

Technical Support Document:
Preparation of Emissions Inventories
for the Version 4.1, 2005-based Platform

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Acronyms

BAFM	Benzene, Acetaldehyde, Formaldehyde and Methanol
BEIS	Biogenic Emissions Inventory System
C3	Category 3 (commercial marine vessels)
CAIR	Clean Air Interstate Rule
CAMD	EPA's Clean Air Markets Division
CAM_x	Comprehensive Air Quality Model with Extensions
CAP	Criteria Air Pollutant
CARB	California Air Resources Board
CEM	Continuous Emissions Monitoring
CHIEF	Clearinghouse for Inventories and Emissions Factors
Cl	Chlorine
CMAQ	Community Multiscale Air Quality
CMV	Commercial marine vessel
CO	Carbon monoxide
EGU	Electric generating units
EPA	Environmental Protection Agency
EMFAC	Emission Factor (California's onroad mobile model)
EEZ	Exclusive Economic Zone
FAA	Federal Aviation Administration
FCCS	Fuel Characteristic Classification System
FIPS	Federal Information Processing Standards
HAP	Hazardous Air Pollutant
HCL	Hydrochloric acid
Hg	Mercury
HGNRVA	Natural recycled, volcanic and anthropogenic Hg
HMS	Hazard Mapping System
ICR	Information Collection Request
IMO	International Marine Organization
IPM	Integrated Planning Model
ITN	Itinerant
MACT	Maximum Achievable Control Technology
MOBILE	OTAQ's model for estimation of onroad mobile emissions factors
MOVES	Motor Vehicle Emissions Simulator -- OTAQ's model for estimation of onroad mobile emissions -- replaces the use of the MOBILE model
NEEDS	National Electric Energy Database System
NEI	National Emission Inventory
NESHAP	National Emission Standards for Hazardous Air Pollutants
NH₃	Ammonia
nm	nautical mile
NMIM	National Mobile Inventory Model
NOAA	National Oceanic and Atmospheric Administration
NONROAD	OTAQ's model for estimation of nonroad mobile emissions
NO_x	Nitrogen oxides
OAQPS	EPA's Office of Air Quality Planning and Standards
OTAQ	EPA's Office of Transportation and Air Quality
ORD	EPA's Office of Research and Development
ORL	One Record per Line
PF	Projection Factor, can account for growth and/or controls
PFC	Portable Fuel Container

PM_{2.5}	Particulate matter less than or equal to 2.5 microns
PM₁₀	Particulate matter less than or equal to 10 microns
RIA	Regulatory Impact Analysis
RFS2	Revised Annual Renewable Fuel Standard
RRF	Relative Response Factor
RWC	Residential Wood Combustion
RPO	Regional Planning Organization
SCC	Source Classification Code
SMARTFIRE	Satellite Mapping Automated Reanalysis Tool for Fire Incident Reconciliation
SMOKE	Sparse Matrix Operator Kernel Emissions
SO₂	Sulfur dioxide
SOA	Secondary Organic Aerosol
SPPD	Sector Policies and Programs Division
TAF	Terminal Area Forecast
TCEQ	Texas Commission on Environmental Quality
TSD	Technical support document
VOC	Volatile organic compounds
VMT	Vehicle miles traveled
WRAP	Western Regional Air Partnership

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1 Introduction

The U.S. Environmental Protection Agency (EPA), hereafter referred to as “we,” has developed an updated version of the 2005-based air quality modeling platform, version 4.1. This document describes the emissions inventory and emissions modeling for this version, focusing on the changes made from version 4. The version 4 platform is documented at the emissions modeling clearinghouse website, <http://www.epa.gov/ttn/chief/emch/>, under the section entitled “2005-Based Modeling Platform” and the subsection entitled “CAP-Hg-BAFM 2005-Based Platform Version 4.1”.

The platform consists of Criteria Air Pollutants (CAPs) and the following select Hazardous Air Pollutants (HAPs): mercury (Hg), chlorine (CL₂), hydrochloric acid or hydrogen chloride (HCL) and benzene, acetaldehyde, formaldehyde and methanol. The latter four are also denoted BAFM. This platform is called the “CAP-Hg-BAFM 2005-Based Platform, Version 4.1” platform (we will use the shortened name “2005v4.1” in this documentation). This platform supports the Regulatory Impact Analysis for National Emission Standards for Hazardous Air Pollutants (NESHAP) for Industrial, Commercial, and Institutional Boilers and Process Heaters (a.k.a. “Boiler MACT”) and the proposal for the Toxics rule.

The underlying 2005 inventories used are: 1) the 2005 National Emission Inventory (NEI), version 2 (<http://www.epa.gov/ttn/chief/net/2005inventory.html>), 2) the 2005 National Air Toxics Assessment (NATA) mercury inventory from June 2010, and 3) an inventory of Hg developed from the Boiler MACT Information Collection Request (ICR) for the National Emission Standards for Major Sources: Industrial/Commercial/Institutional Boilers and Process Heaters (<http://www.epa.gov/ttn/atw/boiler/boilerpg.html>). This document describes the approach and data used to produce the emission inputs to the air quality model used in the 2005v4.1 platform.

Emissions preparation for the 2005v4.1 platform supports the Community Multiscale Air Quality (CMAQ) model (<http://www.epa.gov/AMD/CMAQ/>) and (2) the Comprehensive Air Quality Model, with extensions (CAM_x) (<http://www.camx.com/>). Both models support modeling ozone (O₃), particulate matter (PM) and mercury (Hg), and require hourly and gridded emissions of chemical species from the following inventory pollutants: carbon monoxide (CO), nitrogen oxides (NO_x), volatile organic compounds (VOC), sulfur dioxide (SO₂), ammonia (NH₃), particulate matter less than or equal to 10 microns (PM₁₀), individual component species for particulate matter less than or equal to 2.5 microns (PM_{2.5}) and individual component species of gaseous and particulate mercury (Hg). In addition, the CMAQ Carbon Bond 05 (CB05) chemical mechanism with chlorine chemistry, which is part of the “base” version of CMAQ, allows explicit treatment of BAFM and includes HAP emissions of HCL and CL₂. The platform BAFM emissions come from either the NEI values for benzene, formaldehyde, acetaldehyde and methanol (BAFM) or via speciation of NEI VOC into the component species.

The effort to create the emission inputs for the 2005v4.1 platform included:

- (1) modification of emission inventories used for the 2005v4 base case,
 - (2) updates to the emissions modeling ancillary files used with the emissions modeling tools,
- and

(3) application of the emissions modeling tools.

The primary emissions modeling tool used to create the CMAQ model-ready emissions was the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (<http://www.smoke-model.org/index.cfm>). We used SMOKE version 2.6 to create emissions files for a 36-km national grid, a 12-km Eastern grid and a 12-km Western grid for a 2005 base case (also known as the “2005cr_hg_05b” case for purposes of our directory structure). The purpose of this case is to provide a 2005 case that is consistent with the methods used in the future-year base case and control cases. For regulatory applications, this case is included in the relative response factor (RRF) calculations.

Unlike the version 4 (v4) platform, this platform includes only a base case; it does not include a model evaluation case. The evaluation case in the 2005v4 platform uses 2005-specific fire emissions and 2005 hour-specific continuous emission monitoring (CEM) data for electric generating units (EGUs) whereas the 2005 base case includes an “average year” scenario for fires and a illustrative (rather than year-specific) temporal allocation approach for EGUs to allocate annual 2005 emissions to days and hours. This approach to temporal allocation was used for all base and control cases modeled to provide a temporal consistency that is intended to be a conceivable temporal allocation without tying the approach to a single year.

The 2005v4.1 platform was developed using the concepts, tools and emissions modeling data from EPA’s 2005v4 platform, documented by:
ftp://ftp.epa.gov/EmisInventory/2005v4/2005_emissions_tsd_07jul2010.pdf (main document) ,
ftp://ftp.epa.gov/EmisInventory/2005v4/2005_emissions_tsd_appendices_11may2010.pdf (appendices to the main document), and
http://www.epa.gov/ttn/chief/emch/transport/tr_proposal_emissions_tsd.pdf (future year).

Section 2 provides a summary of the key differences between the two versions of the emissions platform.

This document contains five sections and four appendices. Section 2 describes the 2005 inventories input to SMOKE. Section 3 describes the emissions modeling and the ancillary files used with the emission inventories. The development of the 2016 inventory (projected from 2005) is provided through technical support documents for the specific modeling applications. Section 4 provides references. Appendices A through D provide additional details about specific technical methods.

Electronic copies of the data used with SMOKE for the 2005 platform are available at the emissions modeling clearinghouse, <http://www.epa.gov/ttn/chief/emch/>, under the section entitled “2005-Based Modeling Platform” and the subsection entitled “CAP-Hg-BAFM 2005-Based Platform, Version 4.1”. This is referred to as the “2005v4.1 website” throughout this document. In addition, this data is provided to the electronic docket in support of the Toxics Rule.

