

EPA's MultiPollutant Modeling with the 2002 NEI: Integrating Criteria and Toxics

Madeleine Strum and Marc Houyoux
Office of Air Quality Planning and Standards
U.S. Environmental Protection Agency, Research Triangle Park, NC 27711
strum.madeleine@epa.gov

Rich Mason
Atmospheric Sciences Modeling Division, Air Resources Laboratory, National Oceanic and
Atmospheric Administration, (On Assignment to the Office of Air Quality Planning and Standards,
U.S. Environmental Protection Agency), Research Triangle Park, NC 27711

Allan Beidler and Cliff Stanley
Computer Sciences Corporation, P.O. Box 12804, Research Triangle Park, NC 27709.

Deborah Luecken
Office of Research and Development
U.S. Environmental Protection Agency, Research Triangle Park, NC 27711

ABSTRACT

EPA is embarking on a multipollutant approach to address air quality problems. Under such an approach, EPA aims to better understand the link between criteria air pollutants (CAPs) and hazardous air pollutants (HAPs), including their spatial and temporal variations on both regional and local scales. This understanding will promote the development of control strategies across multiple pollutants, including PM, ozone and toxics, to reduce emissions. As part of the multipollutant approach, EPA is building a multipollutant modeling capability, utilizing a version of the CMAQ model to which numerous toxics have been added. In preparing the emissions platform to use for this approach, we are working to maximize the degree that we use the HAP inventory in combination with the CAP inventory. In particular, we are striving to “integrate” the HAP VOC from the HAP inventory with the CAP VOC from the CAP inventory in order to use HAP emissions directly to generate model species emissions. This paper describes our methodology for modeling HAPs in CMAQ with an updated chemistry mechanism, reviews the approach to combine HAP and CAP inventories (“integrate” and “no-integrate” cases), and examines features of the 2002 NEI’s (February 2006 version) nonpoint, onroad and nonroad inventory sectors to determine the extent to which the “integrate” case could be used.

INTRODUCTION

Air quality management at EPA’s Office of Air Quality Planning and Standards (OAQPS) is moving in a new direction: integrated air quality management across multiple pollutants. Other terms used to describe the approach are “multipollutant” or “one-atmosphere.” Under the current system, air quality management has been compartmentalized. Control programs have focused on individual pollutants, with limited consideration for other pollutants that may be impacted. In their 2004 review of the air quality management system, the National Research Council (NRC) noted that this approach served the nation well, leading to dramatic declines in emissions and air quality concentrations of a number of pollutants, and promoting the advancement of new technologies for pollution control.¹ A key theme of the NRC’s recommendations for sustaining these achievements is to take an integrated multipollutant approach. A stakeholder group charged by the Clean Air Act Advisory Committee to oversee

implementation of the NRC's recommendations published a report that outlined concrete steps that EPA should pursue.² A number of these would be best implemented through multipollutant modeling; specifically, 1.5-"framework for accountability", 4.1-"multipollutant state implementation plans (SIPS)" and 4.2-"multipollutant benefits and disbenefits in standards setting."

We in EPA's OAQPS and EPA's Office of Research and Development (ORD) have been developing the tools and data to perform multipollutant modeling and construct multipollutant inventories for quite some time, long before these reports were published. Witnesses to this include the participants of the International Emission Inventory Conference held in Denver in 2001, entitled, "One Atmosphere, One Inventory, Many Challenges" where the conference title introduced the concept of combining the inventories. Per that theme, the EPA's Emission Inventory and Analysis Group (EIAG) took steps towards this "one inventory" concept: they gave inventories of hazardous air pollutants (HAPs) and criteria air pollutants (CAPs) the same name, the National Emission Inventory (NEI), and the same format, the National Inventory Format (NIF). At the International Emission Inventory Conference held in San Diego in 2003, entitled "Emission Inventories - Applying New Technologies", the authors of this paper implemented and presented enhancements to the Sparse Matrix Operator Kernel Emissions (SMOKE) to allow the use of processing multi-pollutant inventories.³

We developed a version of SMOKE for multipollutant modeling, SMOKE 2.1, and used it to process HAP and CAP emissions from the 1999 NEI for input into the Community Multi-Scale Air Quality (CMAQ) modeling system. CMAQ simulations were performed using two different chemical mechanisms, CB4tx and SAPRC99tx.^{4,5} The focus of these studies was to demonstrate the importance of atmospheric chemistry and long range transport in predicting the HAP concentrations, which would enable accurate estimation of the effect of control strategies on the HAPs and other pollutants. Both the NEI for CAPS and NEI for HAPs were necessary to populate the model species for these mechanisms; however, the HAPS were used minimally due to concerns about the consistency between the CAP and HAP VOC emissions. For example, even though MOBILE6.2 was used for both 1999 CAP and HAP inventories, separate runs were done for HAPs and CAPS, with different input fuel parameters that could have affected the results for VOC and HAP.

In their development of EPA's 2002 NEI, the EIAG has further integrated the CAPs and HAPs in the inventory, which is made difficult considering the lack of requirements for the States to submit HAP inventories. EPA's Office of Transportation and Air Quality (OTAQ) generated much of the mobile source category emissions using the National Mobile Inventory Model (NMIM)⁶. OTAQ used the same model inputs (e.g., activities, fuel parameters, temperatures) to estimate HAP and CAPs with a single run covering CAPs and HAPs. While EIAG allowed State/local agencies to replace the NMIM emissions for CAPs separately for HAPs, EIAG and OTAQ encouraged the State/local agencies to provide NMIM inputs as opposed to replacement emissions, which would enable the HAP/CAP calculations to be consistent. For many of the nonpoint and non-NMIM mobile categories, EIAG multiplied consistent activity values with both HAP and CAP emission factors. While it is not guaranteed HAP emission factors are consistent with the CAP factors, (e.g., they may have been developed from separate studies) the use of consistent activity data is a significant step towards integrated inventories. As with the onroad and nonroad data, however, any replacement of state data for HAPS but not CAPs or vice versa, could lead to estimates that use inconsistent activity data. We expect some 2002 point sources will have consistent CAP and HAP particularly when the emission estimates for CAP and HAP are provided by the same entity using the same facility identifiers.

As a result of these advances towards a consistent inventory for HAPs and CAPs, and EPA's desire to advance the ability to support multi-pollutant modeling and multi-pollutant control strategies, we are working to maximize the degree that the HAP inventory could be used in combination with the CAP inventory for multipollutant modeling of HAPs and CAPs. In particular, we are striving to "integrate"

the HAP VOC from the HAP inventory with the CAP VOC from the CAP inventory in order to use HAP emissions directly with the CAP emissions to generate model species emissions for both toxic and nontoxic model species. We call this method the “integrate” case because we combine the HAP with the VOC in a way that replaces some of the VOC mass with HAP mass prior to the speciation step. The “integrate” case allows us to maximize our ability to capture the impact of HAP emissions and changes in HAP emissions on air quality across multiple pollutants (ozone, particulate matter[PM] and other HAPs). The next section details this approach, and also describes the “no-integrate” approach for combining HAPs and CAPs.

