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A NEW INTERFACE TO MODEL GLOBAL COMMERCIAL AIRCRAFT EMISSIONS FROM THE FAA AVIATION ENVIRONMENTAL DESIGN TOOL (AEDT) IN AIR QUALITY MODELS

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1 ABSTRACT

Commercial aircraft emit substantial amounts of pollutants during their complete activity cycle that ranges from landing-and-takeoff (LTO) at airports to cruising in upper elevations of the atmosphere, and affect both air quality and climate. Since these emissions are not uniformly emitted over the Earth, and have substantial temporal and spatial variability, it is vital to accurately evaluate and quantify the relative impacts of aviation emissions on ambient air quality. Federal Aviation Administration (FAA) has developed the Aviation Environmental Design Tool (AEDT), a software system that dynamically models aircraft performance in space and time to calculate fuel burn and emissions from gate-to-gate for all commercial aviation activity from all airports. To process in-flight aircraft emissions and to provide a realistic representation of these for treatment in grid-based air quality models, we have developed an interface processor called AEDTproc that accurately distributes full-flight chorded emissions in time and space to create gridded, hourly CMAQ-ready emissions input data. Unlike the traditional emissions modeling approach of treating aviation emissions as area sources or processing emissions only from the LTO cycles, AEDTproc distributes chorded aircraft emissions during LTO cycles as well as cruise activities into a time-variant 3-D gridded structure. The main goal of this study is to present results of processed 2006 global emissions from AEDT over a North American CMAQ domain to support a national-scale air quality assessment of the incremental impacts of in-flight emissions on surface air quality, focusing on spatio-temporal variability of these emissions.

2 INTRODUCTION

The Federal Aviation Administration Office of Environment and Energy (FAA-AEE) recognizes that the environmental consequences stemming from the operation of commercial aviation – primarily noise, emissions, and fuel burn – are highly interdependent and occur simultaneously throughout all phases of flight. The Aviation Environmental Design Tool (AEDT) is a software system that is designed to dynamically model full flight gate-to-gate aircraft performance in space and time to compute fuel burn, emissions, and noise from a single flight at an airport to scenarios at the regional, national, and global level. AEDT is currently used by the U.S. government for domestic planning and research analyses and in support of work within the International Civil Aviation Organization (ICAO) Committee on Aviation Environmental Protection (CAEP). It is the next generation aviation environmental consequence tool, and will be the official FAA compliance tool to replace the Emissions and Dispersion Modeling System (EDMS) that is currently designed to model emissions from single airport. In 2007, UNC developed an interface called to EDMS2Inv that converts EDMS's spatially and temporally allocated emissions that were ready for use in AERMOD, into the Sparse Matrix Operator Kernel Emissions (SMOKE)-ready inventory format. By using this interface, we enabled enhanced representation of hourly emissions from aircraft activity at an airport, specifically during LTO activities (Baek *et al.,* 2007).

To process FAA's AEDT in-flight aircraft emissions and to provide a realistic representation of these for treatment in grid-based air quality models, we have developed an interface processor called "AEDTproc", also known as AEDT Processor, that allows the users to accurately distribute full-flight chorded commercial aircraft emissions in time and space to create hourly gridded CMAQ-ready emissions input data. AEDTproc distributes full flight aircraft emissions during LTO cycles as well as cruise activities into a time-variant 3-D gridded structure. This tool follows the guidance developed by FAA on the use of AEDT gridded aircraft emissions in atmospheric models (FAA, 2010) regarding altitude adjustment, chemical speciation of pollutant by altitude, and so on. Above 10,000ft, altitudes are pressure-based altitudes defined relative to the International Standard Atmosphere (ISA).

In this paper, we discuss the AEDT data processing methods used to convert the chorded global-scale emissions from AEDT into a time-variant 3-D gridded emissions over a North American CMAQ domain to support a national-scale air quality assessment of the incremental impacts of in-flight emissions on surface air quality, focusing on spatio-temporal variability of these emissions.