2 2005 emission inventories and approaches

This section describes the 2005 emissions data created for input to SMOKE. As with the 2005v4 platform, the primary basis for the 2005 stationary source emission inputs is the 2005 National Emission Inventory (NEI), version 2, which includes emissions of CO, NO_x, VOC, SO₂, NH₃, PM₁₀, PM_{2.5} and hazardous air pollutants (HAPs). The HAPs we used from this inventory are mercury, chlorine (CL2), hydrogen chloride (HCL), benzene, acetaldehyde, formaldehyde, and methanol. We began with the same SMOKE-formatted inventory inputs as the 2005v4 platform (case name: 2005ck_05b) and made changes described here.

For mercury, the 2005v4.1 platform uses a later version of the 2005v2 NEI inventory prepared for the 2005 National Air Toxics Assessment (NATA). It uses the June 18, 2010 version of the 2005 NATA inventory, with the exception of emissions from commercial, institutional and industrial boilers from the major source information collection request (ICR) database and other changes described later. The NATA inventory started with the 2005v2 NEI, and was updated with data collected for some source categories, which resulted in major updates to mercury emissions for Portland cement and hazardous waste combustion. The NATA inventory was also revised as a result of comments received as part of the state, local and tribal review.

Documentation for the 2005 NEI can be found at: <http://www.epa.gov/ttn/chief/net/2005inventory.html#documentation>. For inventories outside of the United States, which include Canada and Mexico, we used the latest available base-year inventories as discussed in Section 2.6.

The 2005 NEI includes five sectors: nonpoint (formerly called “stationary area”) sources, point sources, nonroad mobile sources, onroad mobile sources, and fires. Because the 2005v4.1 platform includes just a base case, the available day-specific wildfires and prescribed burning data from the 2005 NEI was not used; rather an average fire inventory that is used for both base and future years was used.

For purposes of preparing the air quality model-ready emissions, we used the same split of the 2005 emissions inventory into “platform” sectors for use in emissions modeling as was used in the 2005v4 platform. The significance of an emissions modeling or “platform” sector is that it is run through all of the SMOKE programs except the final merge (Mrggrid) independently from the other sectors. The final merge program combines the sector-specific gridded, speciated and hourly emissions together to create the CMAQ-ready emission inputs, which can be converted to emissions that can be used by CAM_x when needed.

Similarly to 2005v4, we added sectors for biogenic emissions, emissions from the Canadian and Mexican inventories, and augmented with other emissions data to be explained below.

Table 2-1 presents the sectors in the 2005 platform. The sector abbreviations are provided in italics; these abbreviations are used in the SMOKE modeling scripts and inventory file names, and throughout the remainder of this document. Updates from the 2005v4 platform are discussed in Table 2-2.

Table 2-1. Platform sectors used in emissions modeling for the 2005 platform, version 4.1

Platform Sector	2005 NEI Sector	Description and resolution of the data input to SMOKE
EGU sector (also called the IPM sector): <i>ptipm</i>	Point	<p><u>For all pollutants other than mercury (Hg):</u> 2005v2 NEI point source EGUs mapped to the Integrated Planning Model (IPM) model using the National Electric Energy Database System (NEEDS) 2006 version 4.10 database. A few revisions were made to the 2005v2 NEI annual emission estimates as discussed in Table 2-2.</p> <p><u>For Hg:</u> 6/18/2010 version of the inventory used for the 2005 National Air Toxics Assessment (NATA) mapped to IPM using NEEDS version 4.10. The NATA inventory is an update to the 2005v2 NEI and was divided into EGU and non-EGU sectors consistent with the other pollutants (we did not actually map the NATA inventory to IPM, but rather applied the mapping that was done to the 2005 NEIv2 to the NATA Hg inventory). We additionally removed Hg from sources from the National Emission Standards for Hazardous Air Pollutants for Industrial, Commercial, and Institutional Boilers and Process Heaters (aka “Boiler MACT”) Information Collection Request (ICR) database because we included these emissions in the non-EGU sector.</p> <p><u>For both:</u> Day-specific emissions created for input into SMOKE.</p>
Non-EGU sector (also called the non-IPM sector): <i>ptnonipm</i>	Point	<p><u>For all pollutants other than Hg:</u> All 2005v2 NEI point source records not matched to the <i>ptipm</i> sector. Includes all aircraft emissions. Additionally updated inventory to remove duplicates, improve estimates from ethanol plants, and reflect new information collected from industry from the ICR for the Boiler MACT. Includes point source fugitive dust emissions for which county-specific PM transportable fractions were applied.</p> <p><u>For Hg:</u> The 6/18/2010 version of NATA inventory was used except for modifications to gold mine emissions and removal of Hg from facilities that closed prior to 2005. In addition, Hg emissions developed for the Boiler MACT were used</p> <p><u>For both:</u> Annual resolution.</p>
Average-fire sector: <i>avefire</i>	Not applicable	Average-year wildfire and prescribed fire emissions, unchanged from the 2005v4 platform; county and annual resolution.
Agricultural sector: <i>ag</i>	Nonpoint	NH ₃ emissions from NEI nonpoint livestock and fertilizer application, county and annual resolution. Unchanged from the 2005v4 platform.
Area fugitive dust sector: <i>afdust</i>	Nonpoint	PM ₁₀ and PM _{2.5} from fugitive dust sources from the NEI nonpoint inventory after application of county-specific PM transportable fractions. Includes building construction, road construction, paved roads, unpaved roads, agricultural dust), county and annual resolution.
Remaining nonpoint sector: <i>nonpt</i>	Nonpoint	Primarily 2002 NEI nonpoint sources not otherwise included in other SMOKE sectors; county and annual resolution. Also includes updated Residential Wood Combustion emissions, year 2005 non-California WRAP oil and gas Phase II inventory and year 2005 Texas and Oklahoma oil and gas emissions. Removed Hg emissions from boilers to avoid double counting with Hg emissions added to the non-EGU sector from the Boiler MACT ICR.
Nonroad sector: <i>nonroad</i>	Mobile: Nonroad	Monthly nonroad emissions from the National Mobile Inventory Model (NMIM) using NONROAD2005 version nr05c-BondBase, which is equivalent to NONROAD2008a, since it incorporated Bond

Platform Sector	2005 NEI Sector	Description and resolution of the data input to SMOKE
		rule revisions to some of the base case inputs and the Bond rule controls did not take effect until later. NMIM was used for all states except California. Monthly emissions for California created from annual emissions submitted by the California Air Resources Board (CARB) for the 2005v2 NEI.
locomotive, and non-C3 commercial marine: <i>alm_no_c3</i>	Mobile: Nonroad	2002 NEI non-rail maintenance locomotives, and category 1 and category 2 commercial marine vessel (CMV) emissions sources, county and annual resolution. Aircraft emissions are included in the Non-EGU sector (as point sources) and category 3 CMV emissions are contained in the <i>seca_c3</i> sector
C3 commercial marine: <i>seca_c3</i>	Mobile : Nonroad	Annual point source-formatted, year 2005 category 3 (C3) CMV emissions, developed for the rule called “Control of Emissions from New Marine Compression-Ignition Engines at or Above 30 Liters per Cylinder”, usually described as the Emissions Control Area (ECA) study (http://www.epa.gov/otaq/oceanvessels.htm). Utilized final projections from 2002, developed for the C3 ECA proposal to the International Maritime Organization (EPA-420-F-10-041, August 2010).
Onroad California, NMIM-based, and MOVES sources not subject to temperature adjustments: <i>on_noadj</i>	Mobile: onroad	Three, monthly, county-level components: 1) California onroad, created using annual emissions for all pollutants, submitted by CARB for the 2005 NEI version 2. NH ₃ (not submitted by CARB) from MOVES2010. 2) Onroad gasoline and diesel vehicle emissions from MOVES2010 not subject to temperature adjustments: exhaust CO, NO _x , VOC, NH ₃ , benzene, formaldehyde, acetaldehyde, 1,3-butadiene, acrolein, naphthalene, brake and tirewear PM, and evaporative VOC, benzene, and naphthalene. 3) Onroad emissions for Hg from NMIM using MOBILE6.2, other than for California.
Onroad cold-start gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: <i>on_moves_startpm</i>	Mobile: onroad	Monthly, county-level MOVES2010-based onroad gasoline emissions subject to temperature adjustments. Limited to exhaust mode only for PM species and naphthalene. California emissions not included. This sector is limited to cold start mode emissions that contain different temperature adjustment curves from running exhaust (see <i>on_moves_runpm</i> sector).
Onroad running gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: <i>on_moves_runpm</i>	Mobile: onroad	Monthly, county-level draft MOVES2010-based onroad gasoline emissions subject to temperature adjustments. Limited to exhaust mode only for PM species and Naphthalene. California emissions not included. This sector is limited to running mode emissions that contain different temperature adjustment curves from cold start exhaust (see <i>on_moves_startpm</i> sector).
Biogenic: <i>biog</i>	Not applicable	Hour-specific, grid cell-specific emissions generated from the BEIS3.14 model, including emissions in Canada and Mexico.
Other point sources not from the NEI: <i>othpt</i>	Not applicable	Point sources from Canada’s 2006 inventory and Mexico’s Phase III 1999 inventory, annual resolution. Also includes annual U.S. offshore oil 2005v2 NEI point source emissions.