This paper describes our methodology for modeling HAPs in CMAQ with an updated chemistry mechanism, reviews the approach to combine HAP and CAP inventories (“integrate” and “no-integrate” cases), and examines features of the 2002 NEI’s nonpoint, onroad and nonroad inventory sectors to determine the extent to which the “integrate” case could be used. Except for nonroad, the February 2006 version of the inventory was used.

APPROACH

The CMAQ Approach for Modeling Air Toxics

Multipollutant modeling has been accomplished with CMAQ by modifying the standard chemical mechanisms that are normally used for simulations of criteria pollutants, so that they also produce concentrations of certain HAPs along with ozone and PM. To add HAPs, modifications are made to the chemical mechanism to account for the additional production and decay of HAPs, while retaining the chemistry and radical cycling of the original mechanism. HAPS are added to the mechanism as either 1) “active toxics” or “inside-the-mechanism” species where their concentrations are solved at each internal time step (time scale of minutes) and their decay affects the concentrations of other species, or 2.) “tracer toxics” or “outside-the-mechanism species” where their concentrations are only updated at every output time step (time scale of one hour or more). The significance between tracer and active toxics is the influence of the toxic on the mechanism, especially radical levels. As a result, emissions for an active toxic are important not only for estimating the concentrations of that toxic, but also all other species in the model. Other than 1,3-butadiene, which also affects acrolein, the tracer toxics model species do not influence other mechanism species other than the tracer itself. In terms of preparing the emissions for modeling, the difference between active and tracer toxics is particularly significant in that the tracer toxics emissions, by design, are double counted. Tracer toxics emissions are used both for the tracer model species and for other model species that are not by themselves considered air toxics. Active toxics emissions are used only for the active toxics model species.

For the current effort, the above approach utilizes the CB05tx mechanism, an extension of the new CB05 mechanism⁷ in which additional tracer toxics have been added to provide model outputs for these HAPs. Table 1 shows the CB05 (without toxics) model species (excluding biogenic model species). The CB05tx mechanism includes the model species listed in both Table 1 and Table 2. The HAPs in Table 1 (which are those species identified by a “yes” in the “Active HAP?” column) interact with other model species in the mechanism, and are considered “active HAPs”. These are part of the standard CB05 mechanism. The HAPs in Table 2 do not interact with species in Table 1 and are therefore considered tracer HAPs.

Table 1. CB05 Model Species (excluding biogenic species)

CB05 Model species	Description	Active HAP?	Inventory possibilities for generating CBO5 species
NO2	nitrogen dioxide		CAP (NOX)
NO	nitrogen oxide		CAP (NOX)
CO	carbon monoxide		CAP (CO)
FORM	formaldehyde (explicit)	yes	HAP or CAP (VOC speciation)
ALD2	acetaldehyde (explicit)	yes	HAP or CAP (VOC speciation)
ALDX	lumped C3+ aldehydes		CAP (VOC speciation) or combined
CH4	explicit methane		CAP (VOC speciation)
ETHA (ethane)	ethane		CAP (VOC speciation)
PAR	1-carbon paraffin		CAP (VOC speciation) or combined
ETH	ethene		CAP (VOC speciation) or combined
OLE	terminal olefins		CAP (VOC speciation) or combined
IOLE	internal olefins		CAP (VOC speciation) or combined
TOL	toluene (7 carbons) KOH=8.8E3		CAP (VOC speciation) or combined
XYL	xylenes (8-carbons) KOH=3.7E4		CAP (VOC speciation) or combined
ISOP	isoprene		CAP (VOC speciation) or combined
MEOH	methanol	yes	HAP or CAP (VOC speciation)
ETOH	ethanol		CAP (VOC speciation)
TERP	lumped terpene species		CAP (VOC speciation)
NH3	ammonia		CAP (NH3)
PEC	particulate elemental carbon		CAP (PM2.5 speciation)
PMC	PM coarse		CAP (PM10 minus PM2.5)
PMFINE	PM fine		CAP (PM2.5 speciation)
PNO3	particulate nitrate		CAP (PM2.5 speciation)
POA	particulate organic		CAP (PM2.5 speciation)
PSO4	particulate sulfate		CAP (PM2.5 speciation)
SO2	sulfur dioxide		CAP (SO2)
SULF	sulfates		CAP (SO2)

Table 2. Tracer HAP model species in CB05tx

CB05tx Tracer Toxics Species	Name
Cl2	molecular chlorine
HCL	hydrochloric acid
FORM_PRIMARY	primary formaldehyde
ALD2_PRIMARY	primary acetaldehyde
BUTADIENE13	1,3-butadiene
ACROLEIN_PRIMARY	primary acrolein
ACROLEIN	acrolein (includes primary and secondary)
TOLU	toluene
MXYL	m-xylene
OXYL	o-xylene
PXYL	p-xylene
NAPHTHALENE	naphthalene
DICHLOROPROPENE	1,3-dichloropropene, 1,3-dichloropropylene
QUINOLINE	quinoline
CL_ETHE	vinyl chloride, chloroethene
ACRYLONITRILE	acrylonitrile, propenenitrile
CL3_ETHE	trichloroethylene, TCE, ethylene trichloride
BENZENE	benzene
PROPDIChlorIDE	1,2-dichloropropane, propylene dichloride, 1,2-D
ETOX	ethylene oxide, epoxyethane
BR2_C2_12	1,2-dibromoethane, ethylene dibromide
CL2_C2_12	1,2-dichloroethane, ethylene dichloride
CL4_ETHE	tetrachloroethylene, perchloroethylene
CARBONTET	carbon tetrachloride, tetrachloromethane
CL2_ME	dichloromethane, methylene chloride
CL4_ETHANE1122	1,1,2,2-tetrachloroethane
CHCL3	chloroform, trichloromethane
TOL_DIIS	2,4-Toluene Diisocyanate, TDI
HEXAMETHY_DIIS	Hexamethylene 1-6-diisocyanate, HDI, HMDI
MAL_ANHYDRIDE	Maleic anhydride
TRIETHYLAMINE	Triethylamine
HYDRAZINE	Hydrazine, diamine
DICHLOROBENZENE	p-dichlorobenzene, 1,4-dichlorobenzene, PDCB
diesel_pec	Diesel PM - elemental carbon
diesel_poa	Diesel PM - organic carbon
diesel_pso4	Diesel PM - sulfates
diesel_pno3	Diesel PM - nitrate
diesel_pmfine	Diesel PM - other fine particulate
diesel_pmc	Diesel PM - coarse particulate
beryllium_coars	Beryllium compounds - fine particulate
beryllium_fine	Beryllium compounds - coarse particulate
cadmium_coarse	Cadmium compounds -coarse particulate
cadmium_fine	Cadmium compounds - fine particulate
lead_coarse	Lead compounds - coarse particulate
lead_fine	Lead compounds - fine particulate
manganese_coarse	Manganese compounds- coarse PM
manganese_fine	Manganese compounds- fine PM
nickel_coarse	Nickel compounds - coarse PM
nickel_fine	Nickel compounds - fine PM
chrom_tri_coarse	Chromium 3 - coarse PM
chrom_tri_fine	Chromium 3 - fine PM
chrom_hex_coarse	Chromium 6 -coarse PM
chrom_hex_fine	Chromium 6 -fine PM

A key issue in multipollutant modeling is exploring the various inventory options for generating model-ready inputs for the model species. These options are (1) using a CAP inventory only, or (2) using a combination of CAPs and HAPs. For CB05, option 1 involves computing active HAP species and other model species, which we refer to as “nonHAP,” by speciating CAP VOC emissions. Note that TOL is considered a “nonHAP” model species because it is not an individual HAP compound, but rather a lumped species which includes both HAP and nonHAP compounds. Option 2 uses the HAP inventory to provide the emissions for the active toxics and uses a combination of HAP and CAP for the nonHAP model species. The numerous tracer HAPs in CB05tx have similar options, although some of the tracer HAPs are less likely to be included in the speciation profile for the CAP VOC or PM. In addition, some

pollutants (e.g., chlorine or hydrochloric acid) are neither components of VOC nor PM and cannot be generated using speciation.