3 AEDTPROC PROCESSING

Unlike EDMS2Inv developed in 2007 (Baek *et al.,* 2007), the AEDTproc interface tool does not require another emissions processor like SMOKE to create CMAQ-ready 3-D gridded, speciated hourly emissions. Chemical speciation and spatial allocations are driven by the input data within the interface. Modeling domain information (horizontal and vertical) is imported directly from the Meteorology-Chemistry Interface Processor (MCIP) input data files (i.e., GRID_CRO_2D, MET_CRO_3D and MET_COR_2D). GRID_CRO_2D input file contains terrain height information (HT) required for calculations above 10,000 feet above ground level (AGL) altitude (Figure 1). MET_CRO_3D input file provides information on model's vertical layers such as sigma-level (VGTOP3D) and altitude (ZF). Surface pressure (PRSFC) and top pressure (VGTOP) data from MET_CRO_2D are used to compute MCIP modeling sigma layer using AEDT pressure data for optional sigma-layer vertical allocation feature for above LTO altitude.

Chemical speciation is performed using the engine-specific chemical speciation profiles (i.e., piston and turbine engine types) that allow the user to convert AEDT total organic gases (TOG) into air quality model species (i.e., ALD2, ALDX, TOL, FORM, BENZENE, and so on) (Figure 1). The complete list of model species is available in Table 1. This information is based upon the new FAA/EPA TOG speciation profile [USEPA, FAA, 2009].

The AEDTproc also requires airport elevation heights information to convert AEDT-based above mean seal level (AMSL) height to above ground level (AGL) height for accurate vertical allocation in the air quality model.

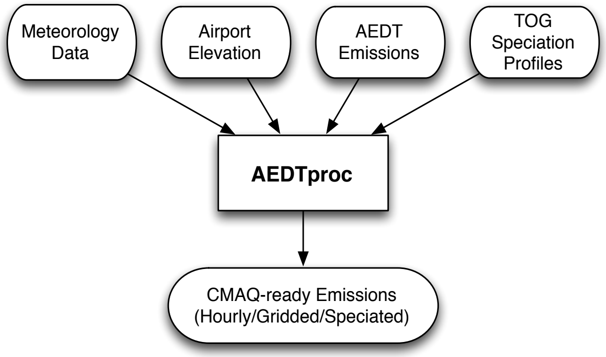

Figure 1. Flowchart of AEDTPROC processing procedure.

3.1 *Spatial Allocation*

For an enhanced vertical and horizontal spatial allocation of AEDT full-flight commercial aircraft emissions for use in regional-scale air quality models, we used "a chorded approach" to distribute link-based AEDT emissions into appropriate grid-cells in the air quality modeling domain. We spatially allocated emissions based on the fraction of time a flight spent in each grid-cell and layer between the start and endpoint of each segment. AEDT output file contains information on date and hour, starting point of segment such as latitude/longitude coordinates, altitude, pressure, fuel burn in unit of kg, and inventory pollutants (CO, HC, NOx as NO2 equivalent, Particulate Organic Carbon [POC], and Particulate Element Carbon [PEC]) in unit of g). Fuel burn is subsequently used to compute emissions of SO2 and primary sulfate (PSO4).

Figure 2 is an illustrative example of a flight segment, which spans multiple grid cells. With a chorded approach, emissions in each AEDT segment would be horizontally allocated to multiple grid cells. Without a chorded approach, emissions would be allocated to the grid-cell with the starting coordinate alone for that segment.

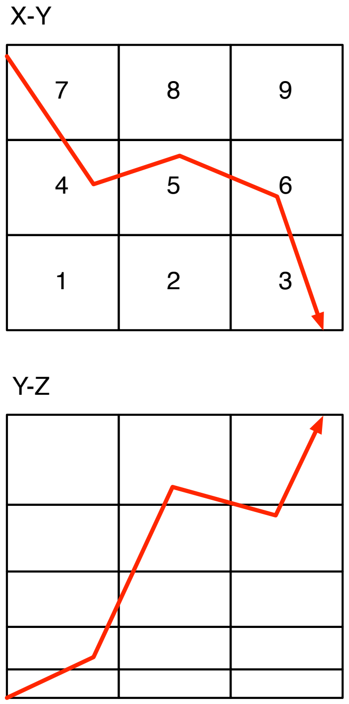

Figure 2. Horizontal and vertical allocation of AEDT link-based emissions.