Platform Sector	2005 NEI Sector	Description and resolution of the data input to SMOKE
Other point sources not from the NEI, Hg only: <i>othpt_hg</i>	Not applicable	Annual year 2000 Canada speciated mercury point source emissions.
Other nonpoint and nonroad not from the NEI: <i>othar</i>	Not applicable	Annual year 2006 Canada (province resolution) and year 1999 Mexico Phase III (municipio resolution) nonpoint and nonroad mobile inventories.
Other nonpoint sources not from the NEI, Hg only: <i>othar_hg</i>	Not applicable	Annual year 2000 Canada speciated mercury from nonpoint sources.
Other onroad sources not from the NEI: <i>othon</i>	Not applicable	Year 2006 Canada (province resolution) and year 1999 Mexico Phase III (municipio resolution) onroad mobile inventories, annual resolution.

The emission inventories in SMOKE input format for the 2005 base case are available at the 2005v4.1 website (see the end of Section 1). The “readme” file provided indicates the particular zipped files associated with each platform sector.

Before discussing the specific components of the 2005v4.1 emissions platform, we provide in Table 2-2 a summary of the significant differences between the 2005v4 emissions platform and this 2005v4.1 platform.

Table 2-2. Summary of significant changes between v4 and v4.1 platforms by sector

Platform Sector	Summary of Significant Inventory Differences from V4 to V4.1																																																												
IPM sector: <i>ptipm</i>	<ul style="list-style-type: none"> - Added or changed ORIS Boiler IDs to some units with missing or incorrect values, and for a subset of these, recomputed annual emissions of NO_x, SO₂ or both using 2005 CEM data, resulting in lower NO_x and/or SO₂ for CA, MA, NY, SC and increasing for MS and WV as shown below <table border="1" data-bbox="480 432 1349 625"> <tbody> <tr> <td>CA</td> <td>NOX down 75.4 tons; SO2 down 21.1 tons</td> </tr> <tr> <td>MA</td> <td>NOX down 483 tons ; SO2 down 1533.4 tons</td> </tr> <tr> <td>NY</td> <td>NOX down 149.3 tons</td> </tr> <tr> <td>SC</td> <td>NOX down 1166.2, tons SO2 down 1.3 tons</td> </tr> <tr> <td>MS</td> <td>SO2 up 929.7 tons</td> </tr> <tr> <td>WV</td> <td>NOX up 142.5 tons</td> </tr> </tbody> </table> <ul style="list-style-type: none"> - Appendix A, Table A-1 provides a facility-level summary of these changes. Only replaced emissions if 2005 CEM data were confirmed to be for the entire year (some CEM is only for the summer season). - Hg emissions from 2005v2 were replaced with Hg emissions from the June 2010 version of the NATA 2005 inventory except for units matched to the Boiler MACT ICR database. - Hg emissions for units matched to units in the Boiler MACT ICR database were removed (summing to 0.045 tons Hg). The Boiler MACT ICR database Hg emissions were used for these in place of the NATA Hg values, but were included in the ptnonipm sector. 	CA	NOX down 75.4 tons; SO2 down 21.1 tons	MA	NOX down 483 tons ; SO2 down 1533.4 tons	NY	NOX down 149.3 tons	SC	NOX down 1166.2, tons SO2 down 1.3 tons	MS	SO2 up 929.7 tons	WV	NOX up 142.5 tons																																																
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Non-IPM sector: <i>ptnonipm</i>	<ul style="list-style-type: none"> - Revised 2005 emissions for many point sources other than EGUs to remove duplicates, improve estimates from ethanol plants, and reflect new emissions and controls information collected from industry and a state through the Boiler MACT ICR. A summary of these NO_x, SO₂, and PM_{2.5} emissions from v4 to v4.1 are listed: <table border="1" data-bbox="513 1150 1325 1696"> <thead> <tr> <th>State</th> <th>NOX change v4 to v4.1</th> <th>SO2 change v4 to v4.1</th> <th>PM2.5 change v4 to v4.1</th> </tr> </thead> <tbody> <tr><td>California</td><td>30</td><td>39</td><td>1</td></tr> <tr><td>Georgia</td><td>-1,242</td><td>-1,614</td><td>-28</td></tr> <tr><td>Indiana</td><td>-4,941</td><td>-7,379</td><td>-1,291</td></tr> <tr><td>Iowa</td><td>2,519</td><td>3,206</td><td>100</td></tr> <tr><td>Kansas</td><td>73</td><td>93</td><td>3</td></tr> <tr><td>Kentucky</td><td>121</td><td>154</td><td>5</td></tr> <tr><td>Nebraska</td><td>31</td><td>39</td><td>1</td></tr> <tr><td>New Mexico</td><td>182</td><td>231</td><td>7</td></tr> <tr><td>North Carolina</td><td></td><td>-6,701</td><td>0</td></tr> <tr><td>North Dakota</td><td>128</td><td>220</td><td>13</td></tr> <tr><td>Ohio</td><td>-366</td><td>-3,303</td><td>0</td></tr> <tr><td>Pennsylvania</td><td>101</td><td>-2,035</td><td></td></tr> <tr><td>South Dakota</td><td>236</td><td>301</td><td>10</td></tr> <tr><td>Tennessee</td><td>-6,098</td><td>-11,046</td><td>-760</td></tr> </tbody> </table> <ul style="list-style-type: none"> - Hg emissions changed to use NATA inventory. Updated NATA inventory to remove closed plants and also replaced boiler Hg with for units mapped to Boiler MACT ICR database with the ICR Hg emissions. 	State	NOX change v4 to v4.1	SO2 change v4 to v4.1	PM2.5 change v4 to v4.1	California	30	39	1	Georgia	-1,242	-1,614	-28	Indiana	-4,941	-7,379	-1,291	Iowa	2,519	3,206	100	Kansas	73	93	3	Kentucky	121	154	5	Nebraska	31	39	1	New Mexico	182	231	7	North Carolina		-6,701	0	North Dakota	128	220	13	Ohio	-366	-3,303	0	Pennsylvania	101	-2,035		South Dakota	236	301	10	Tennessee	-6,098	-11,046	-760
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Average-fire sector: <i>avefire</i>	Unchanged from 2005v4 platform																																																												

Platform Sector	Summary of Significant Inventory Differences from V4 to V4.1
Agricultural sector: <i>ag</i>	Unchanged from 2005v4 platform
Area fugitive dust sector: <i>afdust</i>	Unchanged from 2005v4 platform
Remaining nonpoint sector: <i>nonpt</i>	Added: year 2005 oil and gas data for Texas and Oklahoma provided by these states. Replaced previous Oklahoma oil and gas emissions from this sector (SCC 2310000000). No removals for Texas since the new oil and gas emissions only cover oil rig emissions that are in the nonroad sector. The nonroad sector emissions were not removed because they were very small compared to the newer Texas oil and gas emissions added to this sector and the possibility of double counting was not able to be confirmed by EPA. Changed pesticide category to “no-integrate,” thereby using VOC speciation (rather than the HAP emissions) to compute the BAFM emissions.
Nonroad sector: <i>nonroad</i>	Added PM to 7 California counties which were found to be 0 in the 2005v4 platform. Data used came from an earlier version of the 2005 inventory provided by CARB, which had the same PM values as the 2005v2 NEI other than in the missing counties, for which nonzero PM values were provided.
locomotive, and non-C3 commercial marine: <i>alm_no_c3</i>	Unchanged from 2005v4 platform
C3 commercial marine: <i>seca_c3</i>	Revised 2005 emissions from the category 3 commercial marine sector to reflect the final projections from 2002 developed for the category 3 commercial marine Emissions Control Area (ECA) proposal to the International Maritime Organization (EPA-420-F-10-041, August 2010). Also projected Canada as part of the ECA rather than an “outside the ECA” region, using region-specific growth rates. For example, British Columbia emissions were projected the same as “North Pacific” growth and control used in Washington. Therefore the v4.1 <i>seca_c3</i> inventories contain Canadian province codes. Hg was not used in the 2005v4.1 platform due to uncertainties in the values.
Onroad California, NMIM-based, and MOVES sources not subject to temperature adjustments: <i>on_noadj</i>	For all states except California: All pollutants and modes (exhaust, tire and brake wear) from all vehicle types are now from MOVES2010 except for Hg. Hg is from 2005v2 NEI, based on the MOBILE6 model. In the 2005v4 platform, only exhaust mode onroad gasoline vehicles, other than motorcycles, were included from MOVES in this sector and the rest had been from MOBILE6. For California: Replaced NMIM-based NH ₃ with MOVES2010 emissions for California because California does not provide NH ₃ in its onroad inventory. For the 2005v4 platform, we used NH ₃ from NMIM but since MOVES generates all criteria pollutants, we now use MOVES.
Onroad cold-start gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: <i>on_moves_startpm</i>	For the 2005v4.1 platform, this sector uses MOVES2010 based emissions for all exhaust mode onroad gasoline vehicle types including motorcycles. In the v4 version, motorcycle exhaust mode PM emissions relied on NMIM and were therefore in the <i>on_noadj</i> sector, and other exhaust mode gasoline vehicle PM emissions used the draft version of MOVES. As with v4, these PM and naphthalene cold start mode emissions are subject to grid cell and hourly temperature adjustments.
Onroad running	Same change as “ <i>on_moves_startpm</i> ”