For the purpose of this work, we have chosen an approach that maximizes the use of the HAP inventory for preparing model species emissions using CB05tx. We believe the HAP inventory represents a better choice of emissions data than the CAP inventory for estimating HAP emissions, and our approach centers around this premise. The overall methodology, which includes how to determine a valid way to combine HAPs and CAPS from the 2002 NEI, is presented next.

An Approach to Combine HAP and CAP Inventories

We previously described our approach to combine HAP and CAP inventories for HAP modeling in CMAQ in the previous EI conference paper describing SMOKE2.1; we review this approach below. Although that paper described the use of SMOKE to produce CB4tx model species, our approach is flexible for use with other mechanisms and can be implemented in other emission models. We plan to test this approach using CB05tx which replaces CB4tx and which includes additional HAPs.

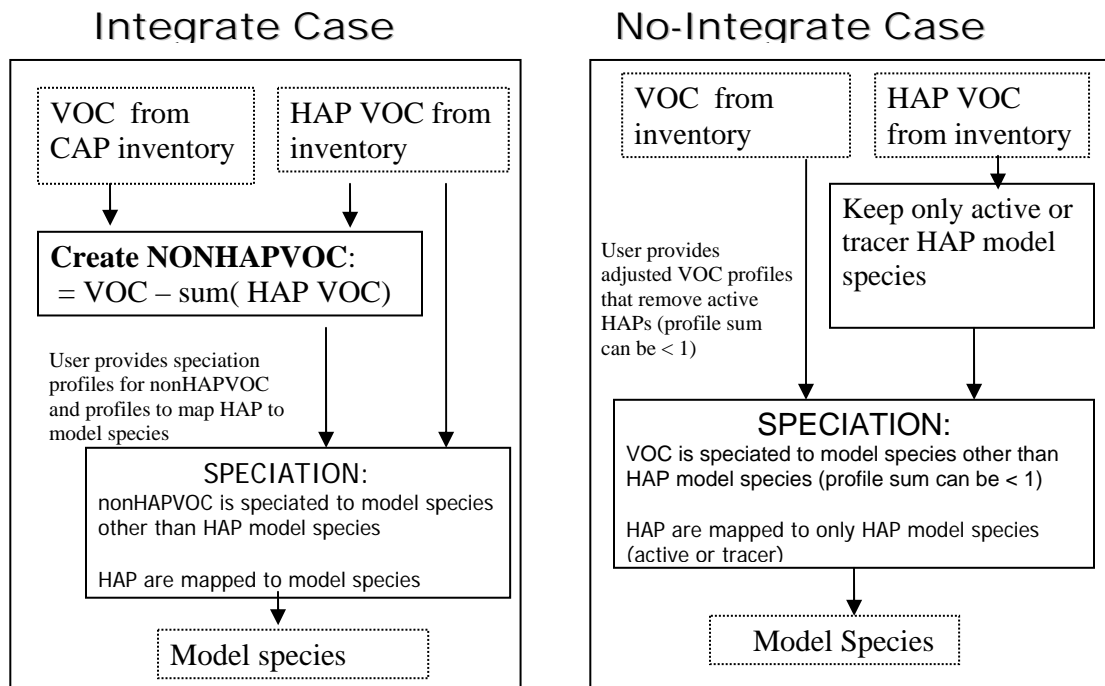
Under this approach, we assume that the HAP inventory is the choice inventory to use for modeling both active and passive HAPs, and we allow the user to choose whether or not to use a combination of the HAP and CAP inventories, or just the CAP inventory, for the nonHAP model species.

The two ways to combine HAP and CAP inventories are the “integrate” case, which we discussed previously, and the “no-integrate” case. For each source with the “integrate” case, the VOC provides the non-HAP part of the mass, the HAP inventory provides the HAP-part of the VOC mass, and the total VOC mass is conserved (neither increased nor decreased). The HAPs and non-HAP part of the VOC are mapped to the appropriate model species in the chemical mechanism. Use of the “integrate” case assumes that the HAPs may be generated with a more detailed methodology than is done using the traditional speciation of VOC and therefore can provide more accurate model species estimates. We have some evidence this is true for some parts of the 2002 NEI. For example, onroad benzene estimated with MOBILE6.2 may be more accurate than speciation of VOC from MOBILE6 due to the complex relationships between fuels and engine parameters included in the model for this pollutant; this complex relationship likely cannot be captured through a speciation profile applied to a mobile source category code and emission process.

For the “no-integrate” case, the HAP inventory provides the mass of the toxics model species only. Because we do use the HAP inventory, we might have named this case the “partial-integrate” case. However, we stick to the word “no-integrate” to be consistent with the current set of SMOKE documentation pertaining to the combination of HAP and CAP inventories. For the “no-integrate” case, the CAP VOC is speciated to provide only those model species that are not explicit toxics. This case is needed when it is impractical or invalid to integrate the inventories.

Figure 1 shows a schematic of the “integrate” and “no-integrate” case, and reflects how SMOKE implements them.

Figure 1. Combining HAP and CAP Inventories



For the “integrate” case, we compute emissions for a new pollutant: NONHAPVOC, which contains that portion of the VOC that are not toxics VOC; the computation is done on a source-by-source basis. When using SMOKE, the user identifies the particular toxics VOC to subtract in the SMOKE input file called the “INVTABLE;” these toxics must be consistent across a single SMOKE run.

SMOKE can use both the “integrate” and “no-integrate” cases within a single run. SMOKE uses the NHAPEXCLUDE file to apply the “no-integrate” case based on a list of county-level inventory (nonpoint, onroad, and nonroad) source information by SCC and state/county FIPS code.

To proceed with the approach to combining HAP and CAP for the 2002 NEI, we need to decide for which sources we can use the “integrate” case. We decided that if the HAP VOC and VOC emissions from a particular source are reasonably consistent, then they could be combined with the “integrate” case. The next section discusses criteria we used to evaluate the consistency in the HAP VOC and VOC estimates in the 2002 NEI how we analyzed the 2002 NEI against these criteria.

The Approach to Determine How Integrated Are the HAP and CAP in the 2002 NEI

For using the 2002 HAP and CAP emissions in the 2002 NEI in multipollutant modeling, we have developed an approach to determine which sources can use the “integrate” case. The approach entails determining, based on the relationship of the CAP and HAP inventory estimates, the potential consistency of the emission estimates of the CAP VOC and the various VOC HAPs from the specific emission sources in the inventory.