The emission in each grid cell is also vertically distributed into air quality model layers. Figures 3 and 4 show an example of 3-D spatial allocation of a full trajectory flight from JFK to LAX with and without a chorded approach. It clearly shows the enhanced representation of the emissions in 3-D space for a full flight trajectory.

3.1.1 Altitude and Elevation Corrections

Because MCIP's sigma levels are based on AGL, one needs to convert altitudes reported as above AMSL by AEDT to AGL by subtracting the elevation of the departure airport for takeoff activities below 10,000 ft., terrain height from MCIP data for activities above 10,000 ft., and the elevation of the arrival airport for landing activities below 10,000 ft. We used a global airport elevation database from Volpe for this step. This database included all but 9 airports in the 2006 AEDT data (5 airports closed since 2006 and 4 were small airports). The elevations for these 9 airports were obtained online and added to the database.

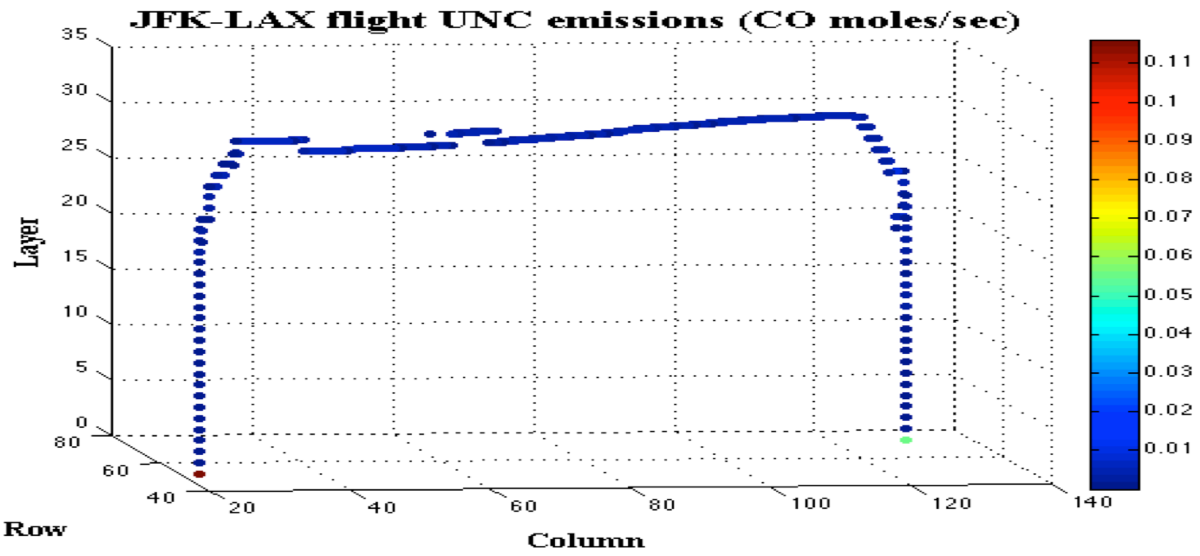

Figure 3. A 3-D spatial allocation of a full trajectory flight from JFK to LAX with a chorded approach.

