Modeling of Mobile Source Air Toxic Emissions Using EPA's National Mobile Inventory Model

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ABSTRACT

EPA's Office of Transportation and Air Quality has recently developed a new emissions modeling system for highway and nonroad sources, the National Mobile Inventory Model (NMIM). NMIM consolidates MOBILE, NONROAD, and a database into one modeling system which creates national, county-level emission inventories. The system can also model hazardous air pollutants (HAPs) not included in MOBILE and NONROAD and aggregate and postprocess the results to a number of formats, including NIF3. NMIM can generate inventories for calendar years 1999 through 2050. It includes all categories of mobile sources except for aircraft, locomotives, and commercial marine vessels.

Presently, NMIM has the capability to estimate county level emissions for all air toxic pollutants with mobile source contributions that are included in the 1999 National Emissions Inventory (NEI). This includes 13 gaseous hydrocarbons, 16 polycyclic aromatic hydrocarbons, 4 metal compounds, and 17 dioxin and furan cogeners. This paper describes the sources of air toxics data used in NMIM and calculation methods.

We also include a brief description of how fuel property information needed to model air toxics was developed and is stored in the NMIM database. For base years, fuel survey data were used, and for future years, refinery modeling, which estimates impacts of fuel controls, was used to develop projected fuel properties.

Finally, we discuss how this tool will be used by the Agency to develop mobile source inventories for the National Emissions Inventory and support programmatic needs, and the Agency's plans to develop guidance for States on how to provide improved local and regional data inputs for the model.

INTRODUCTION

EPA's Office of Transportation and Air Quality has recently developed a new emissions modeling system for highway and nonroad sources, the National Mobile Inventory Model (NMIM). NMIM consolidates the following components into one modeling system which creates national, county-level emission inventories:

1) MOBILE6.2 – U. S. EPA's highway vehicle emission factor model[1]

2) NONROAD – U.S. EPA's emission inventory model for nonroad equipment.[2] NONROAD

includes the following equipment categories: recreational, contruction, industrial, lawn and garden, farm, light commercial, logging, airport service, railway maintenance, recreational marine vessels.

3) County Level Database – Includes county level input data such as temperatures, fuel properties, vehicle registration distributions, inspection and maintenance programs, and toxics inputs in the form of toxic to volatile organic compound (VOC) ratios, toxic to particulate matter (PM) ratios, or toxic emission factors.

These components are consolidated into a Java modeling framework. NMIM can estimate county mobile source inventories in the Continental U.S., Alaska, and Hawaii, and highway vehicle inventories for Puerto Rico and the U. S. Virgin Islands for any year from 1999 to 2050. The model estimates emissions for all nonroad sources except for aircraft, locomotives, and commercial marine vessels. Results can be aggregated and postprocessed into to a number of formats, including NIF3.

Presently, NMIM has the capability to estimate county level emissions for all of the HAPs with mobile source contributions that are included in the 1999 NEI. These pollutants are listed in Table 1.

Table 1. HAPs Included in NMIM

1,3-Butadiene	Benzo(a)pyrene	Fluoranthene	Nickel
2,2,4-Trimethylpentane	Benzo(b)fluoranthene	Fluorene	Phenanthrene
Acenaphthene	Benzo(g,h,i)perylene	Formaldehyde	Propionaldehyde
Acenaphthalene	Benzo(k)fluoranthene	Hexane	Pyrene
Acetaldehyde	Chromium	Indeno(1,2,3,c,d)pyrene	Styrene
Acrolein	Chrysene	Manganese	Toluene
Anthracene	Debenzo(a,h)-anthracene	MTBE	Xylene
Benzene	Ethylbenzene	Naphthalene	Dioxins and Furans (17 cogeners)
Benz(a)anthracene			

In this paper, we briefly describe the methods and data NMIM uses to estimate county level emission of mobile source hazardous air pollutants. We also include a brief description of how fuel property information needed to model air toxics was developed and is stored in the

NMIM database. For base years, fuel survey data were used, and for future years, refinery modeling, which estimates impacts of fuel controls, was used to develop projected fuel properties.

In addition, we discuss how this tool will be used by the Agency to develop mobile source inventories for the National Emissions Inventory and support programmatic needs, and the Agency's plans to develop guidance for States on how to provide improved local and regional data inputs for the model.

