The 2011 National Air Toxics Assessment (2011 NATA): Emissions and Modeling Approach

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ABSTRACT

The National-Scale Air Toxics Assessment (NATA) is a modeling assessment which combines a detailed emissions inventory, atmospheric fate and transport modeling, exposure modeling, and health risk criteria to characterize the risks associated with inhalation of air toxics of outdoor origin. A national-scale effort was conducted for the years 1996, 1999, 2002, and 2005, and included a nationwide characterization of the ambient levels and associated risks from hazardous air pollutants listed in Section 112 of the Clean Air Act plus diesel PM. The 2011 assessment is expected to be completed and released later in 2015. The analysis will include a series of improvements to the assessment methodology in past NATA analyses including: improvements to the national emissions inventory and source characterization including spatial and temporal allocation data and methods, and the use of a hybrid approach that utilizes a photochemical grid model and dispersion model to more accurately account for impacts of atmospheric chemistry and long range transport. This presentation will review the updated modeling methodology being utilized for the 2011 NATA and present some of the preliminary emissions results.

INTRODUCTION

The National Air Toxics Assessment (NATA) is a model-based characterization of air toxics, also known as hazardous air pollutants (HAPs), across the nation. It estimates risks associated with the inhalation of toxics pollutants from outdoor air at the census tract level. The U.S. Environmental Protection Agency (EPA) developed NATA as a state-of-the-science screening tool for State/Local/Tribal Agencies to prioritize pollutants, emission sources and locations of interest for further study in order to gain a better understanding of HAP risks.

NATA is used by the EPA, state and local governments, health researchers and the public. The EPA most recently used it to inform the Second Integrated Urban Air Toxics Report to Congress[1] (EPA 2014). The EPA also used NATA in the school air toxics monitoring effort, to determine which schools and pollutants to monitor (http://www.epa.gov/schoolair/). The EPA's Office of Transportation and Air Quality (OTAQ) cited NATA in major rulemakings, including its Mobile Source Air Toxics Rule (which resulted in a large reduction of benzene and other air toxics), heavy-duty vehicle and engine regulations, Renewable Fuels Standard 2, and Tier 3 light-duty vehicle standards. The EPA's Office Environmental Justice is developing tools that link demographic data to NATA (EJ Screen). The EPA's Office of Research and Development (ORD) uses NATA to set their research agenda and includes NATA as one of its data layers in its Community-Focused Exposure and Risk Screening Tool (CFERST, http://www.epa.gov/heasd/c-ferst/). EPA's Office of Enforcement and Compliance assurance uses NATA as one of many tools for prioritization in enforcement targeting efforts.

State and local governments also use NATA to prioritize pollutants and sources (Weinhold, 2011) and to initiate their own modeling assessments (e.g., Portland Air Toxics Assessment, 2006). It is also used by EPA and State and local agencies to compare against monitoring data, e.g., the Dears Study (George, 2011), Las Vegas Near Road Study (Kimbrough, 2014), Pittsburgh, (Logue, 2011), California (Garcia, 2014) and Houston (Whitworth, 2011). Researchers are using NATA in health studies investigating linkages of HAP exposures to breast cancer (Garcia, 2015), autism (University of Pittsburgh Schools of the Health Sciences, 2014 and Roberts, 2013) and other health issues (Stoner, 2013 and Swartz, 2015). Authors of roughly a hundred published papers have cited NATA in their research.

The NATA is also used to help improve the National Emission Inventory (NEI) and emissions processing approaches. Reviews of NATA risk results have led to improved emission estimates, geographic coordinates and release parameter characteristics for point sources. These changes are incorporated in the Emission Inventory System (EIS) that is used to build the NEI, so that subsequent inventories will automatically have the corrected information. In addition the approach currently used in the NEI for allocating commercial marine emissions to shapes (as opposed to census tracts) resulted from issues found in previous NATAs with this category.

[1] Major findings in the report regarding NATA: "The EPA's 2005 National Air Toxics Assessment (NATA) estimated that based on 2005 conditions, the national average cancer risk was about 50 in a million due to emissions of air toxics from all outdoor sources (i.e., all stationary sources and mobile sources as well as background and secondary formation). NATA also estimated that based on 2005 conditions, more than 13.8 million people, mainly in urban locations, were exposed to cancer risks greater than 100 in a million due to these emissions of air toxics. While emissions from three pollutants, namely formaldehyde, benzene and acetaldehyde, contributed to about two-thirds of the total risks at a national level; each urban area had a unique set of sources and pollutants that drive the risk."

The first national scale modeling-based assessment was EPA's Cumulative Exposure Project (Caldwell, 1998) which assessed toxics for the year 1990 and was conducted by EPA's Office of Policy. Subsequently, the concept of NATA became one of the components of EPA's Integrated Urban Air Toxics Strategy, which recommended a broad umbrella of national air toxics assessment activities including air toxics monitoring, emission inventories, national and local scale air quality modeling, multi-media and exposure modeling, and research. The first NATA was conducted with EPA's model-ready national emission inventory for the year 1996 (the "National Toxics Inventory") and covered 32 urban HAPs and diesel PM. Subsequent NATAs covered all of the HAPs[2] and diesel PM, and used emissions data for 1999, 2002 and 2005. Each NATA uses updated emissions inventory data, emissions processing and modeling techniques and uses the EPA's most recent health risk estimates. The results of each of the NATAs, including emission inputs, ambient concentrations and cancer and noncancer risks at the census tract level are provided on the EPA's NATA website. A technical methods document, also available on the NATA website (ICF, 2011) outlines the approaches used in the 1996-2005 NATAs.

The 2011 NATA uses a hybrid approach that was demonstrated for the Detroit Multipollutant Project (Wesson, 2010). This technique combines the results of the chemical transport model, the Community Multiscale Air Quality (CMAQ) Modeling System and a dispersion model, the American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD). The photochemical transport model provides mass conservation while treating secondary pollutant formation, transport, chemistry, and deposition all within a multipollutant system that includes emissions of anthropogenic emissions, biogenic emissions and fires. The dispersion model quantifies the sub-grid cell variability, capturing the highly resolved spatial resolution of the inventoried point sources. The use of this approach also alleviates the need for background concentrations to be added to the model estimates and provides census tract resolution and source attribution, similar to that provided in previous NATA analyses.

This paper discusses the 2011 NATA analysis design, focusing on the preparation of emission inputs for the air quality modeling.

DESIGN

Figure 1 shows the model design for NATA. The starting point is the 2011 NEI. NATA uses the 2011 NEI version 2[3]. For CMAQ, emissions from all sources are processed by the Sparse Matrix Operator Kernel Emissions (SMOKE), version 3.6, within a multipollutant emissions platform framework that provides speciated, hourly and gridded emissions of HAPs and criteria air pollutants (CAPs) to CMAQ (version MPv5.0.2). AERMOD (version 12345) uses point, nonpoint, onroad and nonroad emissions. While not shown in the figure, AERMOD is run through the Human Exposure Model (HEM) interface, which uses input files that are similar to the inputs to SMOKE. The annual concentrations from CMAQ and AERMOD are combined via the hybrid equation discussed in detail later. Background concentrations, representing the contribution of the total concentration due to long range transport, including from outside the modeling domain, are added only to those HAPs that are not run through CMAQ. Exposure concentrations are estimated by multiplying the ambient modeled concentrations by exposure-to-ambient ratios that were derived from the Hazardous Air Pollutant Exposure model

[2] For which the inventory has emissions.
[3] Post model corrections are made to address comments received after the 2011 NEI v2 was processed through CMAQ.