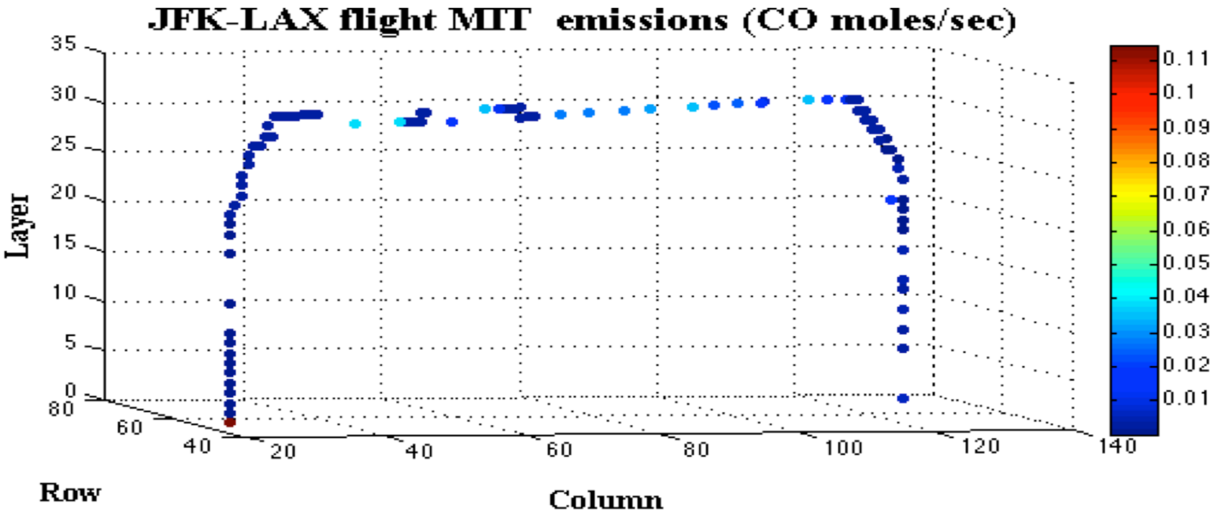

Figure 4. A 3-D spatial allocation of a full trajectory flight from JFK to LAX without a chorded approach.

AEDT emissions are initially gridded onto a regular polar 3-D array. Altitudes are in increments of 500 ft (nominal) starting at 0.0 ft as AMSL. Depending on the altitude, altitude definitions are treated differently in AEDT. Following the guidance on the use of AEDT gridded aircraft emissions in atmospheric models, all emissions below 10,000 ft (nominal) correspond to true altitude. Altitude above 10,000 ft (nominal) is estimated as a function of pressure (FAA, 2010). For segments below 10,000 ft. AMSL, we used the AEDT reported altitude values and layer heights given by the MCIP meteorological files to allocate emissions vertically. For segments above 10,000 ft. AMSL, we converted atmospheric pressures in the AEDT data to altitudes and used sigma layers from MCIP modeling domain to allocate emissions vertically. The following equation was used to convert atmospheric pressure (in hPa) to altitudes (in ft).

$$\begin{aligned} Altitude \ &= -4.384385x10^{-13}\ x\ P^5 + 1.368174x10^{-9}\ x\ P^4 \\ &\quad - 1.650600x10^{-6}\ x\ P^3 + \ 9.902038x10^{-4}\ x\ P^2 \\ &\quad -3.488077x10^{-1}\ x\ P\ +\ 7.99345x10^1 \end{aligned}$$

where P is the atmospheric pressure reported by AEDT. This is a 5th order polynomial with an r^2 value of 0.9998 fit to the equation

$$Altitude = \frac{T_o}{LR}\ x\ \left(1 - \frac{P}{P_o}\right)^{R_d\ x\ \frac{LR}{g}}$$

where T_o is the sea level standard temperature, LR is the temperature lapse rate, P is atmospheric pressure, P_o is the sea level standard atmospheric pressure, R_d is the specific gas constant for dry air, and g is the Earth-surface gravitational acceleration. For the ISA, T_o = 288.15 K, LR = 0.0065 K/m, P_o = 1013.25 hPa, R_d = 287.05307 J/(kg K), and g = 9.80065 m/s^2. The polynomial was used because it only requires 1 variable (atmospheric pressure) and is assumed to be more computationally efficient.

We initially processed AEDT altitudes using different approaches to understand the differences in spatial allocation between true altitude and pressure-altitude. Figures 5 and 6 show the differences in vertical profiles of AEDT after processing. "LTO10k$_{\_altitude}$" is based on altitude values throughout using altimeter field elevation (AFE). "LTO10k$_{\_pressure}$" is based on estimated pressure-altitude values throughout. LTO10K$_{\_altitude\_pressure}$ is a combination of true altitude from AEDT up to 10,000 ft and estimated pressure-altitude above 10,000 ft.

We don't see a noticeable difference between these three approaches for two of the pollutants (CO and VOC) except for heights below 10,000 ft, since their emissions calculation does not vary with LTO and non-LTO altitudes. The difference below 10,000 ft is likely driven by high elevation airports from Denver, Salt Lake City, and so on. However, as shown in Figure 6, emissions of POC do vary significantly between non-LTO and LTO altitudes compared to other pollutants because PM emission calculations change depending on LTO altitude. Based on the FAA guidance, the definition of LTO height impacts the NOx speciation profile that converts NOx to NO, NO_2 and HONO and equations to estimate POC and PEC (FAA, 2010).