NMIM has also recently been used to develop a HAP emission inventory for nonroad equipment in 1999 and 2002; we present nationwide inventory totals for those years and compare 1999 NMIM estimates to inventory estimates in the 1999 NEI final version 3 for HAPs.[3]

DATA AND METHODS

Highway Mobile Sources

NMIM estimates HAPs from highway mobile sources using the AIR TOXICS command in MOBILE6.2. Chapter 2 of the MOBILE6 User's Guide describes this command and required input data in detail.[4]

Benzene, 1,3-Butadiene, Formaldehyde, Acetaldehyde, MTBE and Acrolein

MOBILE6.2 explicitly estimates emissions for benzene, 1,3-butadiene, formaldehyde, acetaldehyde, MTBE (methyl tertiary butyl ether), and acrolein when the AIR TOXICS command is selected. Benzene and MTBE are found in both exhaust and evaporative emissions; the others are constituents of exhaust only. Emission factors are reported according to whether they are exhaust, crankcase, diurnal, hot soak, running loss, resting loss or refueling loss emissions. The number of MOBILE6.2 input files required to model all counties in a State were determined based on unique combinations of control programs and local fuel properties.

The exhaust and evaporative components of the toxics module multiply an air toxic to VOC ratio by the MOBILE6.2 VOC to produce an air toxic emission estimate. For light-duty gasoline vehicles and trucks, the product is then multiplied by an off-cycle adjustment factor. Exhaust toxic to VOC ratios for newer technology light-duty gasoline vehicles (those with three-way catalysts or three-way plus oxidation catalysts) vary by technology group, vehicle type, whether a vehicle is a normal or high emitter (same definition as MOBILE6), and fuel characteristics. Evaporative toxic to VOC ratios do not vary among gasoline vehicles. Since toxic emission rates are a product of toxic to VOC ratios and VOC emission rates, anything that reduces VOC will also result in toxic emission reductions. Ratios for individual technology group/vehicle type/emitter class combinations are determined using a series of algorithms which calculate the ratios based on fuel parameter inputs.

Benzene, 1,3-butadiene, formaldehyde, and acetaldehyde exhaust emissions from light-duty gasoline vehicles and trucks with three-way or three-way plus oxidation catalysts were estimated using algorithms developed for the Complex Model for Reformulated Gasoline.[5] For MTBE, a draft fuel effects model based on the Complex Model database was used.[6] For older technology light-duty gasoline vehicles and trucks, and all other vehicle classes in MOBILE6.2, toxic to TOG ratios are based on limited data, and are either calculated as straight fractions by fuel type, or are estimated based only a couple fuel parameters, such as percent benzene, percent aromatics, and type and content of oxygenate.

The gasoline fuel parameters used as inputs to the algorithms for light-duty gasoline vehicles and trucks with three-way or three-way plus oxidation catalysts are: sulfur content, olefins content, aromatics content, benzene content, E200 value, E300 value, oxygenate content by type, and oxygenate sales fraction by type. Since these fuel parameters are area-specific, EPA developed county-level inputs for each of these parameters for summer and winter gasoline. The gasoline fuels associated with every county for every month have a specific identifier which is stored in the CountyYearMonth table of the NMIM database. Fuel parameters associated with these fuels are stored in the Gasoline table of the database. For base years 1999 and 2000 parameters were collected for winter and summer seasons using a number of different data sources. These sources include the Alliance of Automobile Manufacturers, Northrop Grumman Mission Systems (formerly TRW Petroleum Technologies), and EPA reformulated gasoline surveys.[7, 8] All gasoline properties are area-wide averages, except for oxygenates, which are allowed to have market shares. Three fuels (winter, summer, and spring/fall) were determined for each county and assigned to months by season. Months representing seasons varied by location. Spring/fall gasoline properties were derived from summer and winter fuels by interpolation.

Projection year fuel parameters were developed using results of several refinery modeling analyses conducted to assess impacts of fuel control programs on fuel properties. The projection year fuel parameters were calculated by applying adjustment factors to the base year parameters.[9] In general, multiplicative adjustment factors were used to calculate future year gasoline parameters (i.e., future year parameter = base year parameter x adjustment factor). However, additive adjustment factors were used to calculate future year parameters for E200, E300, and oxygenate market shares (i.e., future year parameter = base year parameter + adjustment factor). The current database assumes no Federal ban on MTBE, but does include State bans. An alternative database has been developed which assumes a Federal ban with no oxygenate mandate, but with a renewable fuel requirement.

