in air quality analysis.

Figure 6a. Daily total of CO, NOx, PM$_{2.5}$, PEC, POA, and PSO4 emissions vertical profiles from Atlanta Hartsfield airport (KATL).

- 15 -
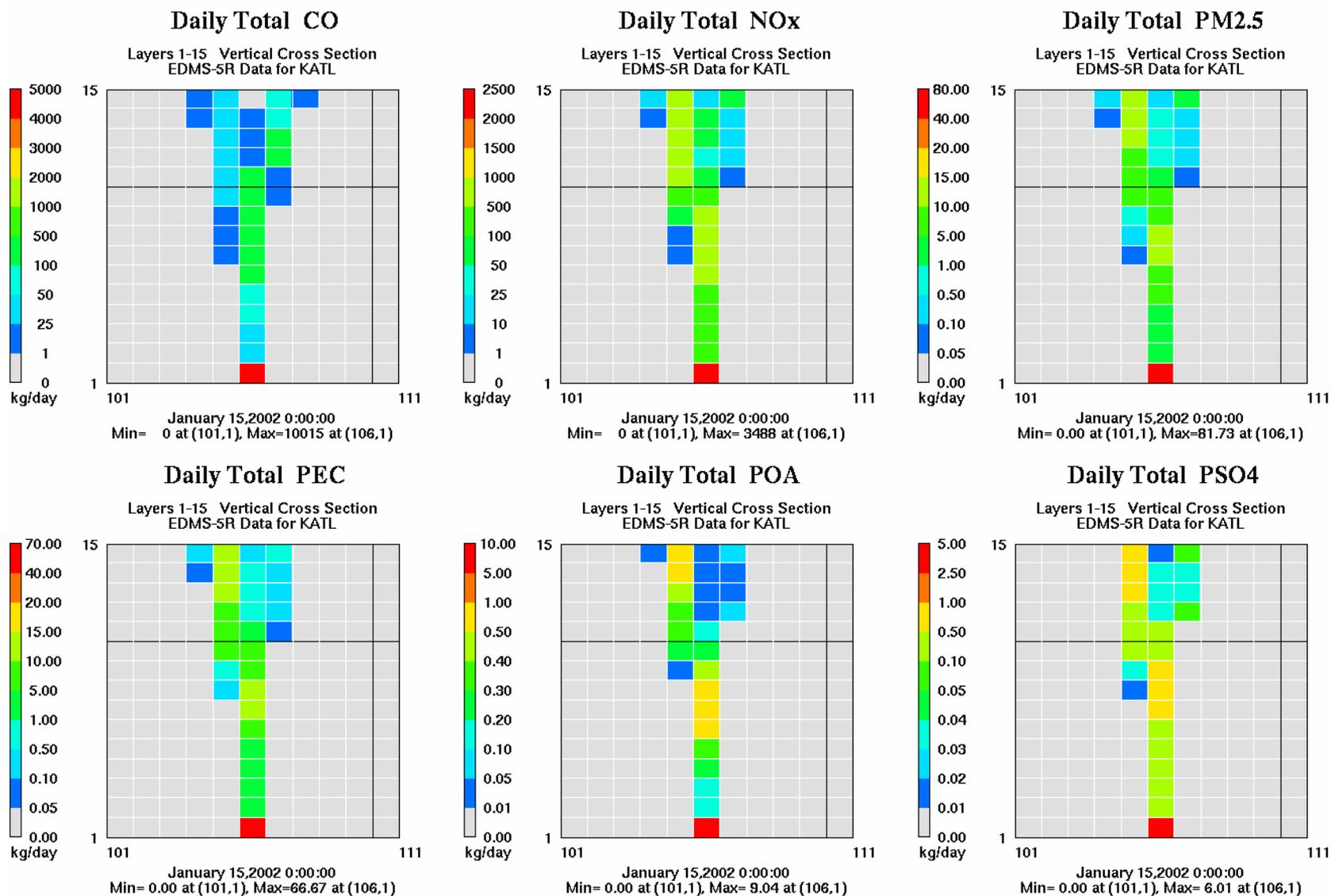
Figure 6b. Daily total of CO, NOx, PM$_{2.5}$, PEC, POA, and PSO4 