(HAPEM, version 7) using a preliminary version of the 2011 NATA ambient levels. Cancer and noncancer and risks are characterized using the exposure concentrations and recent health criteria data.

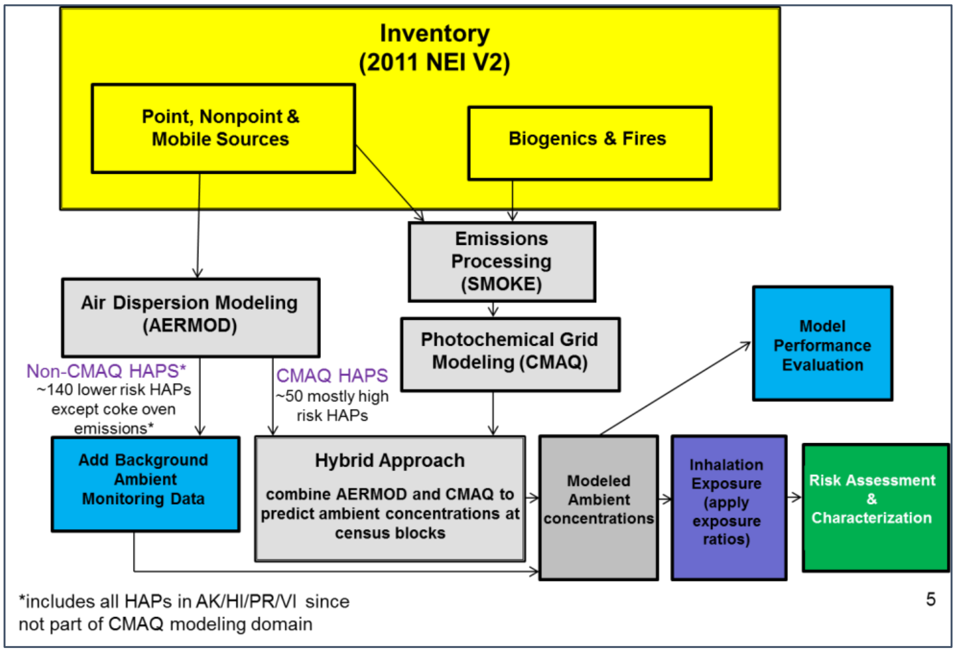

Figure 1. 2011 NATA Design: emissions, air quality modeling, exposure, risk

The hybrid approach is new to the 2011 NATA and combines the annual concentrations from CMAQ and AERMOD to adjust the AERMOD block concentrations in order to impart the spatial variability such that the overall average of the receptors in the grid cell equals the CMAQ concentration, and the variability of concentrations at the receptors in the grid cell is based on the AERMOD concentrations. Figure 2 shows the hybrid conceptual approach.

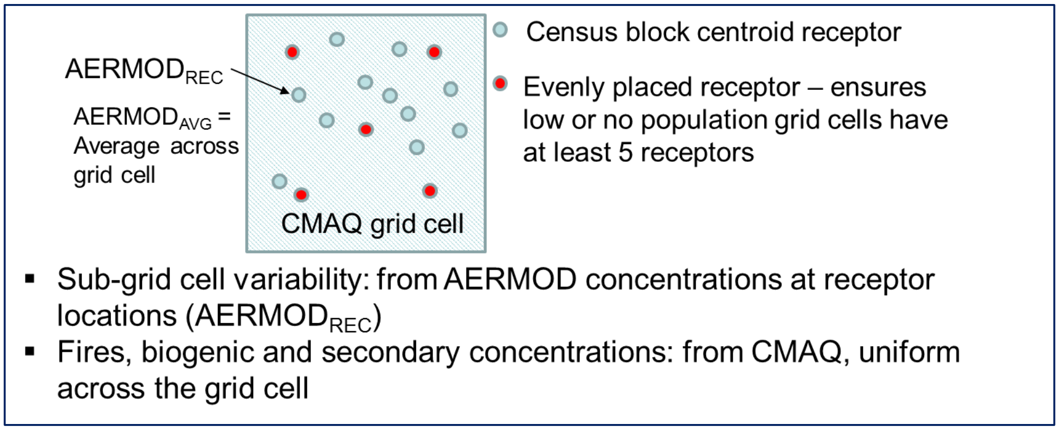

Figure 2. Concept of the hybrid approach

Figure 3 shows the hybrid equation, which is used to calculate a hybrid concentration for each AERMOD receptor that falls within the CMAQ grid cells for pollutants that are modeled in CMAQ.

The hybrid concentration at each AERMOD receptor is computed as the sum of the adjusted $AERMOD_{REC}$ concentration and the CMAQ grid cell concentrations from fires, biogenic emissions and secondary formation. There are approximately 56,500 CMAQ grid cells that cover the continental US. There are approximately 6.7 million AERMOD receptors nationwide (6.6 million within the CMAQ grid cells), including mostly the census block centroids, but also including schools, monitors, and five extra receptors that are equally spaced within each CMAQ grid cell to avoid having grid cells with no receptors.

The adjusted AERMOD concentration in the first term, requires the computation of an average AERMOD concentration across each grid cell. Because most of the AERMOD receptors are census block centroids that may not be spatially well-distributed in the grid cells, an AERMOD grid cell average concentration ($AERMOD_{AVG}$) based on an arithmetic mean of the receptor concentrations in each grid cell may not be spatially representative of the grid cell. Therefore, we use another method to calculate $AERMOD_{AVG}$, which is to create a concentration surface. We create a concentration surface for each CMAQ HAP using inverse-distance weighting interpolation (cell size = 1 km, power = 2) of the AERMOD receptor concentrations. Each HAP surface is continuous nationwide, consisting of 1 km raster cells with concentration values. The mean of these values within each CMAQ grid cell is used as $AERMOD_{AVG}$.

To implement the hybrid equation, the CMAQ concentrations need to be apportioned into a fires and biogenics component. This requires 2 additional runs of CMAQ known as "zero out" runs because CMAQ does not include source attribution for all HAPs at this time. Each receptor within the same grid cell gets a uniform contribution from the fires and biogenics component.

$$\boldsymbol{C_{hybrid,REC} = \underbrace{AERMOD_{REC} \times \frac{CMAQ_{P,NFB}}{AERMOD_{AVG}}}_{\text{Adjusted AERMOD concentration from primary non-fire, non-biogenic sources}} + \underbrace{CMAQ_{SEC,NFB}}_{\text{CMAQ secondary concentration from non-fire, non-biogenic sources}} + \underbrace{CMAQ_{FIRE}}_{\text{CMAQ concentration from fires}} + \underbrace{CMAQ_{BIOG}}_{\text{CMAQ concentration from biogenic emissions}}}$$

Figure 3. Hybrid Equation

The hybrid approach is limited to use for the HAPs in CMAQ and for the CMAQ domain (continental U.S.). Other than coke oven emissions, CMAQ includes the HAPs with greatest risks (based on previous NATA results). The other non-CMAQ pollutants and rest of the NATA domain uses the AERMOD results with a background concentration added, where available.