In the final processing, we consider only the results of "LTO10k$_{\_altitude\_pressure}$" method, as it is the approach suggested in the FAA guidance document of processing AEDT emissions.

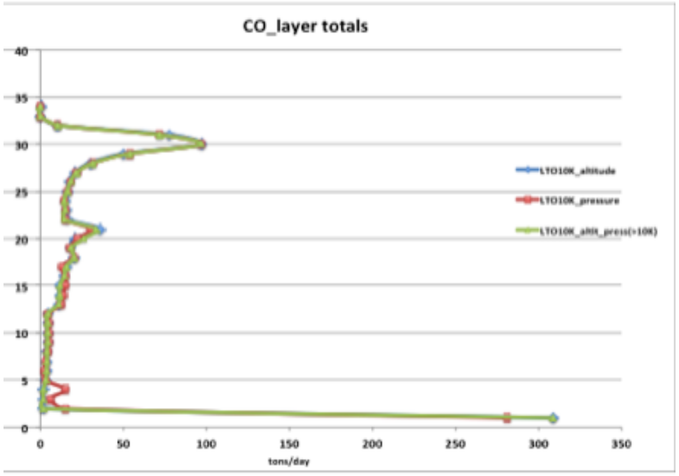

Figure 5. Vertical profiles of CO using three different approaches for computing altitudes.

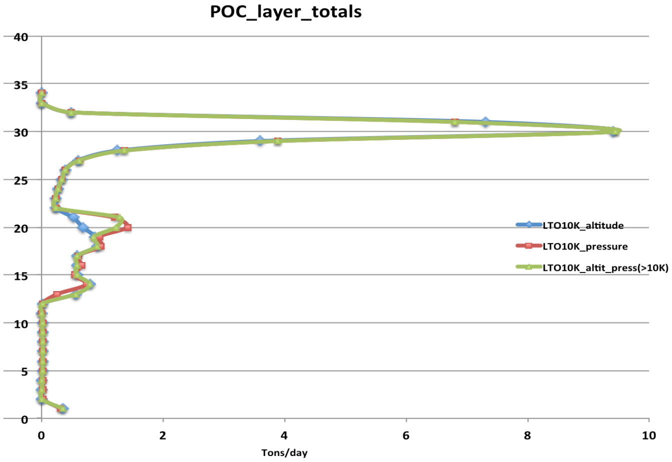

Figure 6. Vertical profiles of POC using three different approaches for computing altitudes.

3.2 Chemical Speciation Allocation

As mentioned, AEDT estimates fuel burn in unit of kg, and inventory pollutants (CO, Hydrocarbon [HC], NOx as NO2 equivalent, POC, and PEC) in unit of g from gate-to-gate for all commercial aviation activity from all airports. Based on FAA guidance document of AEDT processing, the definition of LTO impacts the NOx speciation profile used and equations to estimate PEC and POA and therefore will impact total emissions of NO, NO_2, PEC, and POA. The user can optionally determine the LTO height [`LTO_ALTITUDE`] during AEDTproc processing. It is critical for the user to determine appropriate LTO height for proper processing of AEDT dataset. If LTO height is set to 3,000 ft and AEDTproc processes airports that have elevation heights greater than 3,000 ft, there could be a potential problem in distributing AEDT emissions into model layers.

NOx emissions are given on an NO_2 mass basis. Partitioning at cruise at the engine exit plane by mole fraction is: 90% NO, 9% NO_2, 1% HONO for non-LTO emissions, or 76% NO, 23% NO_2, 1% HONO for LTO emissions. We subsequently converted NO emissions from NO_2 equivalency to NO equivalency.

PEC aerosol emissions below LTO height in g = PEC. For non-LTO, PEC emissions in g = Fuel Burn × 0.03.

POC aerosol emissions below LTO in g = POC. For non-LTO, POC organic carbon emissions in g = Fuel Burn × 0.03.

Unlike the 3 pollutants discussed above (NOx, POC and PEC), TOG, SO_2 and PSO_4 can be estimated following equations using AEDT fuel burn data without LTO height adjustment.