Other Pollutants

For other pollutants in Table 1, except for dioxins and furans, we used the ADDITIONAL HAPS command in MOBILE6.2, which allows the user to enter emission factors or air toxic ratios for additional air toxic pollutants. A number of these compounds have an evaporative as well as an exhaust emissions component. Emission factors must be input in milligrams per mile

and ratios can be input as fractions of VOC, fractions of TOG, or fractions of PM. All user-defined inputs for evaporative emissions must be input as ratios. The input files used were included in the MOBILE6.2 release. Information on the primary data sources can be found in the documentation for the 1999 NEI for HAPs, version 3. Because toxic to VOC ratios for several gaseous HAPs vary between baseline gasoline and gasoline oxygenated with MTBE or ethanol, separate ADDITIONAL HAPS input files were developed as follows:

1. Baseline Gasoline

2. WO (Winter Oxygenate) Gasoline / Ethanol or ETBE - Used where the fuel contains ethanol which is greater than or equal to 5% by volume or ETBE greater than or equal to 5% by volume.

3. WO (Winter Oxygenate) Gasoline / MTBE / TAME - Used where the fuel contains MTBE which is greater than or equal to 12% by volume or TAME greater than or equal to 13% by volume.

4. RFG/MTBE/TAME - Used where the fuel is RFG and where the fuel contains MTBE which is less than 12% by volume or TAME less than 13% by volume.

Emissions of dioxins and furans were not estimated using MOBILE6.2. Instead, emission factors from EPA's draft dioxin reassessment were used.[10] Dioxins were estimated as mass emissions for 17 cogeners rather than as toxic equivalents (TEQs).[a]

Nonroad Mobile Sources

Unlike MOBILE6.2, NONROAD does not currently have the capability to estimate HAP emissions. HAPs are estimated for each equipment type in the NONROAD model using data sources and methods developed for the 1999 NEI for HAPs, version 3.[11] NMIM does not estimate HAP emissions for compressed natural gas (CNG) or liquid propane gas (LPG) vehicles.

Nonroad HAPs are estimated in NMIM using one of three approaches:

1) Gaseous HAPs – Apply toxic to VOC ratios to NONROAD VOC estimates.

2) PAHs – Apply toxic to PM ratios to NONROAD PM estimates.

3) Metals, Dioxins and Furans – Multiply HAP gram per gallon emission factors by county level

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[a]The TEQ is the product of the mass emissions and a toxic equivalence factor (TEF), which compares the toxicity of an individual dioxin or furan cogener to the toxicity of 2,3,7,8-tetrachlorodibenzo-*p*dioxin (TCDD), the most toxic compound in the dioxin group.

fuel consumption estimates.

Gaseous HAPs

As with "additional HAPs" for highway vehicles, because toxic to VOC ratios for several gaseous HAPs vary between fuel types, different toxic to VOC ratios were used for baseline gasoline, winter oxygenated gasoline with ethanol, winter oxygenated gasoline with MTBE, reformulated gasoline with MTBE, and reformulated gasoline with ethanol. It should be noted that NMIM uses a different set of criteria to determine which toxic to VOC ratios to use than in the 1999 NEI final version 3 for HAPs. In that inventory, ratios for different fuel types were weighted according to whether the county participated in the Federal or California Reformulated Gasoline Program or a winter oxygenated fuel program, and the percentage of the year the county participated in these programs. For example, if a county participated in the Federal Reformulated Gasoline Program for 4 months, the RFG/MTBE/TAME fraction would be weighted by a factor of 0.33, and the baseline fraction by 0.67 to develop a composite annual fraction, which would then be applied to VOC. This approach does not adequately account for reformulated and oxygenated gasoline use outside counties participating in the program, or use outside the fuel program season. One result is an underestimate of the nonroad MTBE inventory. Thus, NMIM estimates substantially higher nationwide MTBE than was estimated in the 1999 NEI for HAPs.

In some cases, profiles for specific equipment and engine type combinations were available. However, for many equipment/engine type combinations, no speciation data were available. In such instances, default values for 2-stroke gasoline engines, 4-stroke gasoline engines, and diesel engines were used. These default values represent an average fraction for various equipment types within an engine category.