Platform Sector	Summary of Significant Inventory Differences from V4 to V4.1
gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: <i>on_moves_runpm</i>	
Biogenic: <i>biog</i>	Unchanged from 2005v4 platform
Other point sources not from the NEI: <i>othpt</i>	Unchanged from 2005v4 platform
Other point sources not from the NEI, Hg only: <i>othpt_hg</i>	Unchanged from 2005v4 platform
Other nonpoint and nonroad not from the NEI: <i>othar</i>	Unchanged from 2005v4 platform
Other nonpoint sources not from the NEI, Hg only: <i>othar_hg</i>	Unchanged from 2005v4 platform
Other onroad sources not from the NEI: <i>othon</i>	Unchanged from 2005v4 platform

Annual emission summaries for 2005v4.1, with comparisons to 2005v4 CAPs emissions by emissions modeling sector are provided in Table 2-3. VOC totals are before BAFM speciation (i.e., they are inventory VOC emissions, and not the sum of VOC emissions after BAFM speciation). Summaries of Hg (speciated), HCL and CL2 are provided in Table 2-4, and Table 2-5 provides a summary of natural mercury sources for the modeling domain.

The emission inventories for input to SMOKE for the 2005 base case are available at the 2005v4 website (see the end of Section 1) under the link “Data Files” (see the “2005emis” directory). The inventories “readme” file indicates the particular zipped files associated with each platform sector

Table 2-3. 2005 Emissions by Sector: VOC, NOX, CO, SO2, NH3, PM10, PM2.5

Sector	2005 VOC [tons/yr]		2005 NOX [tons/yr]		2005 CO [tons/yr]		2005 SO2 [tons/yr]		2005 NH3 [tons/yr]		2005 PM10 [tons/yr]		2005 PM2.5 [tons/yr]	
	V4.1	V4	V4.1	V4	V4.1	V4	V4.1	V4	V4.1	V4	V4.1	V4	V4.1	V4
afdust											8,858,992	same	1,030,391	same
ag									3,251,990	same				
alm_no_c3	67,690	same	1,924,925	same	270,007	same	154,016	same	773	same	59,366	same	56,687	same
seca_c3 (US component)	44,990	22,367	647,884	642,088	54,049	53,746	420,110	417,312			53,918	53,580	49,541	49,294
seca_c3 (non-US component)	18,367	18,241	532,181	526,760	43,267	42,959	321,414	319,200			43,326	43014	39,810	39,574
nonpt	7,530,564	7,474,512	1,699,532	1,683,490	7,413,762	7,376,314	1,259,635	1,252,645	134,080	134,080	1,354,638	1,349,685	1,081,816	1,076,954
nonroad	2,691,844	same	2,115,408	same	19,502,718	same	197,341	same	1,972	same	211,807	209,100	201,138	198,734
on_roadj	3,949,362	3,123,642	9,142,274	7,203,876	43,356,130	41,647,066	177,977	144,216	156,528	295,203	308,497	170,554	236,927	115,991
on_moves_runpm											54,071	46,430	49,789	42,753
on_moves_startpm											22,729	23,607	20,929	21,738
ptipm	40,950	same	3,726,459	3,728,190	601,564	same	10,380,786	10,381,411	21,684	same	615,095	same	508,903	same
ptnonipm	1,310,784	1,310,085	2,238,002	2,247,228	3,221,388	3,222,221	2,089,836	2,117,649	158,837	159,003	653,048	653,957	440,714	442,656
avefire	1,958,992	same	189,428	same	8,554,551	same	49,094	same	36,777	same	796,229	same	684,035	same
Canada othar ¹	1,281,095	same	734,587	same	3,789,362	same	95,086	same	546,034	same	1,666,188	same	432,402	same
Canada othon	270,872	same	524,837	same	4,403,745	same	5,309	same	21,312	same	14,665	same	10,395	same
Canada othpt	447,313	same	857,977	same	1,270,438	same	1,664,040	same	21,268	same	117,669	same	68,689	same
Mexico othar	586,842	same	249,045	same	644,733	same	101,047	same	486,484	same	143,816	same	92,861	same
Mexico othon	183,429	same	147,419	same	1,455,121	same	8,270	same	2,547	same	6,955	same	6,372	same
Mexico othpt	113,044	same	258,510	same	88,957	same	980,359	same	0	same	125,385	same	88,132	same
offshore othpt	51,240	same	82,581	same	89,812	same	1,961	same	0	same	839	same	837	same

1. Canada provided 2006 fires but we did not use them in the 2005 platform (for neither v4.1 nor v4)

Table 2-4. Summaries of Hg (speciated), HCL and CL2*

	2005 HGIIGAS (divalent gaseous mercury) [tons/yr]		2005 HGNRVA (elemental mercury) [tons/yr]		2005 PHGI (particulate mercury) [tons/yr]		2005 HCL [tons/yr]		2005 CL2 [tons/yr]	
	V4.1	V4	V4.1	V4	V4.1	V4	V4.1	V4	V4.1	V4
alm_no_c3	0.0411	same	0.0793	same	0.0212	same			1.38	same
seca_c3	**	0.0002	**	0.0004	**	0.0001				
seca_c3 non-US	**	0.0001	**	0.00018	**	0.00007				
Nonpt	1.0605	1.9901	3.1034	4.6528	1.2722	0.6524	29,001	29,364	2,135	same
Nonroad	0.1041	same	0.2105	same	0.0533	0.0533				
on_noadj	0.1402	same	0.5036	same	0.0599	0.0599				
Ptipm	21.096	21.1757	30.1986	30.318	1.6596	1.6136	351,592	same	99	same
Ptnonipm	10.4687	16.4756	29.5686	23.7646	7.4707	6.1291	48,630	48,664	4,174	same
Canada othar_hg	1.08		0.86		0.34					
Canada othpt_hg	1.72		3.59		0.5					
<p>* The sectors afdust, ag, avefire, on_moves_runpm, and on_moves_startpm have no Cl or Hg emissions ** Due to uncertainty in mercury emissions from this sector, they were removed from the inventories and not used for the V4.1 Platform. The amount removed from the 2005 data was the 2005v4 values, and summed to approximately 0.001 tons total mercury for the sum of U.S. and non-U.S. components</p>										

In addition to the anthropogenic sectors, we include speciated hourly emissions for the geogenic categories listed in Table 2-5. These are the same as had been used in the previous platforms except for the land-direct emissions which were reduced by 90% based on updated information from the literature as described in Section 2.7.

Table 2-5. Summaries of the non-anthropogenic mercury across the modeling domain

Region	Species	Land-direct [tons/yr]	Land-recycled [tons/yr]	Ocean Direct [tons/yr]	Ocean Recycled [tons/yr]	Volcanic [tons/yr]
Domain-wide	Elemental Mercury (HGNRVA)	12.077	158.01	7.27	56.51	0.02

The remainder of Section 2 provides details of the data contained in each of the 2005 platform sectors. Different levels of detail are provided for different sectors depending on the availability of reference information for the data, the degree of changes or manipulation of the data needed for preparing it for input to SMOKE, and whether the 2005v4.1 platform emissions changed appreciably since the previously-documented 2005v4 platform.

2.1 2005 NEI Point sources (ptipm and ptnonipm)

Point sources are sources of emissions for which specific geographic coordinates (e.g., latitude/longitude) are specified, as in the case of an individual facility. A facility may have

multiple emission points, which may be characterized as units such as boilers, reactors, spray booths, kilns, etc. A unit may have multiple processes (e.g., a boiler that sometimes burns residual oil and sometimes burns natural gas). Note that this section describes only NEI point sources within the contiguous United States. The offshore oil platform (othpt sector) and category 3 CMV emissions (seca_c3 sector) are also point source formatted inventories that are discussed in Section 2.6 .