We developed a set of criteria which could be automated to determine, source by source, whether the VOC and HAP estimates for nonpoint, nonroad and onroad inventories can be combined. The criteria are aimed at determining the consistency between the VOC and HAP VOC estimates. For this work, we assumed that a source could use the “integrate” case if it met all the following criteria:

- 1) All VOC HAPs and VOC are uniformly submitted by the State or are computed by EPA; for example, if the state submits VOC, it must also submit all VOC HAPs.
- 2) The sum of VOC HAPs is less than or equal to the VOC.
- 3) The particular VOC HAPs can be mapped to model species.

Note that the source can still be integrated if just some of the VOC HAPs cannot be mapped. The HAPs that cannot be mapped must be excluded from the list of VOC HAPs subtracted from VOC to create NONHAPVOC (see Figure 1).

We implemented this approach for several inventory sectors in the final 2002 NEI (February 2006), as discussed below. For the first criterion, we used the “data source code” contained in the NEI Output Format; this code indicates the source of the data, and allows us to distinguish between an EPA-generated and a state-submitted estimate. For the second criterion, we identify which HAPs are VOC HAPs; these are identified in the pollutant code lookup tables as “ozone precursors.” We then summed the VOC HAP and compared the total with the VOC for each different FIPS/SCC combination. For the third criterion, we used data provided by Dr. Bill Carter that maps chemical compounds from the draft SPECIATE4 database to model species. We will need to ensure that the results we obtained with Carter’s data will not change when we use an updated mapping for the CB05 mechanism which is currently under development.

RESULTS

How Integrated is the Nonpoint Inventory?

The non-point inventory, also referred to as the stationary area, contains county-level estimates of stationary source emissions. Examples of source categories included in this sector include residential heating, solvent utilization, livestock and fertilizer emissions, open burning and numerous others.

The nonpoint inventory includes data supplied by several sources. We define consistency as either: (1) all pollutants of interest (VOC and HAP VOC) are EPA derived, or (2) all are not EPA-derived (i.e., state, local, or tribal). We assume state, local, and tribal data are consistent in the rare cases in which data for a single source are submitted by two or more of these origins.

Table 3 shows a summary of the nonpoint inventory across 48 contiguous states and D.C. that shows the amount of HAP and VOC that can and cannot be integrated. By comparing the tons of HAP and VOC that can be integrated with the tons that cannot, it can be seen that more than 70% of the total HAP and VOC in the nonpoint inventory can utilize the “integrate” case for combining CAP/HAP inventories.

Table 3. Nonpoint (February 2006 version) inventory summary of VOC and VOC HAP that can be integrated; excludes Alaska and Hawaii

	Tons of VOC that can be integrated	Tons of HAP that can be integrated	Tons of VOC that CANNOT be integrated	Tons of HAP that CANNOT be integrated	% of VOC mass that can be replaced by HAP mass	% of VOC reported by State	% of HAP reported by State
Stationary Source Fuel Combustion	1,193,445	49,438	517,493	22,943	2.9%	85.2%	76.6%
Mobile Sources	0	0	100	0	0.0%	100.0%	
Industrial Processes	361,903	15,085	274,213	9,585	2.4%	79.8%	83.9%
Solvent Utilization	3,382,877	594,242	563,565	189,514	15.1%	74.2%	68.9%
Storage and Transport	1,003,597	86,025	34,519	757	8.3%	7.1%	16.9%
Waste Disposal, Treatment, Recovery	239,200	19,015	128,196	21,298	5.2%	62.5%	44.0%
Miscellaneous Area Sources	30,195	10,789	261,219	25,507	3.7%	74.1%	83.6%
Total for all Nonpoint Sources	6,211,218	774,595	1,779,305	269,603	9.7%	67.7%	65.1%

As Table 3 shows, the percentage of VOC that can be replaced by HAP is below 10%. This result may be because a large amount of the VOC is not composed of HAPs; this hypothesis may be able to be evaluated by examining the speciation profiles used for the nonpoint inventory.

Most of the VOC mass that could be replaced by HAP in the “integrate” case is from the solvent utilization tier. At the national level, methanol, methyl ethyl ketone, toluene, methyl isobutyl ketone, benzene and xylenes are the largest contributors to solvent utilization HAP emissions; it should be noted however, that MEK was recently removed from the HAP list and will not be present in subsequent inventories. In that these pollutants match to mechanism species, they will be integrated (along with other VOC HAPs) for a sources contributing to most of the solvent utilization emissions.

Table 4 shows the quantities of the top 30 HAPs in the nonpoint inventory that can and cannot be integrated. These HAPs comprise more than 99% of the total HAP emissions in the nonpoint inventory. An additional 112 HAPs comprise the bottom 1% of the emissions. Note that the largest emitting HAP, methanol, is an “active” HAP in the CB05 mechanism. Pollutants inventoried as broad groups such as “glycol ethers” and “PAH, total” cannot be matched to model species, and thus cannot be part of the “integrate” case.

Table 4. Nonpoint Specific HAPs and their “integrate” status (February 2006 version of 2002 NEI), Excludes Alaska and Hawaii

Pollutant Code	Pollutant Name	Tons that Can be Integrated	Tons that Cannot be Integrated	Total Tons	Pct Integrated
67561	Methanol	145,075.26	17,447.63	162,522.89	89.26
108883	Toluene	106,512.09	54,977.51	161,489.60	65.96
1330207	Xylenes (mixture of o, m, and p isomers)	64,573.71	83,463.65	148,037.35	43.62
71432	Benzene	94,958.07	14,368.48	109,326.54	86.86
78933	Methyl ethyl ketone*	92,612.53	4,247.75	96,860.28	95.61
108101	Methyl isobutyl ketone	72,398.75	772.02	73,170.77	98.94
107211	Ethylene Glycol	46,465.17	7,305.48	53,770.64	86.41
110543	Hexane	28,892.86	7,347.42	36,240.28	79.73
1634044	Methyl tert-butyl ether	24,825.20	32.33	24,857.53	99.87
100414	Ethyl Benzene	6,514.74	17,615.18	24,129.92	27.00

Table 4. Nonpoint Specific HAPs and their “integrate” status (February 2006 version of 2002 NEI), Excludes Alaska and Hawaii

Pollutant Code	Pollutant Name	Tons that Can be Integrated	Tons that Cannot be Integrated	Total Tons	Pct Integrated
171	Glycol ethers	0.00	23,717.62	23,717.62	0.00
50000	Formaldehyde	8,946.52	13,370.21	22,316.74	40.09
67663	Chloroform	214.68	15,157.12	15,371.80	1.40
74839	Methyl bromide	10,760.33	3,446.07	14,206.40	75.74
542756	1,3-Dichloropropene	6,645.38	4,869.29	11,514.67	57.71
540841	2,2,4-Trimethylpentane	9,151.25	385.31	9,536.56	95.96
91203	Naphthalene	6,048.33	2,564.59	8,612.92	70.22
75070	Acetaldehyde	5,885.94	2,413.71	8,299.66	70.92
100425	Styrene	4,546.02	3,323.24	7,869.26	57.77
106467	1,4-Dichlorobenzene	5,837.55	1,225.11	7,062.66	82.65
74873	Methyl chloride	3,846.89	2,492.95	6,339.84	60.68
79016	Trichloroethylene	4,678.66	799.44	5,478.10	85.41
95476	o-Xylene	3,747.84	619.62	4,367.46	85.81
108907	Chlorobenzene	1,973.57	1,119.26	3,092.84	63.81
108952	Phenol	2,293.70	729.81	3,023.52	75.86
123386	Propionaldehyde	2,827.88	170.85	2,998.73	94.30
107028	Acrolein	1,990.89	749.70	2,740.59	72.64
84742	Dibutyl phthalate	2,312.98	33.68	2,346.66	98.56
130498292	PAH, Total	0.00	2,184.42	2,184.42	0.00
94757	2,4-Dichlorophenoxy acetic acid	0.00	1,892.88	1,892.88	0.00

* no longer a HAP and will not be in subsequent inventories

Table 5 shows a state-by-state summary of the tonnages in the “integrate” and “no-integrate” cases across all nonpoint sources. Most of the states have a similar percentage of HAP mass that can replace the VOC mass.