Table 1 lists the HAPs in CMAQ MPv5.0.2. Numerous polycyclic aromatic hydrocarbons (PAHs) and arsenic were added to the CMAQ algorithms for the purposes of NATA. The PAHs were added as tracer gases, and arsenic as a tracer metal. Note that the PAHs are modeled as groups of multiple HAPs with the same unit risk estimate (URE), e.g., the CMAQ species named "PAH0E00" has a URE of zero, and "PAH17E2" has a URE of 1.7E-2 m3/ug.

Table 1. HAPs included in CMAQ, and hence, the hybrid approach

Air Toxic	CMAQ species name(s); specific compounds included in parentheses
1,1,2,2-Tetrachloroethane	CL4_ETHANE1122
1,3-Butadiene	BUTADIENE13
1,3-Dichloropropene	DICHLOROPROPENE
1,4-Dichlorobenzene(p)	DICHLOROBENZENE
2,4-Toluene diisocyanate	TOL_DIIS
Acetaldehyde	ALD2,ALD2_PRIMARY
Acrolein	ACROLEIN, ACROLEIN_PRIMARY
Acrylonitrile	ACRYLONITRILE
Arsenic	AASI, AASJ, and ASSK
Benzene (including benzene from gasoline)	BENZENE
Beryllium	ABEK, ABEI, ABEJ
Cadmium	ACDI,ACDJ,ACDK
Carbon tetrachloride	CARBONTET
Chlorine	CL2
Chloroform	CHCL3
Chromium Compounds	ACR_VIK,ACR_VIJ,ACR_VII (Chromium VI, Chromic Acid (VI), chromium trioxide)
Chromium Compounds	ACR_IIIK,ACR_IIII,ACR_IIIJ *we will not provide Chromium III NATA results, only hexavalent (Chromium VI)
Diesel PM *	ADE_ECI,ADE_ECJ,ADE_OCI,ADE_OCJ,ADE_SO4J,ADE_NO3J,ADE_OTHRI, ADE_OTHRK,ADE_K
Ethylene dibromide (Dibromoethane)	BR2_C2_12
Ethylene dichloride (1,2-Dichloroethane)	CL2_C2_12
Ethylene oxide	ETOX
Formaldehyde	FORM, FORM_PRIMARY
Hexamethylene-1,6-diisocyanate	HEXAMETHY_DIIS
Hydrazine	HYDRAZINE
Hydrochloric acid	HCL
Lead Compounds	APBK,APBJ,APBI
Maleic anhydride	MAL_ANHYDRIDE
Manganese Compounds	AMN_HAPSK, AMN_HAPSJ,AMN_HAPSI
Mercury Compounds	HG,HGIIGAS,APHGI,APHGJ (note that there is no APHGK in CMAQ)
Methanol	MEOH
Methylene chloride (Dichloromethane)	CL2_ME
m-Xylenes	MXYL
Naphthalene	NAPHTHALENE
Nickel Compounds	ANIK, ANII, ANIJ (Nickel, Nickel oxide, Nickel refinery dust)
o-Xylenes	OXYL
p-Xylenes	PXYL
Quinoline	QUINOLINE
Tetrachloroethylene (Perchloroethylene)	CL4_ETHE
Toluene	TOLU
Trichloroethylene	CL3_ETHE
Triethylamine	TRIETHYLAMINE
Vinyl chloride	CL_ETHE
Polycyclic Organic Matter, risk group 0	PAH_000E0 (Anthracene, Phenanthrene, Pyrene)
Polycyclic Organic Matter, , risk group 1.76E-5	PAH_176E5 (Carbazole, Chrysene)
Polycyclic Organic Matter, risk group 8.8E-5	PAH_880E5 (12-Methylbenz(a)Anthracene, 1-Methylnaphthalene, 1-Methylphenanthrene, 1-Methylpyrene, 2-Chloronaphthalene, 2-Methylnaphthalene, 9-Methyl Anthracene, Acenaphthene, Acenaphthylene, Benzo(c)phenanthrene, Benzo[e]Pyrene, Benzo[g,h,i,]Perylene ,Coal Tar ,Extractable Organic Matter (EOM),Fluoranthene, Fluorene , Methylanthracene, Methylbenzopyrene, PAH, totalPAH/POM - UnspecifiedPerylene (6) PAH_176E4 1-Nitropyrene, Benz[a]Anthracene, Benzo(a)Fluoranthene, Benzo(g,h,i)Fluoranthene, Benzo[b]Fluoranthene, Benzo[j]fluoranthene, Benzo[k]Fluoranthene,Benzofluoranthenes, Dibenz[a,h]acridine, Dibenzo[a,j]Acridine, Indeno[1,2,3-c,d]Pyrene)
Polycyclic Organic Matter, risk group 1.76-4	PAH_176E4 (1-Nitropyrene, Benz[a]Anthracene, Benzo(a)Fluoranthene, Benzo(g,h,i)Fluoranthene, Benzo[b]Fluoranthene, Benzo[j]fluoranthene,

Air Toxic	CMAQ species name(s); specific compounds included in parentheses
	Benzo[k]Fluoranthene,Benzofluoranthenes, Dibenz[a,h]acridine, Dibenzo[a,j]Acridine, Indeno[1,2,3-c,d]Pyrene)
Polycyclic Organic Matter, risk group 1.76-3	PAH_176E3 5-Methylchrysene, 7H-Dibenzo[c,g]carbazole, Benzo[a]Pyrene, Dibenzo[a,e]Pyrene,7)
Polycyclic Organic Matter, risk group 1.92E-3	PAH_192E3 (Dibenzo[a,h]Anthracene)
Polycyclic Organic Matter, risk group 1.01E-2	PAH_101E2 (3-Methylcholanthrene)
Polycyclic Organic Matter, risk group 1.76E-2	PAH_176E2 (Dibenzo[a,h]Pyrene, Dibenzo[a,i]Pyrene, Dibenzo[a,l]Pyrene)
Polycyclic Organic Matter, , risk group 1.14E-1	PAH_114E1 (7,12-Dimethylbenz[a]Anthracene)
Propylene dichloride (1,2-Dichloropropane)	PROPDICHLORIDE

Another key feature of the design for the 2011 NATA is the ability to present the risk results by source groups for all of the modeled pollutants. AERMOD is run in a way that allows us to save concentrations from sources we group together. This allows risks to be apportioned by source group. For CMAQ pollutants, the source attribution from the AERMOD receptor concentrations is applied to the adjusted AERMOD concentrations (first term of the hybrid equation). The fires, biogenics and secondary source groups are based on the CMAQ concentrations. Table 2 shows the source groups being used in NATA.