After removing offshore oil platforms (othpt sector), we created two platform sectors from the remaining 2005v2 NEI point sources for input into SMOKE: the EGU sector – also called the Integrated Planning Model (IPM) sector (i.e., ptipm) and the non-EGU sector – also called the non-IPM sector (i.e., ptnonipm). This split facilitates the use of different SMOKE temporal processing and future year projection techniques for each of these sectors. The inventory pollutants processed through SMOKE for both ptipm and ptnonipm sectors were: CO, NO_x, VOC, SO₂, NH₃, PM₁₀, PM_{2.5} and the following HAPs: HCL (pollutant code = 7647010), CL2 (code = 7782505) and mercury (codes: 199, 200, 201, 202, 22967926, 593748, 62384, 7439976, and 7487947). We did not utilize BAFM from these sectors as we chose to speciate VOC without any use (i.e., integration) of VOC HAP pollutants from the inventory (integration is discussed in detail in Section 3.1.2.1). We utilized Hg from the NATA Hg point source inventories with the modifications discussed below.

The ptnonipm emissions were provided to SMOKE as annual emissions. The ptipm emissions for the base case were input to SMOKE as daily emissions.

Documentation for the development of the 2005 point source NEI v2, is at: <http://www.epa.gov/ttn/chief/net/2005inventory.html#documentation>. A summary of this documentation describes these data as follows:

1. Electric generating unit (EGU) emissions are obtained from emissions/heat input from EPA's Acid Rain Program for Continuous Emissions Monitoring System (CEMS) reporting. The following approach applied to units in the 2002 NEI that matched to 2005 CEMS units. For pollutants covered by the CEMS, the 2005 CEMS data were used. For CEMS units with pollutants not covered by CEMS (e.g., VOC, PM_{2.5}, HCL) unit-specific ratios of 2005 to 2002 heat input were applied to 2002v3 NEI emissions to obtain 2005 estimates.
2. Non-EGU stationary source development for the 2005 NEI focused on improving the following sectors:
 - a. HAP data received from States and industry to support the MACT program, including the recent Risk and Technology Review rulemaking
 - b. 2005 State, local, and tribal data submitted to EPA under the Consolidated Emissions Reporting Rule (CERR)
 - c. HAP data from Toxic Release Inventory (TRI) for missing facilities and pollutants
 - d. Off-shore platform data from Mineral Management Services (MMS)

The changes made to the 2005v2 NEI non-EGU point inventory prior to modeling are as follows:

- The tribal data, which do not use state/county Federal Information Processing Standards (FIPS) codes in the NEI, but rather use the tribal code, were assigned a state/county FIPS code of 88XXX, where XXX is the 3-digit tribal code in the NEI. We made this change because SMOKE requires the 5-digit state/county FIPS code.
- We defaulted stack parameters for some point sources when modeling in SMOKE. SMOKE uses an ancillary file, called the PSTK file, which provides default stack parameters by SCC code to either gap fill stack parameters if they are missing in the NEI or to correct stack parameters if they are outside the ranges specified in SMOKE as acceptable values. The SMOKE PSTK file is contained in the ancillary file directory of the 2005v4 website (see the end of Section 1).
- We applied a transport fraction to all SCCs that we identified as PM fugitive dust, to prevent the overestimation of fugitive dust impacts in the grid modeling as described in Section 2.2.1.

We also made a changes to the 2005 NATA Hg inventory (June 18, 2010 version) prior to its use in modeling. We removed sources that were discovered to have closed prior to 2005. We modified gold mine emissions based on information collected as part of the data gathering for the proposed gold mine rule. We replaced Hg emissions with values in the Boiler MACT ICR database. Of the 1607 facilities in the Boiler MACT ICR database, all except for 184 facilities (0.177 tons Hg) were matched to inventory (NATA inventory, NEI v2 inventory or both) facilities based on the NEI_UNIQUE_ID code. The 184 facilities without NEI_UNIQUE_IDs were not used in our 2005 Hg inventory for the platform. Since the ICR database contained only emissions by unit and the fuel type, we needed to assign the geographic coordinates and stack parameters needed to transform the Boiler MACT ICR database into a modeling file. We used geographic coordinates and stack parameters from the NATA Hg inventory (or NEI v2 if not in the NATA inventory) by matching the facility and then choosing the parameters from the process/unit that matched the fuel type in the ICR. If more than one unit matched, we used the stack parameters from the unit with the highest emissions. Where there were no fuel matches, we used default parameters. Additional information on these changes is provided in Table 2-6 below. Further details of this procedure, and the other fields we populated to construct the modeling file are provided in Appendix B.

Because the NATA Hg point source emissions were not separated into ptnonipm and ptipm, we applied the same point splits (via the field IPM_YN) to the NATA Hg inventory as were applied to the 2005v2 NEI.

Table 2-6. Hg changes made to the 2005 NATA Hg inventory (June 18, 2010 version) for the 2005 ptnonipm, ptipm, and nonpt sectors.