Table 5. State summary of the amount of VOC and VOC HAPs that can be integrated in the nonpoint sector of the 2002 NEI (February 2006 version of 2002 NEI)

	Tons of VOC "integrate" case	Tons of HAP "integrate" case	Tons of VOC "no-integrate" case	Tons of HAP "no-integrate" case	% VOC replaced by HAP	% VOC reported by State
Alabama	106,028	14,574	102,579	4502	7.0%	88.5%
Arizona	45,010	5927	30,418	5175	7.9%	48.7%
Arkansas	68,352	8564	27,305	2109	9.0%	62.0%
California	379,796	72,686	64,249	4096	16.4%	84.2%
Colorado	58,450	6892	23,956	195	8.4%	0.0%
Connecticut	77,484	7271	66,913	1270	5.0%	83.3%
Delaware	14,455	1359	455	747	9.1%	87.6%
D.C.	2664	443	1187	147	11.5%	41.7%
Florida	357,065	40,960	83,391	114,632	9.3%	75.7%
Georgia	238,130	31,603	51,161	3566	10.9%	57.7%
Idaho	127,766	19,698	12,446	4345	14.0%	91.2%
Illinois	214,308	43,089	57,532	1977	15.9%	66.3%
Indiana	105,593	14,988	69,760	8140	8.5%	81.5%
Iowa	68,974	8500	6481	312	11.3%	0.0%
Kansas	58,378	8107	74,997	1894	6.1%	63.1%
Kentucky	92,153	12,057	9712	2258	11.8%	1.1%
Louisiana	112,155	14,867	18,539	5980	11.4%	6.1%

Table 5. State summary of the amount of VOC and VOC HAPs that can be integrated in the nonpoint sector of the 2002 NEI (February 2006 version of 2002 NEI)

	Tons of VOC "integrate" case	Tons of HAP "integrate" case	Tons of VOC "no-integrate" case	Tons of HAP "no-integrate" case	% VOC replaced by HAP	% VOC reported by State
Maine	81,143	5801	6169	959	6.6%	94.0%
Maryland	118,323	15,370	4206	12,847	12.5%	84.1%
Massachusetts	149,996	15,976	24,546	2786	9.2%	87.8%
Michigan	138,545	18,399	97,129	12,739	7.8%	64.3%
Minnesota	120,255	15,601	1189	208	12.8%	79.3%
Mississippi	89,184	12,921	64,405	2061	8.4%	78.9%
Missouri	122,508	14,945	35,739	2402	9.4%	62.9%
Montana	19,491	2132	3289	381	9.4%	0.0%
Nebraska	33,001	3874	6655	113	9.8%	10.4%
Nevada	15,909	2189	5278	562	10.3%	23.6%
New Hampshire	57,732	4168	3016	583	6.9%	92.6%
New Jersey	48,314	7815	97,599	9306	5.4%	74.1%
New Mexico	31,257	3575	4144	98	10.1%	23.2%
New York	694,832	62,104	44,694	14,676	8.4%	87.2%
North Carolina	192,368	27633	82,370	926	10.1%	0.0%
North Dakota	12,121	1316	2429	1085	9.0%	0.0%
Ohio	255,705	43,797	18,318	6185	16.0%	62.2%
Oklahoma	88,933	7184	107,520	227	3.7%	68.4%
Oregon	240,550	26,317	2007	1556	10.8%	91.3%
Pennsylvania	158,876	22,883	115,324	4770	8.3%	58.8%
Rhode Island	11,027	1242	750	107	10.5%	23.3%
South Carolina	91,705	10,250	89702	2979	5.7%	79.7%
South Dakota	16,440	1786	2629	282	9.4%	0.0%
Tennessee	128,053	16,520	15,021	1493	11.5%	3.8%
Texas	602,694	55,144	81,452	14,913	8.1%	84.1%
Utah	34,736	3610	18,140	3641	6.8%	82.2%
Vermont	12,813	1153	5638	1000	6.3%	56.6%
Virginia	108,176	17,412	88,909	3322	8.8%	74.6%
Washington	154,757	14,946	6453	918	9.3%	60.0%
West Virginia	30185	3751	27062	3929	6.6%	81.4%
Wisconsin	211,321	21,828	13,974	413	9.7%	82.2%
Wyoming	13,503	1366	2469	788	8.6%	0.0%
Total for U.S.	6,211,218	774,595	1,779,305	269,603	9.7%	67.7%

How Integrated Is the Onroad Inventory?

The onroad inventory contains the emissions of onroad vehicles such as cars, trucks, buses and motorcycles. The inventory is developed through the NMIM model, which runs MOBILE6.2 to generate emissions of CAPs and HAPs. States can submit inputs to the NMIM model, such as county-specific fuels, vehicle registration or other inputs that affect emission factors or activity levels. States may also replace NMIM-estimates with their own estimates.

We define consistency as either: (1) all pollutants of interest (VOC and HAP VOC) are NMIM derived using state inputs, or (2) all are NMIM derived using EPA inputs, or (3) all NMIM derived using state inputs, but were subsequently replaced by state emission estimates, or (4) all are state-submitted estimates that replaced EPA default inputs to NMIM .

Table 6 provides a summary of the quantities of HAP and VOC that can and cannot be integrated in the onroad inventory across the 48 contiguous states and D.C. It shows that of the more than 4.5 million tons of VOC and 1 million tons of HAP in the inventory, about half of both the VOC and the VOC HAP can be processed using the “integrate” case. This will result in roughly 13% of the VOC mass being replaced with HAP mass.

Table 6. Onroad VOC and HAP that can be integrated (excludes Alaska and Hawaii), (February 2006 version of NEI)

	Tons of VOC That Can Be Integrated	Tons of HAP That Can Be Integrated	Tons of VOC That Cannot Be Integrated	Tons of HAP That Cannot Be Integrated	% of VOC mass that can be replaced by HAP mass
Light-Duty Gas Vehicles & Motorcycles	1,170,365	307,046	1,212,363	285,097	12.9%
Light-Duty Gas Trucks	877,968	247,146	951,739	245,143	13.5%
Heavy-Duty Gas Vehicles	91,677	22,448	122,878	31,672	10.5%
Diesels	91,376	14,287	81,150	17,391	8.3%
Total	2,231,386	590,927	2,368,130	579,303	12.8%

Table 7 shows a state-level summary of this information.