Table 2. Source groups for nonpoint, nonroad and onroad categories

NEI inventory data category	NATA Broad category	Source group		NEI inventory data category	NATA Broad category	Source group
nonpoint	nonpoint	NP-Bulk_gas_term		nonpoint	nonpoint	NP-Refineries
nonpoint	nonpoint	NP-Chemical_Mfg		nonpoint	nonpoint	NP-Oil/Gas
nonpoint	nonroad	NP-CMV_ports		nonpoint	nonpoint	NP-SfcCoating_IndSolvent
nonpoint	nonroad	NP-CMV_underway		nonpoint	nonpoint	NP-Storage_Transfer
nonpoint	nonpoint	NP-Comm_cooking		nonpoint	nonpoint	NP-WasteDisposal_Other
nonpoint	nonpoint	NP-Consumer_comm_solvent		nonroad	nonroad	NR-Construction
nonpoint	nonpoint	NP-Degreasing		nonroad	nonroad	NR-Diesel/Other
nonpoint	nonpoint	NP-Dry_cleaning		nonroad	nonroad	NR-Gas/Other
nonpoint	nonpoint	NP-Gas_stations (stage 1 only)		nonroad	nonroad	NR-Pleasurecraft
nonpoint	nonpoint	NP-IndComInst_fuel_comb		onroad	onroad	OR-Heavy Duty Diesel
nonpoint	nonpoint	NP-Industrial_NEC		onroad	onroad	OR-Heavy Duty Gasoline
nonpoint	nonpoint	NP-Landfills		onroad	onroad	OR- Light Duty Diesel
nonpoint	nonroad	NP-Locomotives		onroad	onroad	OR- Light Duty Gasoline
nonpoint	nonpoint	NP-Mining		onroad	onroad	OR-Refueling
nonpoint	nonpoint	NP-Misc_non-ind		point	point	POINT
nonpoint	nonpoint	NP-Nonferrous_metals		point	nonroad	Airports
nonpoint	nonpoint	NP-Non-industrial_surface_coating		point	nonroad	Railyards
nonpoint	nonpoint	NP-Residential Wood Combustion (RWC)		Events + nonpoint	FIRES	Fires (prescribed, wild, and agricultural)
nonpoint	nonpoint	NP-Non-RWC_ResFuelComb		nonpoint	BIOGENICS	biogenics

EMISSIONS

National Emission Inventory

The basis of the emissions for NATA is the 2011 NEI v2 (EPA, 2015). The 2011 NEI is a multipollutant inventory containing criteria and hazardous air pollutants. EPA develops year-specific multipollutant inventories every 3 years. EPA uses the EIS to collect, quality assure and store the data. Data are collected in 5 major inventory categories:

1. point - facilities at distinct locations;
2. nonpoint - county level;
3. onroad - county level, based on the sources computed primarily from EPA mobile modeling;
4. nonroad - county level, nonroad equipment, based on the sources computed primarily from EPA mobile modeling; and
5. event – wild and prescribe fires, daily emissions at specific locations.

Emissions for the NEI come from State, local and tribal agencies and other data sources. The Air Emissions Reporting Rule (AERR) requires State and local agencies (SLT) to report point source emissions for CAPs. Hazardous air pollutant (HAP) emissions are submitted voluntarily and are gap filled by EPA using a variety of data sources and approaches, primarily: the Toxics Release Inventory, "hap augmentation" by multiplying state-reported CAP by the ratio of the HAP and CAP emission factors[4], and data collected for rule development via information collection requests. SLT also report nonpoint categories or use the EPA-developed estimates. Similar to point sources, EPA conducts hap augmentation on nonpoint categories for which SLT submitted CAP but no HAP. Excluding California, which uses different models for mobile sources, onroad mobile emissions are computed using EPA's MOVES2014 model. Excluding California and Texas, nonroad equipment emissions (i.e., construction equipment, lawn mowers, small boats) are computed using EPA's NONROAD model (via the National Mobile Inventory Model). Both of these data categories use state-reported inputs where provided. Both models provide CAP and HAP emissions. EPA develops emissions at specific "shapes" within the county for locomotives, commercial marine vessels and facility (point) emissions for airports and large rail yards. For NATA, diesel PM emissions were assigned to all PM_{10} emitted by diesel engines in the onroad and nonroad inventories, all residual oil and diesel fueled commercial marine vessels, diesel ground support equipment at airports and all locomotive emissions (both nonpoint and at point rail yards).

EPA provided preliminary AERMOD modeling for the 2011 NEI v1 point and nonpoint sources and provided to states for their review between November 2013 and March 2014. TRI facilities that were not in 2011 NEI v1 but were added to the NEI v2 were provided as part of this review. There were numerous improvements in the 2011 NEI over previous year inventories used in NATA, including:

- The oil and gas emissions are more complete since data not provided by states were gap filled with estimates from the new EPA oil and gas tool (Pring, 2015); in addition, spatial allocation of this sector is improved by using the same database of wells as in the tool;
- the generation of port and underway commercial marine emissions as shapes within counties, which allows proper spatial allocation of the emissions in modeling;
- the use of MOVES2014 and an update to the default inputs from a study conducted by the Coordinated Research Council (Koupal, 2014); and
- stakeholder review of modeled risks based on the 2011 NEI v1.

We also conducted a review of the 2011 NEI v2 risks from point sources from AERMOD modeling. While the emission and facility changes resulting from this review were not incorporated into the 2011

[4] Emission factor ratios are computed by source classification code using emission factors from the WebFire database (http://cfpub.epa.gov/webfire/)

NEI v2 or the subsequent CMAQ modeling (which was completed with the 2011 NEI v2) they were re-run in AERMOD and will be incorporated into the hybrid results prior to the final NATA tract risk calculations. All facility inventory changes (geographic coordinated and stack parameter changes) are being incorporated into the EIS so that they will be used in the 2014 NEI unless states make additional changes.

Emissions Processing

Because the hybrid approach combines the results of the two models, efforts are made to keep the inputs to the models as consistent as possible. In addition to use of the same inventory, 2011 NEI v2, the emissions processing use the same or similar underlying data.

Key emissions processing steps to prepare emissions for input into the models are temporalization and spatial allocation.

For CMAQ, SMOKE is used to create gridded, hourly emissions of CAPs and HAPs for continental US domain at 12 km resolution. SMOKE is run by modeling platform sectors. Spatial allocation for county total emissions (i.e., nonpoint, onroad and nonroad data categories) is done using spatial surrogate data which vary in underlying data resolution.

Table 3 shows the total HAP and toxicity weighted HAP emissions used by the various surrogates used in the platform by modeling platform sector. As shown in the table, a key surrogate is “Residential + Commercial + Industrial + Institutional + Government” which is based on a combination of Federal Emergency Management Agency (FEMA) building square footages summed by census tract for all FEMA-defined categories of Commercial, Residential, Industrial, Institutional and Government.