emissions vertical profiles from Chicago O'Hare airport (ORD).
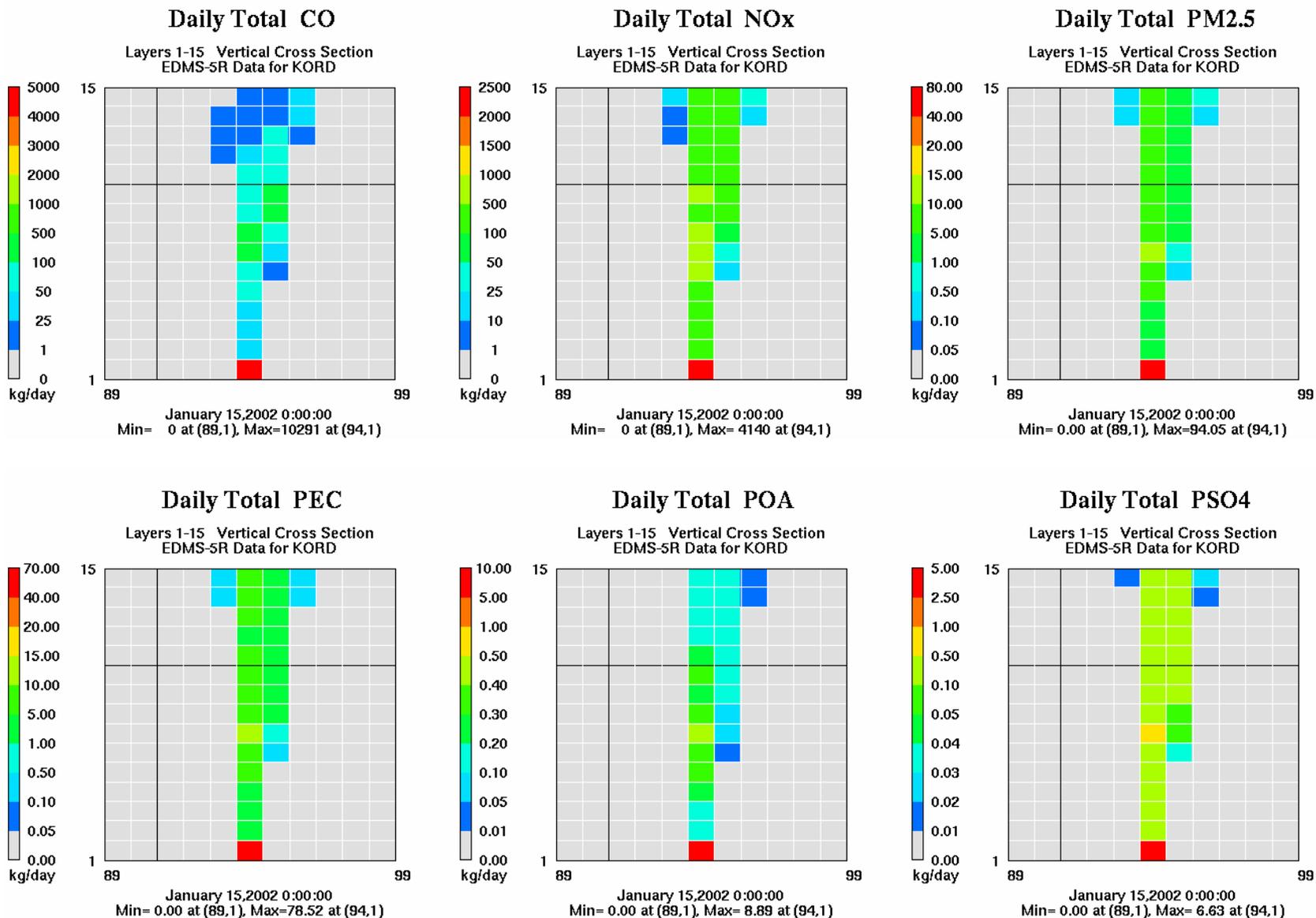
Figure 6c. Daily total of CO, NOx, PM$_{2.5}$, PEC, POA, and PSO4 emissions vertical profiles from Providence/TF Green (PVD).
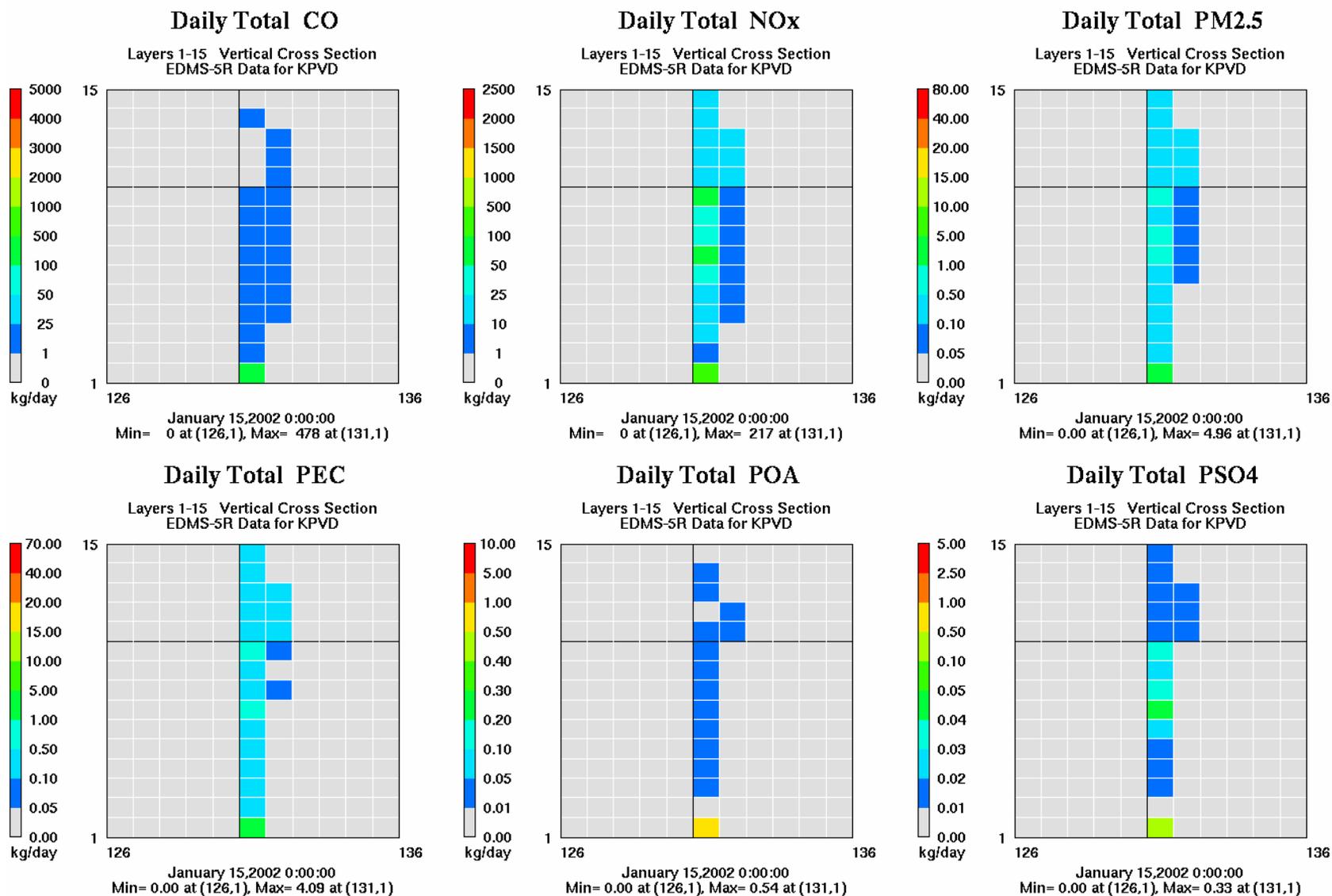
CONCLUSIONS