PAHs

As with highway vehicles, all PAHs were estimated as fractions of PM, although the data used to calculate mass ratios included both gas and particle phase PAH emissions. The data used to develop the PAH to PM fractions are described in the documentation for the 1999 NEI for HAPs. NMIM does not currently estimate evaporative naphthalene emissions for nonroad equipment.

Metals, Dioxins, and Furans

The approach used by NMIM to estimate county level metal emissions differs in a number of respects from the approach used in the 1999 NEI for HAPs, version 3.

In the 1999 NEI, nationwide metal emissions for gasoline engines were obtained by applying a mass per gallon emission factor by nationwide gasoline consumption from the NONROAD model. For diesel engines, a mass per brake-horsepower emission factor was

multiplied by nationwide energy output. The resultant nationwide emission estimates were then spatially allocated to counties relative to the county proportion of PM_{10} emissions compared to the national PM_{10} emissions, as obtained from the NONROAD model.

In contrast, NMIM multiplies mass per gallon emission factors for gasoline engines by county level fuel consumption to obtain a county level inventory estimate. For diesel engines, mass per brake horsepower emission factors were converted to mass per gallon emission factors using the following equation:

grams per gallon = (micrograms per brake-horsepower hour (µg/bhphr) * average fuel density (lb/gallon))/(fuel consumption per brake-horsepower hour (lb fuel/bhphr)*1,000,000)

where:

average fuel density = 7.01 lb/gal

fuel consumption per brake horsepower hour = 0.408 lb/bhphr for engines less than 100 hp
= 0.367 lb/bhphr for engines greater than 100 hp

The fuel consumption per brake horsepower hour estimates are from the NONROAD model.[12]

Mass per gallon emission factors for dioxins and furans were calculated for nonroad equipment by multiplying the highway vehicle emission factors by fleet average fuel economy estimates.

NATIONWIDE NONROAD INVENTORY FOR 1999 AND 2002 USING NMIM

To date, NMIM has not been used to develop nationwide highway mobile source inventories for the NEI. However, NMIM has recently been used to develop HAP inventories for equipment in the NONROAD model in 1999 and 2002. The calendar year 2002 numbers will be used for the NEI. Table 2 presents the 1999 and 2002 nationwide estimates for gaseous HAPs using NMIM, along with a comparison to national totals from the 1999 National Emission Inventory (NEI) final version 3 for HAPs. All gaseous HAPs are estimated using toxic to VOC ratios. For most gaseous HAPs, NMIM predicts inventory totals for 1999 that are very similar to what is in the 1999 NEI final version 3 for HAPs. NMIM predicts a significantly higher MTBE inventory, due to differences in the criteria used to determine which toxic to VOC ratios are used, as discussed previously. 2002 inventory estimates are slightly lower than 1999 estimates for all gaseous HAPs. Table 3 presents similar comparisons for PAHs, which are all estimated by applying PAH to PM ratios to PM estimates, except for evaporative napthalene which is calculated using a toxic to VOC ratio.

Table 2. 1999 and 2002 nationwide nonroad inventory estimates (tons) for gaseous HAPs using NMIM, and comparison to national totals from the 1999 National Emission Inventory (NEI) final version 3 for HAPs (does not include commercial marine vessels, locomotives, or aircraft).

Pollutant	1999 NMIM	2002 NMIM	1999 NEI final version 3	1999 NMIM/NEI	2002/1999 NMIM
Acetaldehyde	15,453	13,949	15,819	0.98	0.90
Acrolein	1,432	1,337	1,572	0.91	0.93
Benzene	60,534	57,361	62,498	0.97	0.95
1,3-Butadiene	8,266	7,828	8,619	0.96	0.95
Formaldehyde	36,277	32,902	36,868	0.98	0.91
MTBE	67,174	64,617	38,894	1.73	0.96
2,2,4-Trimethylpentane	89,233	87,839	98,859	0.90	0.98
Ethyl Benzene	39,431	38,709	43,633	0.90	0.98
Hexane	29,703	28,813	28,828	1.03	0.97
Propionaldehyde	3,826	3,470	3,749	1.02	0.91
Styrene	2,420	2,375	2,496	0.97	0.98
Toluene	205,746	202,379	209,190	0.98	0.98
Xylene	179,048	175,499	185,034	0.97	0.98
Total	**738,543**	**717,080**	**736,058**	**1.00**	**0.97**

Table 3. 1999 and 2002 nationwide nonroad inventory estimates (tons) for PAHs using NMIM, and comparison to national totals from the 1999 National Emission Inventory (NEI) final version 3 for HAPs (does not include commercial marine vessels, locomotives, or aircraft).