Table 3. Surrogates used in NATA – total and toxicity weighted emissions based on CMAQ HAPs

		Total CMAQ emissions (HAP and diesel PM): fraction of sector and total									Cancer-weighted CMAQ emissions fraction of sector and total									Respiratory-weighted CMAQ emissions fraction of sector and total								
code	SURROGATE DESCRIPTION	agfire	c1c2rail	c3marine	nonpt	nonroad	np_oilgas	onroad	rwc	Total (tons)	agfire	c1c2rail	c3marine	nonpt	nonroad	np_oilgas	onroad	rwc	Total (tons)	agfire	c1c2rail	c3marine	nonpt	nonroad	np_oilgas	onroad	rwc	Total (tons)
100	Population				0.99	0.01				216,700				0.92	0.08				18,074				0.57	0.43				22,562
140	Housing Change and Population				0.11	0.89				60,448				0.07	0.93				16,629				0.00	1.00				170,238
150	Residential Heating - Natural Gas				1.00					591				1.00					2,960				1.00					1,543
165	0.5 Residential Heating - Wood plus 0.5 Low Intensity Residential								1.00	58,529								1.00	263,784								1.00	107,990
170	Residential Heating - Distillate Oil				1.00					99				1.00					5,490				1.00					315
180	Residential Heating - Coal				1.00					148				1.00					17				1.00					533
190	Residential Heating - LP Gas				1.00					49				1.00					248				1.00					173
200	Urban Primary Road Miles							1.00		59,697							1.00		63,561							1.00		123,133
205	Extended Idle Locations							1.00		21,888							1.00		59,215							1.00		70,100
210	Rural Primary Road Miles							1.00		37,604							1.00		34,492							1.00		93,523
221	Urban Unrestricted Roads							1.00		133,013							1.00		138,931							1.00		211,287
231	Rural Unrestricted Roads							1.00		81,752							1.00		83,453							1.00		153,654
240	Total Road Miles				1.00					2,557				1.00					261				1.00					133
250	Urban Primary plus Rural Primary				1.00					2,306				1.00					942				1.00					1
256	Off-Network Short-Haul Trucks							1.00		3,651							1.00		5,057							1.00		2,841
257	Off-Network Long-Haul Trucks							1.00		317							1.00		817							1.00		686
258	Intercity Bus Terminals							1.00		7							1.00		22							1.00		20
259	Transit Bus Terminals							1.00		24							1.00		70							1.00		63
260	Total Railroad Miles				1.00					58				1.00					24				0.00					0
261	NTAD Total Railroad Density		0.59			0.41				916		0.82			0.18				556		0.60			0.40				3,083
271	NTAD Class 1 2 3 Railroad Density		1.00							28,137		1.00							15,144		1.00							98,881
280	Class 2 and 3 Railroad Miles		1.00							1,155		1.00							541		1.00							4,074
300	Low Intensity Residential				0.31	0.65			0.03	36,870				0.53	0.39			0.08	71,144				0.74	0.13			0.12	21,011
310	Total Agriculture	0.53			0.02	0.46				101,453	0.93			0.01	0.06				226,969	0.48			0.02	0.50				305,616
312	Orchards/Vineyards	0.97			0.03					539	0.61			0.39					3,502	1.00			0.00					1,424
320	Forest Land	0.99			0.01					97	1.00			0.00					391	0.99			0.01					264
330	Strip Mines/Quarries				1.00					9				1.00					302				1.00					6
340	Land					1.00				643					1.00				641					1.00				759
350	Water					1.00				87,373					1.00				53,031					1.00				8,205
400	Rural Land Area				0	1.00	0			119,240				0.00	1.00	0.00			43,368				0.00	1.00	0.00			7,442
500	Commercial Land				1.00					4,292				1.00					14,162				1.00					7,080
505	Industrial Land				0.74	0.26				21,496				0.84	0.16				15,594				0.35	0.65				25,782
506	Education							1.00		229							1.00		424							1.00		301
507	Heavy Light Construction Industrial Land							1.00		21							1.00		40							1.00		30
510	Commercial plus Industrial				0.11	0.31		0.59		82,646				0.02	0.30		0.67		86,727				0.17	0.49		0.34		61,363
515	Commercial plus Institutional Land				1.00					1,144				1.00					9,169				1.00					2,249
520	Commercial plus Industrial plus Institutional				0.04	0.96				44,805				0.00	1.00				42,735				0.00	1.00				13,253
526	Residential - Non-Institutional							1.00		473							1.00		352							1.00		128
527	Single Family Residential				1.00					9,681				1.00					2,103				1.00					1
535	Residential + Commercial + Industrial + Institutional + Government				0.13			0.87		345,828				0.00			1.00		319,891				0.05			0.95		112,380
540	Retail Trade (COM1)				1.00					48				1.00					15				1.00					29
545	Personal Repair (COM3)				1.00					11,879				1.00					1,019				1.00					780
555	Professional/Technical (COM4) plus General Government (GOV1)				1.00					90				1.00					67				1.00					63
560	Hospital (COM6)				1.00					10				1.00					337				0.00					0
575	Light and High Tech Industrial (IND2 + IND5)				1.00					239				1.00					28				1.00					50
580	Food, Drug, Chemical Industrial (IND3)				1.00					554				1.00					1,777				1.00					490
585	Metals and Minerals Industrial (IND4)				1.00					10				1.00					4				1.00					1

		Total CMAQ emissions (HAP and diesel PM): fraction of sector and total									Cancer-weighted CMAQ emissions fraction of sector and total									Respiratory-weighted CMAQ emissions fraction of sector and total								
code	SURROGATE DESCRIPTION	agfire	c1c2rail	c3marine	nonpt	nonroad	np_oilgas	onroad	rwc	Total (tons)	agfire	c1c2rail	c3marine	nonpt	nonroad	np_oilgas	onroad	rwc	Total (tons)	agfire	c1c2rail	c3marine	nonpt	nonroad	np_oilgas	onroad	rwc	Total (tons)
590	Heavy Industrial (IND1)				1.00					25,345				1.00					22,024				1.00					291
595	Light Industrial (IND2)				1.00					21,569				1.00					885				1.00					987
596	Industrial plus Institutional plus Hospitals				1.00					0				0.00					0				0					0
600	Gas Stations				0.23			0.77		51,562				0.84			0.16		10,963				1.00			0.00		5
650	Refineries and Tank Farms				1.00					3,087				1.00					1,660				1.00					1
675	Refineries and Tank Farms and Gas Stations				1.00					16				1.00					9				0					0
680	Oil and Gas Wells						1.00			0						1.00			1						1.00			0
681	Spud count - Oil Wells						1.00			14						1.00			24						0			0
682	Spud count - Horizontally-drilled wells						1.00			70						1.00			202						1.00			201
683	Produced Water at all wells						1.00			107						1.00			202						0.00			0
684	Completions at Gas and CBM Wells						1.00			212						1.00			597						1.00			256
685	Completions at Oil Wells						1.00			309						1.00			835						1.00			328
686	Completions at all wells						1.00			1,053						1.00			2,434						1.00			1,321
687	Feet drilled at all wells						1.00			627						1.00			1,935						1.00			1,747
688	Spud count - Gas and CBM Wells						1.00			35						1.00			42						0.00			0
689	Gas production at all wells						1.00			36,433						1.00			31,775						1.00			1,131
692	Spud count - all wells						1.00			254						1.00			709						1.00			707
693	Well count - all wells						1.00			835						1.00			1,895						1.00			663
694	Oil production at oil wells						1.00			8,720						1.00			15,982						1.00			1,648
695	Well count - oil wells						1.00			3,518						1.00			8,951						1.00			4,431
697	Oil production at gas and CBM wells						1.00			4,666						1.00			5,980						1.00			1,042
698	Well count - gas and CBM wells						1.00			13,023						1.00			40,438						1.00			28,683
700	Airport area				1.00					54				1.00					72				1.00					3
801	Port Areas				1.00					44				1.00					31				1.00					3
806	Offshore Shipping NEI2011 NOx		0.76	0.24						25,173		0.56	0.44						22,225		0.76	0.24						89,752
820	Ports NEI2011 NOx		0.34	0.66						6,620		0.08	0.92						17,240		0.34	0.66						23,643
850	Golf Courses					1.00				1,135					1.00				1,674					1.00				200
860	Mines					1.00				414					1.00				104					1.00				1,388
870	Wastewater Treatment Facilities				1.00					692				1.00					357				1.00					257
880	Drycleaners				1.00					8,300				1.00					830				1.00					0
890	Commercial Timber					1.00				2,263					1.00				1,313					1.00				3,233