Table 7. Onroad source HAP and VOC emissions that can and cannot be integrated by State. February 2006 version of 2002 NEI
I, E, S and SI are data source codes: I=NMIM with state inputs, E=NMIM with EPA defaults, SI= state data replaced NMIM with State inputs, and S=state data replaced EPA defaults

State	"Integrate" (rounded to the nearest ton)								"No-Integrate" (rounded to the nearest ton)							
	HAP				VOC				HAP				VOC			
	I	E	S or SI	Total	I	E	S or SI	Total	I	E	S or SI	Total	I	E	S or SI	Total
Alabama	0	0	0	0	0	0	0	0	25,759	0	0	25,759	0	0	99,650	99,650
Arizona	9,578	6,226	0	15,803	35,698	27,686	0	63,385	2,987	0	0	2,987	0	0	1,089	1,089
Arkansas	0	0	0	0	0	0	0	0	14,013	0	0	14,013	0	0	69,955	69,955
California	0	0	0	0	0	0	0	0	16,850	0	75,802	92,652	0	0	343,902	343,902
Colorado	19,344	0	0	19,344	75,106	0	0	75,106	0	0	0	0	0	0	0	0
Connecticut	0	0	0	0	0	0	0	0	11,057	0	0	11,057	0	0	30,911	30,911
Delaware	0	0	2,860	2,860	0	0	10,564	10,564	0	0	0	0	0	0	0	0
DC	1,278	0	0	1,278	4,884	0	0	4,884	0	0	0	0	0	0	0	0
Florida	33,633	49,726	0	83,358	132,007	191,877	0	323,884	4,831	0	0	4,831	0	0	14,779	14,779
Georgia	0	0	0	0	0	0	0	0	45,687	0	0	45,687	0	0	218,729	218,729
Idaho	0	0	0	0	0	0	0	0	5,267	0	1,561	6,828	0	0	35,343	35,343
Illinois	0	0	0	0	0	0	0	0	35,589	0	0	35,589	0	0	116,717	116,717
Indiana	0	33,217	0	33,217	0	125,549	0	125,549	0	0	0	0	0	0	0	0
Iowa	19,022	0	0	19,022	70,810	0	0	70,810	0	0	0	0	0	0	0	0
Kansas	0	13,089	0	13,089	0	47,251	0	47,251	0	0	0	0	0	0	0	0
Kentucky	0	17,968	2,594	20,562	0	65,205	9,997	75,201	0	0	0	0	0	0	0	0
Louisiana	0	19,304	0	19,304	0	74,865	0	74,865	0	0	0	0	0	0	0	0
Maine	0	0	0	0	0	0	0	0	6,052	0	0	6,052	0	0	23,037	23,037
Maryland	16,927	0	0	16,927	62,982	0	0	62,982	0	0	0	0	0	0	0	0
Massachusetts	0	0	0	0	0	0	0	0	15,726	0	0	15,726	0	0	59,897	59,897
Michigan	26,708	0	0	26,708	94,219	0	0	94,219	24,650	0	0	24,650	0	0	61,056	61,056
Minnesota	22,252	0	0	22,252	89,562	0	0	89,562	0	0	0	0	0	0	0	0
Mississippi	0	0	0	0	0	0	0	0	14,868	0	0	14,868	0	0	68,508	68,508
Missouri	0	0	0	0	0	0	0	0	30,623	0	0	30,623	0	0	133,733	133,733
Montana	0	4,960	0	4,960	0	17,163	0	17,163	0	0	0	0	0	0	0	0
Nebraska	0	7,461	0	7,461	0	27,313	0	27,313	1,242	0	0	1,242	0	0	7,063	7,063
Nevada	0	1,212	0	1,212	0	4,360	0	4,360	4,941	0	0	4,941	0	0	46,611	46,611
New Hampshire	0	5,096	0	5,096	0	18,366	0	18,366	0	0	0	0	0	0	0	0
New Jersey	23,029	0	0	23,029	88,848	0	0	88,848	0	0	0	0	0	0	0	0
New Mexico	2,417	8,474	0	10,891	9,034	32,360	0	41,393	0	0	0	0	0	0	0	0

Table 7. Onroad source HAP and VOC emissions that can and cannot be integrated by State. February 2006 version of 2002 NEI
 I, E, S and SI are data source codes: I=NMIM with state inputs, E=NMIM with EPA defaults, SI= state data replaced NMIM with State inputs, and S=state data replaced EPA defaults

	"Integrate" (rounded to the nearest ton)								"No-Integrate" (rounded to the nearest ton)							
	I	E	S	SI	I	E	S	SI	I	E	S	SI	I	E	S	SI
New York	0	0	0	0	0	0	0	0	46,764	0	0	46,764	0	0	287,845	287,845
North Carolina	0	0	0	0	0	0	0	0	35,315	0	0	35,315	0	0	148,046	148,046
North Dakota	0	3,598	0	3,598	0	12,517	0	12,517	0	0	0	0	0	0	0	0
Ohio	47,360	0	0	47,360	184,072	0	0	184,072	0	0	0	0	0	0	0	0
Oklahoma	0	21,043	0	21,043	0	77,443	0	77,443	0	0	0	0	0	0	0	0
Oregon	24,022	0	0	24,022	86,016	0	0	86,016	0	0	0	0	0	0	0	0
Pennsylvania	0	0	0	0	0	0	0	0	43,585	0	0	43,585	0	0	176,090	176,090
Rhode Island	3,406	0	0	3,406	12,827	0	0	12,827	0	0	0	0	0	0	0	0
South Carolina	22,215	0	0	22,215	84,640	0	0	84,640	0	0	0	0	0	0	0	0
South Dakota	0	3,706	0	3,706	0	13,631	0	13,631	0	0	0	0	0	0	0	0
Tennessee	5,868	0	0	5,868	22,658	0	0	22,658	28,952	0	0	28,952	0	0	110,857	110,857
Texas	16,376	0	0	16,376	64,087	0	0	64,087	59,393	0	0	59,393	0	0	209,529	209,529
Utah	0	0	0	0	0	0	0	0	10,801	0	3,182	13,983	0	0	53,296	53,296
Vermont	0	0	0	0	0	0	0	0	3,196	0	1,074	4,270	0	0	17,288	17,288
Virginia	28,834	0	0	28,834	113,830	0	0	113,830	0	0	0	0	0	0	0	0
Washington	0	0	42,227	42,227	0	0	150,428	150,428	0	0	0	0	0	0	0	0
West Virginia	0	0	0	0	0	0	0	0	9,539	0	0	9,539	0	0	34,197	34,197
Wisconsin	21,521	0	0	21,521	78,397	0	0	78,397	0	0	0	0	0	0	0	0
Wyoming	0	4,379	0	4,379	0	15,133	0	15,133	0	0	0	0	0	0	0	0
Total	343,789	199,457	47,681	590,927	1,309,677	750,720	170,989	2,231,386	497,684	0	81,619	579,303	0	0	2,368,130	2,368,130

Table 8 lists VOC HAPs in the onroad inventory, in descending amount of emissions, and provides the associated quantities of the amount of emissions that can and cannot be integrated.