Change																					
<p>Incorporated Boiler MACT ICR emissions</p>	<p>Added 4.66 tons Hg from ICR unit-level emissions data. Generated modeling parameters (latitudes/longitudes, stack parameters) from the NATA Hg or NEI inventories, by matching ICR facilities/fuel information to matching facility identifiers (the NEI_UNIQUE_ID) and fuel types in these other modeling inventories.</p> <p>Removed 0.045 tons Hg from ptipm which is the sum of Hg from sources that and matched a facility in the ICR based on the NEI_UNIQUE_ID and either (1) had a design capacity of less than 25 MW and matched a facility in the ICR or (2) had no design capacity listed had a MACT code beginning with 0107, which is the general code for identify industrial, commercial, institutional boilers and process heaters.</p> <p>Removed 1.71 tons Hg from ptnonipm - we used a crosswalk that link combinations of Maximum Achievable Control Technology (MACT) code, standard industrial code (SIC), NAICS (North American Industrial Classification System) code and source classification code (SCC) to identify industrial, commercial, institutional (ICI) boilers and process heaters, and removed all records that matched the ICR facilities based on the NEI_UNIQUE_ID.</p> <p>Removed 3.15 tons Hg from nonpt – we used a crosswalk that link combinations of MACT and SCC to ICI boilers and process heaters and removed all records 4.68 to in the nonpt sector that matched.</p>																				
<p>Changed Gold Mine Emissions, geographic coordinates and stack parameters</p>	<p>Changed facility emissions for nine out of 19 facilities in the ptnonipm sector based on data collected for the proposed National Emission Standards for Hazardous Air Pollutants for Gold Mine Ore Processing and Production, provided by the EPA Sector Policies and Programs Division (SPPD) project lead Chuck French.</p> <p>These changes are summarized below, and result in an overall total change of Hg emissions from Goldmines from 2.35 to 2.50 tons.</p> <table border="1" data-bbox="571 1596 1438 1871"> <thead> <tr> <th data-bbox="571 1596 803 1627">State facility ID</th> <th data-bbox="803 1596 1104 1627">Facility name</th> <th data-bbox="1104 1596 1242 1627">Updated Hg emissions</th> <th data-bbox="1242 1596 1438 1627">BASIS</th> </tr> </thead> <tbody> <tr> <td data-bbox="571 1627 803 1659">89406KNNCT55MIL</td> <td data-bbox="803 1627 1104 1659">KENNECOTT RAWHIDE MINING CO</td> <td data-bbox="1104 1627 1242 1659">0.02</td> <td data-bbox="1242 1627 1438 1659">based on 2007 emissions test data</td> </tr> <tr> <td data-bbox="571 1659 803 1690">89045SMKYV1SMOK</td> <td data-bbox="803 1659 1104 1690">SMOKY VALLEY COMMON OPERATION</td> <td data-bbox="1104 1659 1242 1690">0.03</td> <td data-bbox="1242 1659 1438 1690">based on 2007 emissions test data</td> </tr> <tr> <td data-bbox="571 1690 803 1722">T\$18242</td> <td data-bbox="803 1690 1104 1722">RUBY HILL MINE</td> <td data-bbox="1104 1690 1242 1722">0.018</td> <td data-bbox="1242 1690 1438 1722">emissions test data based on 2008</td> </tr> <tr> <td data-bbox="571 1722 803 1753">89418FLRDCEXIT1</td> <td data-bbox="803 1722 1104 1753">STANDARD MINING INC</td> <td data-bbox="1104 1722 1242 1753">0.08</td> <td data-bbox="1242 1722 1438 1753">emissions test data</td> </tr> </tbody> </table>	State facility ID	Facility name	Updated Hg emissions	BASIS	89406KNNCT55MIL	KENNECOTT RAWHIDE MINING CO	0.02	based on 2007 emissions test data	89045SMKYV1SMOK	SMOKY VALLEY COMMON OPERATION	0.03	based on 2007 emissions test data	T\$18242	RUBY HILL MINE	0.018	emissions test data based on 2008	89418FLRDCEXIT1	STANDARD MINING INC	0.08	emissions test data
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	<p>89419CRRCH180EX COEUR ROCHESTER INC 0.069 based on 2007 emissions test data</p> <p>89438NWMNTSTONE NEWMONT MINING CORP 0.311 based on 2006 emissions test data is for the 2004-05 timeframe based on the estimate submitted to Nevada DEP in response to ICR survey sent to the company.</p> <p>89801JRRRT50MIL JERRITT CANYON MINE 0.23 based on 2008 emissions test data</p> <p>89803BLDMN70MIL BALD MOUNTAIN MINE 0.14 based on 2007 emissions test data</p> <p>89803BRRCK27MIL BARRICK GOLDSTRIKE MINES INC 0.35 based on 2007 emissions test data</p> <p>Also changed geographic coordinates and stack parameters for 10 facilities based on information provided by Chuck French that was used in local scale modeling done in support of the NESHAP in early 2010.</p> <table border="1" data-bbox="586 800 1446 1230"> <tr> <th>Facility Name</th> <th></th> </tr> <tr> <td>GLAMIS MARIGOLD MINE</td> <td>Refinery building operations</td> </tr> <tr> <td>NEWMONT MINING CORP CARLIN SOUTH</td> <td>Refinery and roasting operations</td> </tr> <tr> <td>NEWMONT MINING CORP TWIN CREEKS MINE</td> <td>Refinery and autoclave operations</td> </tr> <tr> <td>SMOKY VALLEY COMMON OPERATION</td> <td>Refinery building operations</td> </tr> <tr> <td>CORTEZ GOLD MINES</td> <td>Refinery building operations</td> </tr> <tr> <td>RUBY HILL</td> <td>Refinery building operations</td> </tr> <tr> <td>BARRICK GOLDSTRIKE</td> <td>Refinery, autoclave & roasting operations</td> </tr> <tr> <td>WESTERN MESQUITE MINES</td> <td>Refinery building operations</td> </tr> <tr> <td>CRIPPLE CREEK COLORADO</td> <td>Refinery building operations</td> </tr> <tr> <td>GREENS CREEK WA</td> <td>Refinery building operations</td> </tr> </table>	Facility Name		GLAMIS MARIGOLD MINE	Refinery building operations	NEWMONT MINING CORP CARLIN SOUTH	Refinery and roasting operations	NEWMONT MINING CORP TWIN CREEKS MINE	Refinery and autoclave operations	SMOKY VALLEY COMMON OPERATION	Refinery building operations	CORTEZ GOLD MINES	Refinery building operations	RUBY HILL	Refinery building operations	BARRICK GOLDSTRIKE	Refinery, autoclave & roasting operations	WESTERN MESQUITE MINES	Refinery building operations	CRIPPLE CREEK COLORADO	Refinery building operations	GREENS CREEK WA	Refinery building operations
Facility Name																							
GLAMIS MARIGOLD MINE	Refinery building operations																						
NEWMONT MINING CORP CARLIN SOUTH	Refinery and roasting operations																						
NEWMONT MINING CORP TWIN CREEKS MINE	Refinery and autoclave operations																						
SMOKY VALLEY COMMON OPERATION	Refinery building operations																						
CORTEZ GOLD MINES	Refinery building operations																						
RUBY HILL	Refinery building operations																						
BARRICK GOLDSTRIKE	Refinery, autoclave & roasting operations																						
WESTERN MESQUITE MINES	Refinery building operations																						
CRIPPLE CREEK COLORADO	Refinery building operations																						
GREENS CREEK WA	Refinery building operations																						
<p>Removed Hg emissions for sources closed or not operating in 2005</p>	<p>Removed 0.342 tons, most of which (0.337 tons) is associated with the removal of Northwestern Steel & Wire Co, Illinois (NEI_UNIQUE_ID NEIL1955ABD), which shut down prior to 2005. Other removals were:</p> <ul style="list-style-type: none"> • Arkwright, Georgia (NEI12787) • CPSG Gould Street, Maryland (NEI7008) State sent article written in 2008 (http://www.thefreelibrary.com/Constellation+Energy+Restarts+Gould+Street+Power+Plant+in+Baltimore.-a0179900776) that said it had been shut down for the last 5 years and would be re-opening as a gas fired plant only. • Midwest Generation LLC, Illinois (NEIIL0638266). • Northwestern Steel & Wire Co, Illinois (NEIIL1955ABD) 																						

2.1.1 IPM sector (ptipm)

The ptipm sector contains emissions from EGUs in the 2005v2 NEI point inventory that we were able to match to the units found in the NEEDS database. While we originally used version 3.02 of NEEDS to split out the ptipm sector for v4 of the platform, there were no changes to the mapping when we moved to NEEDS version 4.10

(<http://www.epa.gov/airmarkets/progsregs/epa-ipm/index.html>). The IPM model provides future-year emission inventories for the universe of EGUs contained in the NEEDS database. As described below, this matching was done to (1) provide consistency between the 2005 EGU sources and future year EGU emissions for sources which are forecasted by IPM and (2) avoid double counting in projecting point source emissions.

The 2005v4 platform document provides additional details on how the 2005 NEI point source inventory was split into the ptipm and ptnonipm sectors.

Although we used the same ptipm split as was used for the v4 platform, we changed some emissions values based on updates we made to some ORIS identifiers in the ptipm file. For a subset of the units for which we added or changed ORIS identifiers, we recomputed annual emissions for SO₂, NO_x or both using the CEMS data available at the EPA's data and maps website.² The impact of these changes is summarized in Table 2-2 and detailed changes are provided in Appendix A.

Creation of temporally resolved emissions for the ptipm sector

Another reason we separated the ptipm sources from the other sources was due to the difference in the temporal resolution of the data input to SMOKE. For the base case 2005 run, the ptipm sector uses daily emissions input into SMOKE. The daily emissions are computed from the annual emissions. First, we allocate annual emissions to each month (this process occurs outside of SMOKE). To do this, we created state-specific, three-year averages of 2004-2006 CEM data. These average annual-to-month factors were assigned to sources by state. To allocate the monthly emissions to each day, we used the 2005 CEM data to compute state-specific month-to-day factors, averaged across all units in each state. The resulting daily emissions were input into SMOKE. The daily-to-hourly allocation was performed with SMOKE using diurnal profiles. The development of these diurnal ptipm-specific profiles, which are considered ancillary data for SMOKE, is described in Section 3.2.3.

2.1.2 Non-IPM sector (ptnonipm)

The non-IPM (ptnonipm) sector contains all 2005v2 NEI point sources that we did not include in the IPM (ptipm) sector.³ The ptnonipm sector contains fugitive dust PM emissions from vehicular traffic on paved or unpaved roads at industrial facilities or coal handling at coal mines.⁴ Prior to input to SMOKE, we reduced the fugitive dust PM emissions to estimate the emissions

² <http://camddataandmaps.epa.gov/gdm/index.cfm?fuseaction=emissions.wizard>

³ Except for the offshore oil and day-specific point source fire emissions data which are included in separate sectors, as discussed in sections 2.6 and 2.3.1, respectively.

⁴ Point source fugitive dust emissions, which represent a very small amount of PM, were treated the same way in the 2002 platform but were treated as a separate sector in the 2001 Platform.

that remain aloft by applying county-specific fugitive dust transportable fraction factors. This is discussed further in Section 2.2.1.

For some geographic areas, some of the sources in the ptnonipm sector belong to source categories that are contained in other sectors. This occurs in the inventory when states, tribes or local programs report certain inventory emissions as point sources because they have specific geographic coordinates for these sources. They may use point source SCCs (8-digit) or non-point, onroad or nonroad (10-digit) SCCs. In the 2005 NEI, examples of these types of sources include: aircraft emissions in all states, waste disposal emissions in several states, firefighting training in New Mexico, several industrial processes and solvent utilization sources in North Carolina and Tennessee, livestock (i.e., animal husbandry) in primarily Kansas and Minnesota, and petroleum product working losses.

The modifications between the published 2005v2 NEI and the 2005 inventory we used for modeling are summarized here:

Ptnonipm changes from the original 2005v2 inventory for the v4 platform development

- Removed duplicate annual records. We did not delete some apparent duplicates because they were in fact covering different parts of the year (i.e., the emissions in the inventory file were sub-annual).
- Removed a source with a state/county FIPS code of 30777; the “777” county FIPS represents portable facilities that move across counties, but is not currently a valid state/county FIPS code in the SMOKE ancillary file “COSTCY”. This Montana FIPS code was located in northern Wyoming and contained very small emissions.
- Dropped sources with coordinates located well into the oceans or lakes.
- Fixed the coordinates for several larger sources that had a state/county FIPS code mismatch with their inventory coordinates greater than 10 km and emissions greater than 10 tons per year of either NOX, VOC, SO₂, or 5 tons/yr of PM_{2.5}. These corrections were limited to a small number of plants in Arizona, Indiana, Kentucky, Ohio, and Virginia.