Sectors: "agfire"-agricultural fires, "c1c2rail"= c1/c2 marine vessels and locomotives, "nonpt" is other nonpoint sources, "np_oilgas" is oil and gas production emissions in the NEI's nonpointdata category, "rwc" is residential wood combustion
Note: point sources including fires do not need to be spatially allocated using surrogates so are exluded from this table.

For AERMOD, emissions inventoried at county resolution (i.e., all sectors in the nonpoint data category other than commercial marine vessels and locomotives, and the onroad and nonroad data categories) are allocated to tracts using the same surrogates as are used in CMAQ. The tract shapes are then modeled as polygons in AERMOD. Commercial marine vessel (CMV) emissions are modeled at the actual shapes of the ports and underway shapes provided in the NEI (as opposed to being allocated to census tracts). Some simplification of the tract and NEI shapes was done to reduce computational resources needed to run AERMOD.

SMOKE generates hourly emissions starting with the inventory data, which is primarily annual but also includes some hourly data. Hourly data are used for electric generating units (EGUs) that have continuous emission monitors that provide hourly emissions and heat input. SMOKE-MOVES (Baek, et. al, 2015) estimates hourly onroad emissions incorporating both the temperature effects on emission factors and the temporal variation in vehicle activity. General information of the preparation of the CMAQ emissions is provided in documentation for the emision platforms at www.epa.gov/ttn/chief/emch. Detailed documentation for the 2011 NATA will be released with the final NATA.

For AERMOD, we used the same temporal allocation approaches for point sources were used for CMAQ. For the other sectors, simplifications were made to the CMAQ temporalization approaches to reduce the number of tract-level emission groups would have to be modeled separately. A few examples are provided below.

Residential wood combustion (RWC) sources (i.e., fireplaces, woodstoves, outdoor hydronic heaters) comprise a tract-level emission group that is run separately from other tract-level emission sources due to its unique emissions characterization. The RWC temporal allocation method used in SMOKE to generate the CMAQ hourly gridded emissions is based on meteorological conditions (more activity on days with cold temperatures) for the daily variation, overlayed with a diurnal variation which places more of the RWC emissions in the morning and the evening when people are typically using these sources. Outdoor hydronic heaters use a different profile based on data on their use. In order to run RWC as a single group in AERMOD, we develop a county-specific hourly profile for all RWC sources, computed by summing the hourly emissions of VOC and $PM_{2.5}$ from SMOKE across all RWC sources. We used the 2011 NEI v1 for computing the profile. It was discovered that the diurnal variation was time shifted from the day to day variation due to an inconsistency in the use of local and Greenwich Mean Time between the hourly and daily temporal allocation. This inconsistency was fixed for the CMAQ run (2011 NEI v2) but not for the AERMOD run which used the 2011 NEI v1-based hourly emissions to create the profile. Because we are combining the CMAQ and AERMOD results at the annual level and we generally capture the daily fluctuation, we don't expect this inconsistency in the temporal allocation to have a significant impact on the annual hybrid values.

Onroad hourly profiles for AERMOD were also generated from the SMOKE hourly emissions used for CMAQ. Unlike for RWC, we used 2011 NEI v2 hourly emissions for onroad since we used a different mobile source model between the 2011 NEI v1 and 2011 NEI v2. Hourly profiles were generated by month, weekday, Saturday and Sunday for each county and for light duty versus heavy duty vehicles. No day-to-day variation was used. Although these hourly emissions could vary for different pollutants, we used the hourly emissions for $PM_{2.5}$ for all HAPs for heavy duty vehicles and hourly emissions of benzene for all HAPs from light duty vehicles. Sample profiles for Wake County, North Carolina, are shown in Figures 4 and 5. Light duty weekday peaks are at 8am and 6pm. Heavy duty weekday peaks are at noon.