Table 8. Onroad HAPs and their “integrate” status (excludes Alaska and Hawaii); February 2006 version of 2002 NEI

Pollutant Code	Pollutant Name	Tons that can be integrated	Tons that cannot be integrated	Total Tons	Percent that can be integrated
108883	Toluene	195,271	180,605	375,876	52%
1330207	Xylenes (Mixture of o, m, and p Isomers)	110,287	107,798	218,084	51%
71432	Benzene	77,888	68,766	146,654	53%
540841	2,2,4-Trimethylpentane	71,929	64,296	136,225	53%
50000	Formaldehyde	30,133	31,627	61,761	49%
100414	Ethyl Benzene	29,125	27,812	56,937	51%
110543	Hexane	25,803	27,717	53,520	48%
1634044	Methyl Tert-Butyl Ether	18,429	39,888	58,317	32%
75070	Acetaldehyde	12,135	11,181	23,316	52%
106990	1,3-Butadiene	9,187	9,307	18,494	50%
100425	Styrene	5,739	5,098	10,837	53%
91203	Naphthalene	1,724	1,661	3,385	51%
123386	Propionaldehyde	1,630	1,690	3,320	49%
107028	Acrolein	1,435	1,636	3,071	47%
208968	Acenaphthylene	65	67	132	49%
85018	Phenanthrene	42	44	86	49%
86737	Fluorene	25	26	52	49%
129000	Pyrene	21	22	43	49%
206440	Fluoranthene	15	16	31	49%
120127	Anthracene	15	15	30	49%
83329	Acenaphthene	12	13	25	49%
191242	Benzo[g,h,i]Perylene	4	4	9	49%
56553	Benz[a]Anthracene	3	4	7	48%
205992	Benzo[b]Fluoranthene	2	3	5	49%
207089	Benzo[k]Fluoranthene	2	3	5	49%
50328	Benzo[a]Pyrene	2	2	4	49%
218019	Chrysene	2	2	4	49%
193395	Indeno[1,2,3-c,d]Pyrene	1	1	3	49%
53703	Dibenzo[a,h]Anthracene	0.0017	0.0034	0.0051	34%
SUM	All Onroad HAPs	590,927	579,303	1,170,230	50%

How Integrated is the Nonroad Inventory (Sources Other than Aircraft, Locomotive and Commercial Marine Emissions)?

We used a different approach to determine the mass that can be integrated for this sector because the nonroad 2002 inventory is based on NMIM runs using the new NONROAD2005 model. Except for California, all nonroad emissions are computed with NMIM using either EPA or State-provided inputs. We also determined that the NMIM nonroad HAPs can be mapped to model species.

We thus consider this sector to use the “integrate” case. Table 8 summarizes the quantities of VOC and HAP that can be integrated, and the percent of replacement of VOC mass with HAP mass. Even with 100% of the emissions using the “integrate” case, there is still no more than about 28% replacement of VOC mass with HAP because HAPs do not comprise the majority of the VOC. Note that California quantities in Table 9 are

based on NMIM; the actual modeling files (not available at the time of this paper) will include the California data.

Table 9. Summary of Nonroad HAP emissions that can be integrated based on NONROAD2005 model executed in NMIM

State	Tons of HAP "integrate"	Tons of VOC "integrate"	% VOC replaced by HAP
ALABAMA	156,69.5	58,996.6	26.6%
ARIZONA	12,422.7	55,724.3	22.3%
ARKANSAS	98,94.7	37,298.0	26.5%
CALIFORNIA	93,849.3	294,341.4	31.9%
COLORADO	11,122.2	43091.4	25.8%
CONNECTICUT	10,722.8	34,050.4	31.5%
DELAWARE	2416.4	7722.7	31.3%
DISTRICT OF COLUMBIA	640.5	20,83.5	30.7%
FLORIDA	68,652.9	258,471.7	26.6%
GEORGIA	22,103.5	858,97.8	25.7%
IDAHO	6703.0	23,705.8	28.3%
ILLINOIS	22,02.8	97,490.4	23.0%
INDIANA	13,119.8	55,632.9	23.6%
IOWA	11,808.1	45,992.6	25.7%
KANSAS	6375.2	25,634.3	24.9%
KENTUCKY	11,299.4	41,901.4	27.0%
LOUISIANA	17,901.3	66,205.3	27.0%
MAINE	99,18.0	30,663.3	32.3%
MARYLAND	17,041.9	54,322.4	31.4%
MASSACHUSETTS	17,658.9	55,465.2	31.8%
MICHIGAN	43813.5	158,787.2	27.6%
MINNESOTA	23,912.0	98,973.2	24.2%
MISSISSIPPI	10,247.8	38,302.4	26.8%
MISSOURI	18,639.1	66,536.6	28.0%
MONTANA	36,44.9	13,225.8	27.6%
NEBRASKA	4693.1	18,945.7	24.8%
NEVADA	5972.7	23,469.2	25.4%
NEW HAMPSHIRE	7115.9	22,526.1	31.6%
NEW JERSEY	26,303.9	83,112.4	31.6%
NEW MEXICO	3620.6	14,095.2	25.7%
NEW YORK	47,511.2	158,160.3	30.0%
NORTH CAROLINA	24,315.3	93,455.5	26.0%
NORTH DAKOTA	3679.1	13,764.0	26.7%
OHIO	22,729.3	98,868.2	23.0%
OKLAHOMA	105,36.7	39,782.0	26.5%
OREGON	11,042.4	41,107.2	26.9%
PENNSYLVANIA	28,050.7	100,479.3	27.9%
RHODE ISLAND	2427.8	7805.6	31.1%
SOUTH CAROLINA	13,947.8	53,101.1	26.3%
SOUTH DAKOTA	3216.3	12,570.3	25.6%

Table 9. Summary of Nonroad HAP emissions that can be integrated based on NONROAD2005 model executed in NMIM

State	Tons of HAP "integrate"	Tons of VOC "integrate"	% VOC replaced by HAP
TENNESSEE	16,526.3	63,058.2	26.2%
TEXAS	51,770.3	18,5714.8	27.9%
UTAH	7167.4	26,261.4	27.3%
VERMONT	3055.5	10,646.8	28.7%
VIRGINIA	18,408.2	70,173.3	26.2%
WASHINGTON	18,217.6	66,697.2	27.3%
WEST VIRGINIA	4669.4	17,630.0	26.5%
WISCONSIN	27382.8	98,053.2	27.9%
WYOMING	2652.9	9239.5	28.7%
Total	846,993.8	3,079,233.5	27.5%

Table 10 lists the HAPs along with the quantity in the inventory- which is the same as the quantity that can be integrated (48 state totals).