Ptnonipm updates from 2005v4 platform used in creating the 2005v4.1 platform

Found and removed additional duplicate records. These records were duplicates caused by records from both 2002 and 2005 being in the inventory. These were caught after ignoring leading zeroes in the plant IDs, point IDs, etc. that were present for only one of the years of data. There were a total of 175 records removed. A summary of the emissions removed is provided below. Due to the small mass of duplicate HAP records and the fact that most were not being used in the platform, no HAP records were removed.

CO	3,520 tons
NH ₃	166 tons
NO _x	13,421 tons
PM ₁₀	3,858 tons
PM _{2.5}	3,444 tons
SO ₂	21,061 tons
VOC	1,504 tons

- Removed duplicate emissions for Blue Ridge Paper (FIPS=37087). For the same unitid, stackid and SCC there were two records for the same pollutant with different data source codes but similar emissions values. They appeared to be duplicates so they were removed.
- Updated boiler emissions at Domtar Paper/Johnsonburg Mill (FIPS code =42047), which included 2002 emissions values to 2005 emissions values based on information provided by the Department of Environmental Protection in Pennsylvania. They had put on scrubbers between 2002 and 2005 and that was not reflected in the platform 2002-based emissions. Rather than apply the reductions, we updated the emissions to better reflect 2005. Note: We only changed NO_x, SO₂ and HCL even though the facility representative send information for all pollutants plant because of the effort involved with converting the information provided into a form usable for modeling.
- Removed unit-level emissions from plants for units determined to have shut down between 2002 and 2005. In all situations, the state inventory representative was contacted to confirm that the unit actually shut down. Plants impacted were: LaFarge Cement Plant in Atlanta Georgia, Domtar Paper, Tennessee, FIPS=47163 and P. H. Glatfelter Company in Chillicothe, Ohio.
- Added North Dakota ADM facility (FIPS code = 38067) that was in the 2005v1 NEI but was missing from the 2005v2 NEI and was not determined to have shut down. Added the 2002-based emissions to the ptnonipm file, since 2005 data were not available.
- Added an inventory of 2005 ethanol plants using plant names and data provided by EPA's Office of Transportation and Air Quality for use in a previous modeling effort (Renewable Fuel Standards 2), which included these with the 2005v1 inventory. The list below includes only the ethanol plants that were used in the previous modeling effort but were missing from the 2005v2 NEI.

State/County FIPS code	Plant Name	CO (tons/yr)	NOX (tons/yr)	PM10 (tons/yr)	PM2_5 (tons/yr)	SO2 (tons/yr)	VOC (tons/yr)
06065	Golden Cheese Company of CA	10.47	30.31	12.13	1.29	38.58	14.33
13205	Wind Gap Farms (Anheuser/Miller Brewery)	0.84	2.43	0.97	0.10	3.09	1.15
19033	Golden Grain Energy LLC	146.60	424.38	169.75	15.33	540.12	200.62
19035	Little Sioux Corn Processors	184.30	533.51	213.40	19.27	679.01	252.20
19055	Permeate Refining	3.14	9.09	3.64	0.39	11.57	4.30
19057	Big River Resources, LLC	108.91	315.26	126.10	13.43	401.23	149.03
19083	Hawkeye Renewables, LLC	115.19	333.44	133.38	14.21	424.38	157.63
19093	Quad-County Corn Processors	56.55	163.69	65.48	6.97	208.33	77.38
19167	Siouxland Energy & Livestock Coop (SELC)	209.44	606.26	242.50	25.83	771.60	286.60
21047	Commonwealth Agri-Energy, LLC	46.08	133.38	53.35	4.82	169.75	63.05
31047	Cornhusker Energy Lexington (CEL)	25.13	72.75	29.10	3.10	92.59	34.39
31145	SW Energy, LLC.	41.89	121.25	48.50	5.17	154.32	57.32
35041	Abengoa Bioenergy Corporation	10.47	30.31	12.13	1.09	38.58	14.33
46005	Heartland Grain Fuels, LP	0.21	0.61	0.24	0.03	0.77	0.29
46109	North Country Ethanol (NCE)	62.83	181.88	72.75	6.57	231.48	85.98
19109	Global Ethanol	29.32	84.88	33.95	3.07	108.02	40.12
20055	Reeve Agri-Energy	52.36	151.57	60.63	6.46	192.90	71.65
	TOTAL TONS	1103.73	3195.00	1278.00	127.13	4066.36	1510.36

2.2 2005 Nonpoint sources (afdust, ag, nonpt)

The 2005v2 NEI generally did not include updated nonpoint emissions from values used in the 2002 NEI, and this modeling platform took a similar approach. Consequently, we created several sectors from the 2002 nonpoint NEI. We removed the nonpoint tribal-submitted

emissions to prevent possible double counting with the county-level emissions. Because the tribal nonpoint emissions are small, we do not anticipate these omissions having an impact on the results at the 36-km and 12-km scales used for modeling. This omission also eliminated the need for us to develop spatial surrogate data for allocation of tribal data to grid cells during the SMOKE processing, with little expected impact.

The documentation for the nonpoint sector of the 2005 NEI is available at:
<http://www.epa.gov/ttn/chief/net/2005inventory.html>

In the rest of this section, we describe in more detail each of the platform sectors into which we separated the 2005 nonpoint NEI, and the changes we made to these data. We will refer to the 2002 platform documentation for sectors that did not change.

2.2.1 Area Fugitive dust sector (afdust)

The emissions for this sector are unchanged from the 2005v4 platform, and the documentation is repeated here for convenience. However, we changed the temporal allocation of the emissions to account for day-of-week variation. In particular, we used updated dust profiles that are consistent with the activity related to non-dust profiles for similar processes. The processes and profiles updated are provided in Pouliot, et. al., 2010. Previously, all days within the same month had the same emissions.

The area-source fugitive dust (afdust) sector contains PM₁₀ and PM_{2.5} emission estimates for 2002 NEI nonpoint SCCs identified by EPA staff as dust sources. This sector is separated from other nonpoint sectors to make it easier to apply a “transport fraction,” which reduces emissions to reflect observed diminished transport from these sources at the scale of our modeling. Application of the transport fraction prevents the overestimation of fugitive dust impacts in the grid modeling as compared to ambient samples. Categories included in this sector are paved roads, unpaved roads and airstrips, construction (residential, industrial, road and total), agriculture production and all of the mining 10-digit SCCs beginning with the digits “2325.” It does not include fugitive dust from grain elevators because these are elevated point sources.

We created the afdust sector from the 2002 NEI based on SCCs and pollutant codes (i.e., PM₁₀ and PM_{2.5}) that are considered “fugitive”. A complete list of all possible fugitive dust SCCs (including both 8-digit point source SCCs and 10-digit nonpoint SCCs) is provided at: http://www.epa.gov/ttn/chief/emch/dustfractions/tf_scc_list2002nei_v2.xls. However, not all of the SCCs in this file are present in the 2002 NEI. The SCCs included in the 2002 NEI that comprise the 2005 (and 2002) platform afdust sector (which are a subset of the SCCs in the web link) are provided in Table 2-7.

Table 2-7. SCCs in the afdust platform sector

SCC	SCC Description
2275085000	Mobile Sources;Aircraft;Unpaved Airstrips;Total
2294000000	Mobile Sources;Paved Roads;All Paved Roads;Total: Fugitives
2296000000	Mobile Sources;Unpaved Roads;All Unpaved Roads;Total: Fugitives
2296005000	Mobile Sources;Unpaved Roads;Public Unpaved Roads;Total: Fugitives
2296010000	Mobile Sources;Unpaved Roads;Industrial Unpaved Roads;Total: Fugitives
2311000000	Industrial Processes;Construction: SIC 15 - 17;All Processes;Total
2311010000	Industrial Processes;Construction: SIC 15 - 17;Residential;Total
2311010040	Industrial Processes;Construction: SIC 15 - 17;Residential;Ground Excavations
2311010070	Industrial Processes;Construction: SIC 15 - 17;Residential;Vehicle Traffic
2311020000	Industrial Processes;Construction: SIC 15 - 17;Industrial/Commercial/Institutional;Total
2311020040	Industrial Processes;Construction: SIC 15 - 17;Industrial/Commercial/Institutional;Ground Excavations
2311030000	Industrial Processes;Construction: SIC 15 - 17;Road Construction;Total
2325000000	Industrial Processes;Mining and Quarrying: SIC 14;All Processes;Total
2801000000	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Total
2801000002	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Planting
2801000003	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Tilling
2801000005	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Harvesting
2801000007	Miscellaneous Area Sources;Agriculture Production - Crops;Agriculture - Crops;Loading
2805000000	Miscellaneous Area Sources;Agriculture Production - Livestock;Agriculture - Livestock;Total
2805001000	Miscellaneous Area Sources;Agriculture Production - Livestock;Beef cattle - finishing operations on feedlots (drylots);Dust Kicked-up by Hooves (use 28-05-020, -001, -002, or -003 for Waste

Our approach was to apply the transportable fractions by county such that all afdust SCCs in the same county receive the same factor. The approach used to calculate the county-specific transportable fractions is based on land use data and is described by:

http://www.epa.gov/ttn/chief/emch/dustfractions/transportable_fraction_080305_rev.pdf

As this paper mentions, a limitation of the transportable fraction approach is the lack of monthly variability, which would be expected due to seasonal changes in vegetative cover. Further, the variability due to soil moisture, precipitation, and wind speeds is not accounted for by the methodology. An electronic version of the county-level transport fractions can be found at:

<http://www.epa.gov/ttn/chief/emch/dustfractions/transportfractions052506rev.xls>

The 2002 platform documentation describes an error in which the transportable fraction application for PM_{2.5} was not applied. This error was fixed for the 2005v4.1 platform, and 2005 PM_{2.5} afdust emissions are therefore correctly about 43% less than those in the 2002 platform.