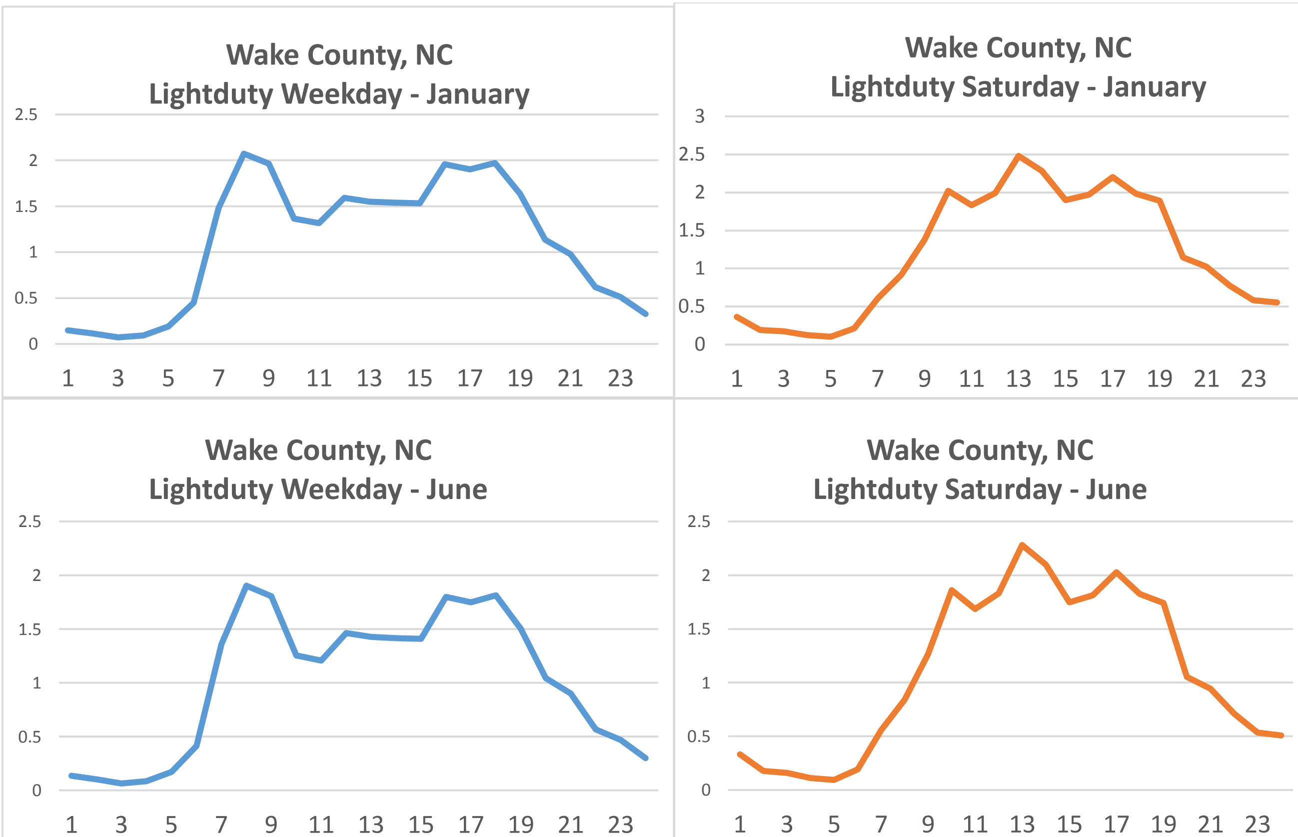

Figure 4. Diurnal Profile for weekday and Saturday emissions, Light Duty Vehicles, Wake County

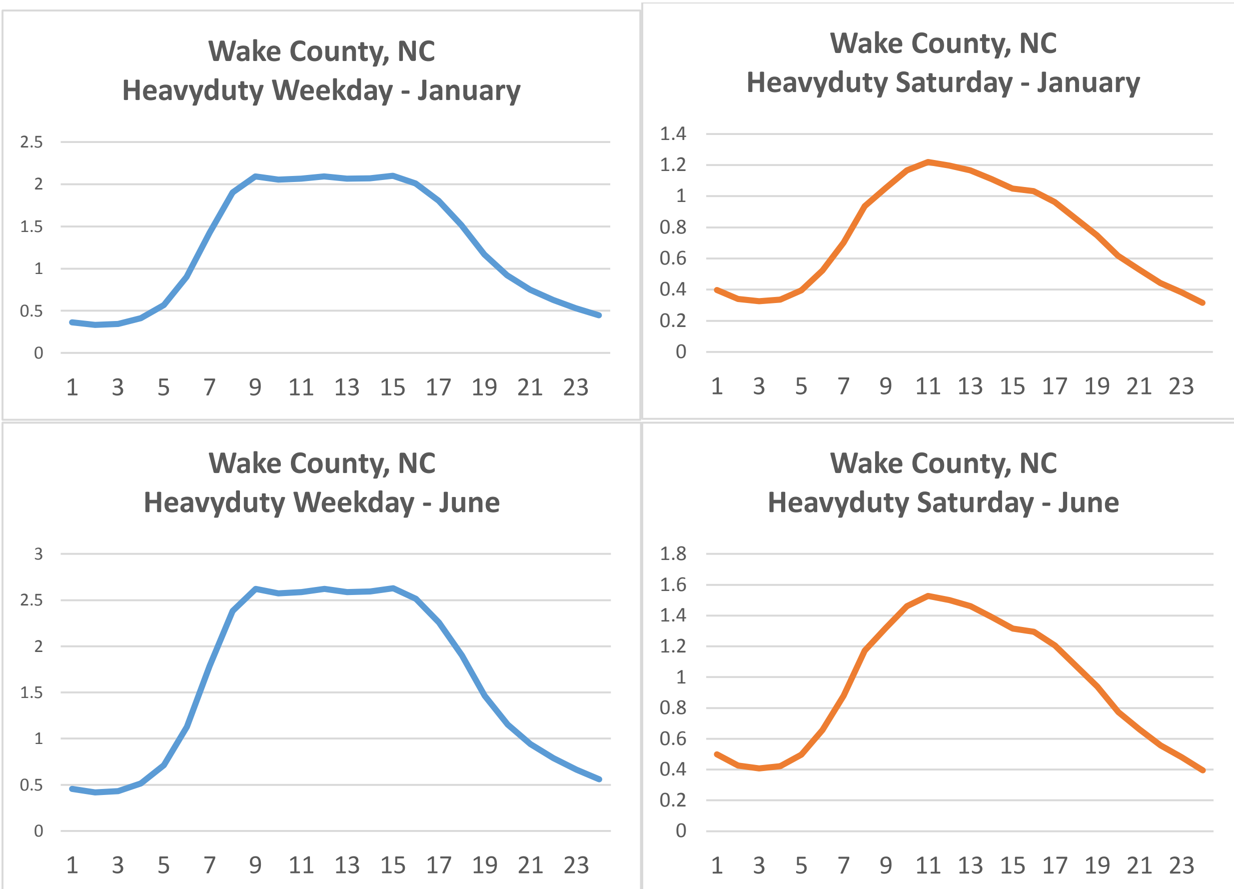

Figure 5. Diurnal Profile for weekday and Saturday emissions, Heavy Duty Vehicles, Wake County, NC

Emissions Review

The CMAQ modeling used a version of the 2011 NEI v2 that was prepared in September 2014. The September 2014 version was modeled through AERMOD, and results for stationary point sources were shared with state, local and tribal agencies via a secure EPA SharePoint site. This review resulted in approximately 200 changes, including emissions, geographic coordinates and release point parameters. Because of resource limitations, CMAQ could not be re-run for these changes. As a result, for the hybrid approach, we developed an AERMOD average that also did not incorporate these changes and utilized this AERMOD average to get the CMAQ/AERMOD ratio as is depicted in the equation shown in Figure 3. All such changes were then remodeled in AERMOD to get the corrected AERMOD receptor concentration which is utilized in the final hybrid calculations. Additional changes resulting from the NATA preview are expected to be incorporated in a similar way.

PRELIMINARY EMISSIONS RESULTS

Figures 5 through 7 show the gridded emissions (12 km) input to CMAQ for benzene, formaldehyde, and diesel PM, respectively. Benzene is highest in the northeast and in areas of high population.

Formaldehyde is highest in the south east and central U.S. due to biogenic emissions and fires, which are both important sources of formaldehyde. Diesel particulate matter emissions are most prevalent on heavily traveled roads, railways and in areas with ports and waterways (Figure 6).