Table 10. Specific nonroad** HAPs in the 2002 NEI – all can be integrated based on NONROAD2005 model executed in NMIM

Pollutant code	Pollutant Name	Total* (includes CA emissions generated by NMIM, which will be replaced)
108883	Toluene	233,817.5
1330207	Xylenes (Mixture of o, m, and p Isomers)	205,048.4
540841	2,2,4-Trimethylpentane	108,542.7
1634044	Methyl Tert-Butyl Ether	80,025.4
71432	Benzene	70,282.1
100414	Ethyl Benzene	45,424.8
110543	Hexane	37,051.3
50000	Formaldehyde	34,620.0
75070	Acetaldehyde	14,802.5
106990	1,3-Butadiene	8746.7
123386	Propionaldehyde	3674.2
100425	Styrene	2671.9
107028	Acrolein	1434.8
91203	Naphthalene	605.1
85018	Phenanthrene	69.1
208968	Acenaphthylene	42.0
86737	Fluorene	38.3
129000	Pyrene	24.9
206440	Fluoranthene	22.5
83329	Acenaphthene	20.9
120127	Anthracene	8.6
191242	Benzo[g,h,i,j]Perylene	7.8

Table 10. Specific nonroad** HAPs in the 2002 NEI – all can be integrated based on NONROAD2005 model executed in NMIM

Pollutant code	Pollutant Name	Total* (includes CA emissions generated by NMIM, which will be replaced)
56553	Benz[a]Anthracene	2.5
193395	Indeno[1,2,3-c,d]Pyrene	2.4
50328	Benzo[a]Pyrene	2.2
218019	Chrysene	2.0
205992	Benzo[b]Fluoranthene	1.6
207089	Benzo[k]Fluoranthene	1.5
53703	Dibenzo[a,h]Anthracene	0.1
TOTAL		846993.8
<ul style="list-style-type: none"> • (includes CA emissions generated by NMIM, which will be replaced) • ** excludes aircraft, commercial marine and locomotive categories 		

Aircraft, Locomotive and Commercial Marine and point sources

Analyses for the aircraft, locomotive and commercial marine (ALM) and point source sectors will be performed at a later date. Note that the VOC emissions for ALM total roughly 100,000 tons across the 48 contiguous states and D.C., and the point source VOC emissions total roughly 1.7 million tons. We have not yet produced summaries for the 2002 NEI prescribed and wildfires which we have received in a day-specific point source emission format. Similar to nonroad sources, these point sources will fully utilize the “integrate” case because the VOC and HAP emission estimation methodology uses the same activity data.

Limitations of the Approach

The method we developed to determine how to combine HAP/CAP from the 2002 NEI is fairly straightforward to implement, since the criteria for the “integrate” case utilizes codes (i.e. data source codes) and cross references (VOC HAP identifiers and mapping data) that can be analyzed using in an automated approach (we developed various SAS programs for this effort). In utilizing such an approach we have made several assumptions which, at some point, should be further investigated. A key assumption is that HAP emissions estimates are more accurate than the speciation of the VOC estimates. Case studies to explore the underlying data used for estimating the HAP emissions, and the speciation profile data for the CAP emissions, could be undertaken for key source categories to evaluate this assumption.

We also assume that if the same entity (i.e., state or EPA) generates both the CAP and HAP emissions for a particular source, then the pollutants are consistent with each other. A more comprehensive investigation of the consistency of HAP and CAP estimates would require gathering additional information on the emission estimation methodology for each pollutant at each source. For example, when emission factors are used, what is

the source of factors? What specific test programs and measurement methods are involved, and are they consistent across the HAPs and CAPs? Even with the detailed documentation provided with EPA estimates, it is difficult to determine the consistency of a HAP and VOC estimate for a particular source. For state-submitted estimates, the emission estimation methods are not provided, and so it is not possible to determine the consistency. In addition, between a third to a half of the state and local agencies prepare separate HAP and CAP emission inventories, and thus even if the same agency reports HAPs and CAPs, they still may not be consistent if different staff work separately on them.

Further, we assume that for a particular source that can be integrated (an “integrate” source), that the VOC HAPs contained in the HAP inventory constitute all of the VOC HAP associated with that source. If a particular VOC HAP is not estimated for a particular “integrate” source, we assume it is not a component of the VOC for that particular source. This assumption is questionable when the SCC for an “integrate” source in one location (e.g., state or county) has a different set of HAPs for that same SCC for an “integrate” source in a different location. In this case, our methodology will produce different speciation for these “integrate” source even though they have the same SCC. Depending on the SCC, such a difference may not be sensible. Geographic inconsistency in the specific pollutants emitted by a source category, however, is not limited to HAPs, thus this limitation is broader than the context of the HAP/CAP “integrate” case.

CONCLUSIONS

We are developing a multipollutant modeling platform with the 2002 NEI which utilizes both HAP and CAP inventories. We developed an approach to maximize the use of the HAP inventory has been developed to maximize the use of the HAP inventory for use in populating both HAP and non HAP model species. Under this approach we have found that for the largest inventory sector of VOC, non-point, about 80% of the VOC and CAP emissions can be combined utilizing the “integrate” case whereby HAP VOC from the HAP inventory is used to replace VOC mass. For the non-point inventory, this integration results in the replacement of approximately 10 % of the VOC mass with HAP mass.

Due to the consistency of the nonroad NMIM-based inventory, 100% of the VOC and HAPs could be integrated, resulting in 27% of the VOC mass using the HAP emissions for speciation and the remainder using NONHAPVOC profiles.

In that the onroad inventory has a large number of state-submitted emissions of VOC, but model generated emissions for HAP, only half of the VOC could be integrated, and in some states, none of the VOC could be integrated. This will result in approximately 10% of the VOC mass being replaced with the HAP.

The next steps will be to determine the sensitivity on air quality model predictions of the use of the HAP inventory in the model species preparation.

DISCLAIMER

This paper has been reviewed in accordance with the U.S. EPA peer and administrative review policies and approved for presentation and publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for their use.

REFERENCES

1. National Research Council, *Air Quality Management in the United States*, Washington, D.C.; National Academies Press, 2004.
2. Air Quality Management (AQM) Work Group. Recommendations to the Clean Air Act Advisory Committee, Phase I and Next Steps. January 2005. Available from <http://www.epa.gov/air/caaac/aqm/report1-17-05.pdf>
3. Strum, M.; Driver, L.; Gipson, G.; Benjey, W.; Cook, R.; Houyoux, M.; Seppanen, C.; Stella, G.; "The Use of SMOKE to Process Multi-pollutant Inventories - Integration of Hazardous Air Pollutant And Volatile Organic Compound Emissions", Presented at the 12th International Emission Inventory Conference, "Emission Inventories – Applying New Technologies" of the Environmental Protection Agency, San Diego, CA, April 2003.
4. Luecken, D.J. and W.T. Hutzell, 2004. Concentrations of toxic air pollutants in the U.S. simulated by an air quality model, Proceedings of the 27th NATO/CCMS International Technical Meeting on Air Pollution Modeling and its Application, Banff, Canada, October, 2004.
5. Luecken, D.J., W.T. Hutzell and G.L. Gipson, 2006. Development and analysis of air quality modeling simulations for hazardous air pollutants, Atmospheric Environment, in press.
6. Michaels, H.; Brzezinski, D.; Cook, R. *EPA's National Mobile Inventory Model (NMIM), A Consolidated Emissions Modeling System for MOBILE6 and NONROAD*, U. S. Environmental Protection Agency, 2005; EPA-420-R-05-003. Available from <<http://www.epa.gov/otaq/nmim.htm>>
7. Yarwood, G., Rao, S., Yocke, M., and G. Whitten. 2005. Updates to the Carbon Bond Mechanism: CB05. Yocke and Company, final report to the U.S. Environmental Protection Agency, December 5, 2005. Available at http://www.camx.com/publ/pdfs/CB05_Final_Report_120805.pdf