We have developed EDMS2Inv, a new interface to process commercial aviation emissions in the LTO cycle (up to 10,000 ft) from EDMS through SMOKE, and then through CMAQ. We performed extensive quality assurance of the processed results to make sure that the speciation, and the spatial and temporal allocation of these emissions were performed accurately. We processed criteria air pollutant emissions for three airports [Atlanta Hartsfield (ATL), Chicago O'Hare (ORD), and Providence T.F. Green (PVD)] through the new interface, and this work can be easily extended to process HAP estimates as well using SMOKE's 'integrate' option. These airport emissions will be merged with the baseline emissions (which do not contain aviation emissions) to prepare inputs for a nested CMAQ application over the Eastern United Sates. This research version of EDMS is an improvement from the publicly released version, which models emissions only upto 3,000 feet, and also estimates emissions at heights that are consistent with the CMAQ modeling application.

The new interface EDMS2Inv allows a spatially enhanced vertical representation of emission inputs by allocating emissions into the appropriate CMAQ modeling layers aloft and a temporally enhanced representation by allocating hourly EDMS emissions into regional air quality models instead of using uniform seasonal or monthly profiles. The availability of such an interface with improved representation of aviation emissions in air quality models will help support the design of new sensitivity scenarios to assess the impacts of the rapid growth of aviation in the United States and for improved air quality management.

The availability of such an interface to process EDMS outputs (which are also used as AERMOD inputs) also facilitates comparison of AERMOD outputs with CMAQ outputs (after they have been processed through the interface) in the immediate vicinity of the airports. Since AERMOD does not treat chemical transformations and CMAQ does, and the two modeling systems have vastly different resource requirements, such comparisons using consistent input emissions to the models will be valuable. Further, we can develop hybrid modeling applications of these airport sources using a combination of AERMOD and CMAQ outputs that have a consistent emissions inputs basis.

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ACKNOWLEDGMENTS AND DISCLAIMER

KEY WORDS

SMOKE
CMAQ
EDMS
Emission Modeling
Aviation
Commercial Aircraft
HAPs
Air Toxics