SO_2 and SO_4 emissions are scaled from fuel burn assuming a fuel sulfur concentration. Fuel sulfur concentration (FSC) = 600 [400-800] in mg/kg-fuel, and a mole fraction (E) = 2.0 in % of the fuel sulfur is emitted as SO^{VI}, with the remaining (100-E) % being emitted as SO_2. Therefore emissions of SO_2 in g = (FSC/1000) × [(100-E)/100] × Fuel Burn × (64/32), where it should be recalled that Fuel Burn is in kg. Emissions of SO^{VI} as SO_4 in g = (*FSC*/1000) × (*E*/100) × Fuel Burn × (98/32).

HC emissions are in CH_4 equivalent, which is converted to total organic gases (TOG) as TOG = HC × 1.16.

3.2.1 TOG Split Factors

Once TOG is estimated based on HC, AEDTproc can convert TOG into air quality model species (e.g., ALD2, ETOH, FORM, PAR, XYL, and so on depending on the choice of chemical mechanism) by aircraft engine type (turbine and piston) using engine-specific TOG chemical speciation profiles [`TURBINE_SPC` and `PISTON_SPC`] developed by EPA (Table 1).

To prepare CMAQ-ready emissions, we need to chemically speciate TOG into model species. Table 1 indicates the splitting factors (SF=mass fraction of total VOC emissions/molecular weight) to speciate TOG emissions from turbine engines, which are based on the chemical speciation profile #5565 (1099 was used for piston engines) based on U.S. EPA National Emission Inventory modeling 2005 platform version 4.2 (U.S. EPA, 2012).

Table 1. TOG speciation factors for turbine and piston engines (for Carbon Bond 2005 chemical mechanism).

Model Species	Turbine Engine [TURBINE_SPC]		Piston Engine [PISTON_SPC]	
	Mass Fraction	Molecular Weight	Mass Fraction	Molecular Weight
ALD2	0.0435	43.6298	0.0444	43.3667
ALDX	0.0585	35.2256	0.0264	37.2487
CH4	NA	NA	0.1095	16.0425
ETH	0.1546	28.0532	0.155	28.0532
ETHA	0.0052	30.0690	0.0091999	30.069
ETOH	NA	NA	4.00E-05	28.7623
FORM	0.1389	29.3904	0.1543	29.8843
IOLE	0.0246	56.1063	0.0090426	56.1092
MEOH	0.0181	32.0419	4.46E-06	14.3811
OLE	0.0876	28.5737	0.0848	29.894
PAR	0.3729	14.3326	0.1818	15.4652
TOL	0.0223	98.1480	0.0175	96.2053
UNR	0.0430	13.4366	0.1961	27.7326
XYL	0.0278	105.7999	0.0119	104.3208

3.3 *AEDTproc Input Files*

This section lists all the input files required to run AEDTproc program and Figure 7 is a flow diagram of AEDTproc program.

- `APRT_ELEVATION`: Global airport elevation height information. Arrival and departure airport elevation heights are required to convert AEDT MSL altitudes to AGL up to 10,000 feet AGL altitude.
- `FLIGHT_FILELIST`: AEDT raw flight data including flight ID, latitude/longitude coordinates of origin location, altitude, pressure, fuel burn in unit of kg, and inventory pollutants (CO, HC, NOx as NO2 equivalent, POC, and PEC) in unit of g.
- `SEGMENT_FILELIST`: AEDT raw segment data including types of aircraft, departure/arrival airports, and engine types.
- `GRIDDESC`: Horizontal modeling domain information.
- `GRID_CRO_2D`: Terrain height information required for AGL calculations above 10,000 feet AGL altitude.
- `MET_CRO_3D`: Vertical modeling layer information (sigma-level (VGTOP_3D) and altitude (ZF))
- `MET_CRO_2D`: Surface pressure (PRSFC) and top pressure (VGTOP) data. PRSFC and VGTOP values are used to compute modeling sigma layer using AEDT pressure for optional sigma-layer vertical allocation feature.
- `PISTON_HAP`: FAA piston-engine pollutant profiles reported by FAA
- `PISTON_SPC`: Chemical speciation profiles that convert piston-engine specific pollutants (TOG, CO, NOx, SO_2, PEC and POC) estimated by PISTON_HAP input file to model species (e.g., ALD2, FORM, PAR, XYL, and so on)
- `TURBINE_HAP`: FAA turbine-engine pollutant profiles measured by FAA
- `TURBINE_SPC`: Chemical speciation profiles that convert turbine-engine specific pollutants (TOG, CO, NOx, SO_2, POC, and PEC) estimated by TURBINE_HAP input file to model species (e.g., ALD2, FORM, PAR, XYL, and so on)