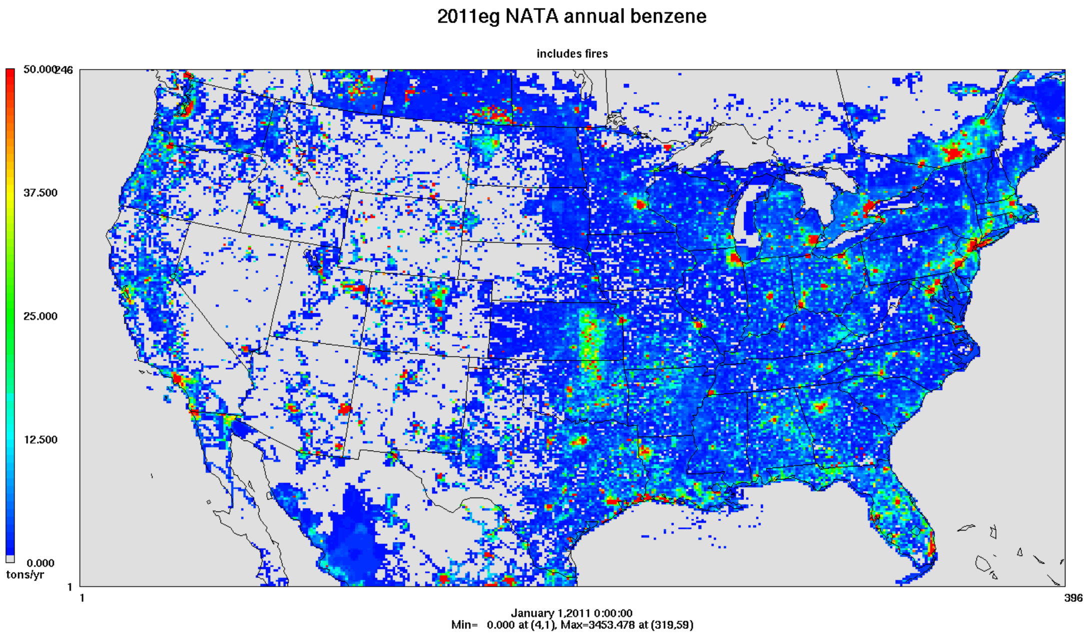

Figure 5. Gridded benzene emissions

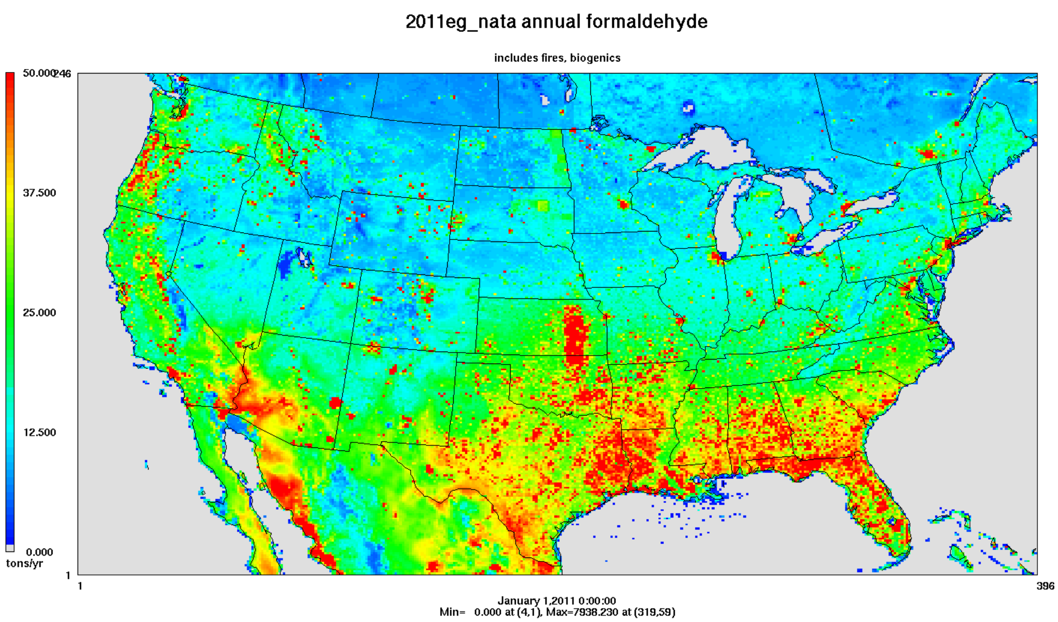

Figure 6. Gridded formaldehyde emissions

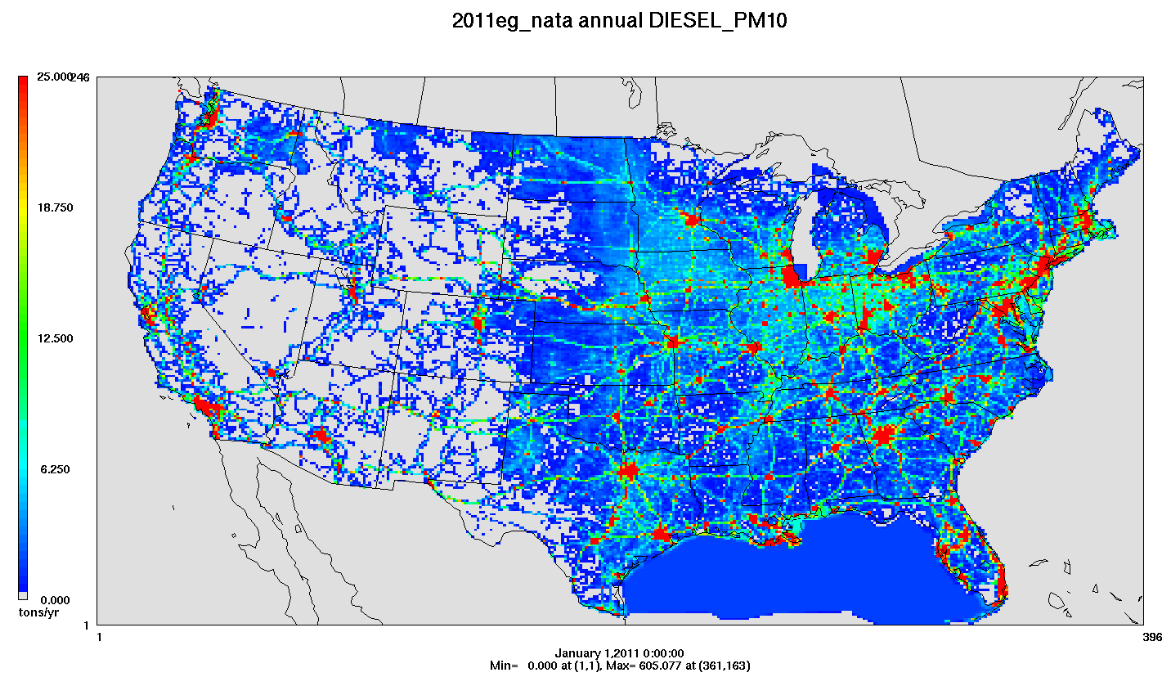

Figure 7. Gridded diesel emissions

CONCLUSIONS

NATA provides useful information to EPA, SLT and researchers for prioritizing air toxics efforts and improving air toxics information.

EPA is conducting a 2011 NATA using the 2011 NEI v2 to update the information from the 2005 NATA. The 2011 NATA uses a different modeling approach from previous NATAs, the hybrid approach, which combines the results from CMAQ and AERMOD models. The approach was tested using the 2011 NEI v1 which led to an improvement in the computation of the AERMOD average used in the hybrid equation. Emissions plots show the importance of including all emissions (e.g., biogenics for formaldehyde) in NATA, which is a feature of the hybrid approach.

Emissions reviews with SLTs have been conducted on the 2011 NEI using AERMOD modeling results. Comments from the 2011 NEI v1 resulted in corrections incorporated into the 2011 NEI v2. SLTs also provided a significant number of comments/changes to emissions resulting from the 2011 NEI v2 AERMOD modeling. In addition to improved emission estimates, these comments result in improved emission release characteristics, which can be utilized in subsequent NEIs. Although we cannot rerun the CMAQ model, we have developed a method to adjust the NATA results to reflect these additional changes.

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