Pollutant	1999 NMIM	2002 NMIM	1999 NEI final version 3	1999 NMIM/NEI	2002/1999 NMIM
Acenaphthene	22.14	20.36	22.59	0.98	0.92
Acenaphthylene	41.19	39.25	41.36	1.00	0.95
Anthracene	8.76	8.64	8.76	1.00	0.99
Benz(a)anthracene	2.85	2.82	2.85	1.00	0.99
Benzo(a)pyrene	2.46	2.44	2.46	1.00	0.99
Benzo(b)fluoranthene	1.74	1.72	1.74	1.00	0.99
Benzo(g,h,i)perylene	8.91	8.85	8.92	1.00	0.99
Benzo(k)fluoranthene	1.59	1.56	1.59	1.00	0.99
Chrysene	2.22	2.18	2.24	0.99	0.98
Dibenzo(a,h)anthracene	0.07	0.07	0.07	1.00	1.00
Fluoranthene	25.12	24.68	25.16	1.00	0.98
Fluorene	41.54	39.62	41.62	1.00	0.95
Indeno(1,2,3,c,d)pyrene	2.70	2.68	2.70	1.00	0.99
Naphthalene	545.39	526.54	546.85	1.00	0.97
Phenanthrene	74.02	69.28	74.28	1.00	0.94
Total	**781**	**751**	**783**	**1.00**	**0.96**

NMIM predicts very similar PAH totals to what is in the 1999 NEI final version 3 for HAPs, and 2002 inventory estimates are slightly lower than the 1999 estimates. Finally, Table 4 presents results for metals, dioxins, and furans, which are all estimated by applying emission factors to activity estimates. 1999 inventory estimates generated using NMIM are lower than estimates form the 1999 NEI final version 3 for HAPs due to differences in activity, and 2002 estimates are higher than 1999 due to an increase in nonroad activity.

Table 4. 1999 and 2002 nationwide nonroad inventory estimates (tons) for metals, dioxins, and furans using NMIM, and comparison to national totals from the 1999 National Emission Inventory (NEI) final version 3 for HAPs (does not include commercial marine vessels, locomotives, or aircraft).

Pollutant	1999 NMIM	2002 NMIM	1999 NEI final version 3	1999 NMIM/NEI	2002/1999 NMIM
Chromium (Cr3+)	0.47	0.48	0.56	0.84	1.02
Chromium (Cr6+)	0.24	0.25	0.29	0.84	1.02
Manganese	0.53	0.57	0.57	0.94	1.06
Nickel	0.96	1.01	1.04	0.92	1.05
Dioxins and furans (17 cogeners)	8.9075E-04	9.6851E-04			1.09

CONCLUSIONS

NMIM uses a combination of toxic to VOC ratios, toxic to PM ratios, and emission factors in conjunction with activity data to develop HAP inventories for highway vehicles and nonroad mobile sources in the NONROAD model. This capability streamlines the development process for the NEI and reduces costs. NMIM has already been used to develop nonroad equipment inventory estimates for the 2002 draft NEI, and comparisons of 1999 NMIM HAP inventory estimates for nonroad equipment are very close to those in the 1999 NEI final version 3 for HAPs. The one major exception is for MTBE, where changes in criteria used to determine which toxic to VOC ratio is used results in a larger inventory.

FUTURE USE OF NMIM IN DEVELOPING HAP INVENTORIES

In addition to its use in developing the nonroad inventory for the draft 2002 National Emissions Inventory, the U.S. EPA plans to use NMIM to estimate HAPs in subsequent NEI development efforts. The Agency plans to make this tool publicly available in the near future, and also to provide written guidance to States on how to provide improved local and regional data inputs for the model. In addition, the Agency plans to use the model to develop projected inventories to inform the regulatory decision-making process, to help support local assessments, and to measure progress toward achieving reduction goals the Agency has set in compliance with the Government Performance Results Act (GPRA).

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