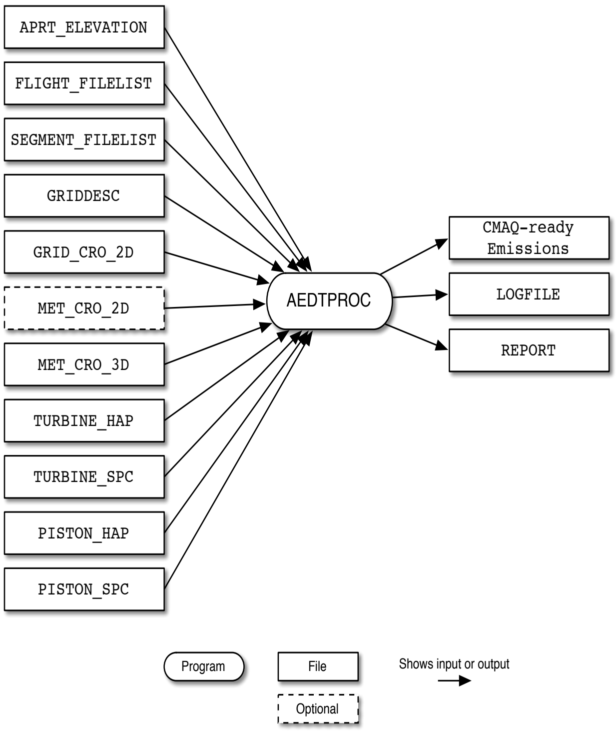

Figure 7. Flow diagram of AEDTproc program.

3.4 *Environment Variables*

- `CUTOFF_ALTITUDE [default: 70,000]`

: Determines the cutoff height in unit of feet. This option will allow users to discard AEDT data above cutoff height.

- `LTO_ALTITUDE [Default: 10,000]`

  : Determines the LTO height in unit of feet. The definition of LTO height impacts the NOx speciation profile that converts NOx to NO, NO2 and HONO and equations to estimate PEC and POA.

- `SIGMA_VERT_ALLOC_YN [default: Y]`
  : Determines whether sigma-layer vertical allocation or not. If this flag is set to Y, user must provide MET_CRO_2D input file to provide surface pressure (PRSFC) and top pressure (VGTOP) data to compute sigma layer.

4 RESULTS

We have completed developing this tool, and processed CMAQ-ready emissions for 2 months. Given its flexibility, this tool can be easily adapted for processing AEDT-based aircraft emissions to any CMAQ modeling domain in the world. Figure 8 presents a daily total NO emissions across all model vertical layers.

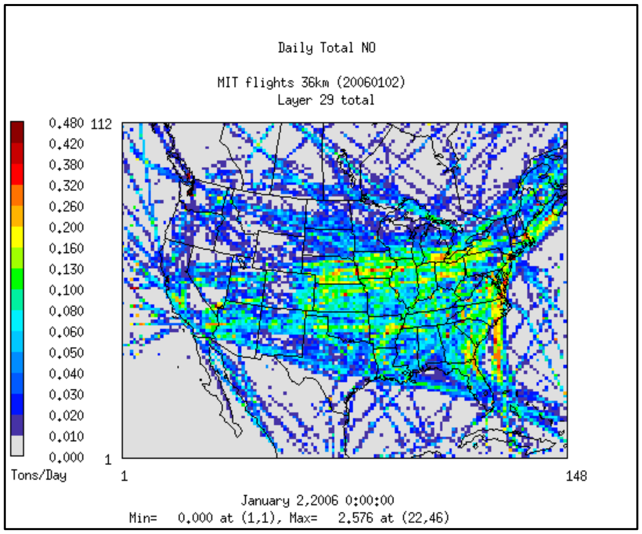

Figure 8. Horizontal spatial distribution with daily vertical total values.

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