2.2.2 Agricultural Ammonia sector (ag)

This sector is unchanged from the 2005v4 platform; the documentation is repeated here for completeness.

The agricultural NH₃ “ag” sector is comprised of livestock and agricultural fertilizer application emissions from the nonpoint sector of the 2002 NEI. This sector is unchanged in the 2005

platform. The rest of this section documentation is therefore very similar to that in the 2002 documentation.

In building this sector we extracted livestock and fertilizer emissions based on the SCC. The livestock SCCs are listed in Table 2-8, and the fertilizer SCCs are listed in Table 2-9.

Table 2-8. Livestock SCCs extracted from the 2002 NEI to create the ag sector

SCC	SCC Description*
2805000000	Agriculture - Livestock;Total
2805001100	Beef cattle - finishing operations on feedlots (drylots);Confinement
2805001200	Beef cattle - finishing operations on feedlots (drylots);Manure handling and storage
2805001300	Beef cattle - finishing operations on feedlots (drylots);Land application of manure
2805002000	Beef cattle production composite;Not Elsewhere Classified
2805003100	Beef cattle - finishing operations on pasture/range;Confinement
2805007100	Poultry production - layers with dry manure management systems;Confinement
2805007300	Poultry production - layers with dry manure management systems;Land application of manure
2805008100	Poultry production - layers with wet manure management systems;Confinement
2805008200	Poultry production - layers with wet manure management systems;Manure handling and storage
2805008300	Poultry production - layers with wet manure management systems;Land application of manure
2805009100	Poultry production - broilers;Confinement
2805009200	Poultry production - broilers;Manure handling and storage
2805009300	Poultry production - broilers;Land application of manure
2805010100	Poultry production - turkeys;Confinement
2805010200	Poultry production - turkeys;Manure handling and storage
2805010300	Poultry production - turkeys;Land application of manure
2805018000	Dairy cattle composite;Not Elsewhere Classified
2805019100	Dairy cattle - flush dairy;Confinement
2805019200	Dairy cattle - flush dairy;Manure handling and storage
2805019300	Dairy cattle - flush dairy;Land application of manure
2805020001	Cattle and Calves Waste Emissions;Milk Cows
2805020002	Cattle and Calves Waste Emissions;Beef Cows
2805020003	Cattle and Calves Waste Emissions;Heifers and Heifer Calves
2805020004	Cattle and Calves Waste Emissions;Steers, Steer Calves, Bulls, and Bull Calves
2805021100	Dairy cattle - scrape dairy;Confinement
2805021200	Dairy cattle - scrape dairy;Manure handling and storage
2805021300	Dairy cattle - scrape dairy;Land application of manure
2805022100	Dairy cattle - deep pit dairy;Confinement
2805022200	Dairy cattle - deep pit dairy;Manure handling and storage
2805022300	Dairy cattle - deep pit dairy;Land application of manure
2805023100	Dairy cattle - drylot/pasture dairy;Confinement
2805023200	Dairy cattle - drylot/pasture dairy;Manure handling and storage
2805023300	Dairy cattle - drylot/pasture dairy;Land application of manure
2805025000	Swine production composite;Not Elsewhere Classified (see also 28-05-039, -047, -053)
2805030000	Poultry Waste Emissions;Not Elsewhere Classified (see also 28-05-007, -008, -009)
2805030001	Poultry Waste Emissions;Pullet Chicks and Pullets less than 13 weeks old
2805030002	Poultry Waste Emissions;Pullets 13 weeks old and older but less than 20 weeks old
2805030003	Poultry Waste Emissions;Layers
2805030004	Poultry Waste Emissions;Broilers
2805030007	Poultry Waste Emissions;Ducks
2805030008	Poultry Waste Emissions;Geese
2805030009	Poultry Waste Emissions;Turkeys
2805035000	Horses and Ponies Waste Emissions;Not Elsewhere Classified

SCC	SCC Description*
2805039100	Swine production - operations with lagoons (unspecified animal age);Confinement
2805039200	Swine production - operations with lagoons (unspecified animal age);Manure handling and storage
2805039300	Swine production - operations with lagoons (unspecified animal age);Land application of manure
2805040000	Sheep and Lambs Waste Emissions;Total
2805045000	Goats Waste Emissions;Not Elsewhere Classified
2805045002	Goats Waste Emissions;Angora Goats
2805045003	Goats Waste Emissions;Milk Goats
2805047100	Swine production - deep-pit house operations (unspecified animal age);Confinement
2805047300	Swine production - deep-pit house operations (unspecified animal age);Land application of manure
2805053100	Swine production - outdoor operations (unspecified animal age);Confinement

* All SCC Descriptions begin "Miscellaneous Area Sources;Agriculture Production – Livestock"

The "ag" sector includes all of the NH₃ emissions from fertilizer from the NEI. However, the "ag" sector does not include all of the livestock ammonia emissions, as there are also significant NH₃ emissions from livestock in the point source inventory that we retained from the 2002 NEI. Note that in these cases, emissions were not also in the nonpoint inventory for counties for which they were in the point source inventory; therefore no double counting occurred. Most of the point source livestock NH₃ emissions were reported by the states of Kansas and Minnesota. For these two states, farms with animal operations were provided as point sources using the following SCCs⁵:

- 30202001: Industrial Processes; Food and Agriculture; Beef Cattle Feedlots; Feedlots General
- 30202101: Industrial Processes; Food and Agriculture; Eggs and Poultry Production; Manure Handling: Dry
- 30203099: Industrial Processes; Food and Agriculture; Dairy Products; Other Not Classified

There are also livestock NH₃ emissions in the point source inventory with SCCs of 39999999 (Industrial Processes; Miscellaneous Manufacturing Industries; Miscellaneous Industrial Processes; Other Not Classified) and 30288801 (Industrial Processes; Food and Agriculture; Fugitive Emissions; Specify in Comments Field). We identified these sources as livestock NH₃ point sources based on their facility name. The reason why we needed to identify livestock NH₃ in the ptnonipm sector was to properly implement the emission projection techniques for livestock sources, which cover all livestock sources, not only those in the ag sector, but also those in the ptnonipm sector.

⁵ These point source emissions are also identified by the segment ID, which is one of the following: "SWINE", "CATTLE", "DAIRY", or "PLTRY".

Table 2-9. Fertilizer SCCs extracted from the 2002 NEI for inclusion in the “ag” sector

2002 SCC	2002 SCC Description*
2801700001	Anhydrous Ammonia
2801700002	Aqueous Ammonia
2801700003	Nitrogen Solutions
2801700004	Urea
2801700005	Ammonium Nitrate
2801700006	Ammonium Sulfate
2801700007	Ammonium Thiosulfate
2801700010	N-P-K (multi-grade nutrient fertilizers)
2801700011	Calcium Ammonium Nitrate
2801700012	Potassium Nitrate
2801700013	Diammonium Phosphate
2801700014	Monoammonium Phosphate
2801700015	Liquid Ammonium Polyphosphate
2801700099	Miscellaneous Fertilizers

* All descriptions include “Miscellaneous Area Sources; Agriculture Production – Crops; Fertilizer Application” as the beginning of the description.

2.2.3 Other nonpoint sources (nonpt)

Nonpoint sources that were not subdivided into the afdust, ag, or avefire sectors were assigned to the “nonpt” sector.

The 2002 platform documentation describes the creation of the 2002 nonpt sector in great detail, but the rest of this section will simply document what has changed for the 2005v4.1 platform. Below is a list of changes made from the 2002 platform both for the v4 platform and for the v4.1 platform. Details on the changes to 2002 for the version 4 platform are in the v4 documentation.

Updates to the nonpt sector from 2002 platform made for creation of the nonpt sector of the 2005v4 platform

- The 2005 platform replaces 2002v3 NEI non-California Western Regional Air Partnership (WRAP) oil and gas emissions (SCCs beginning with “23100”) with WRAP year 2005 Phase II oil and gas emissions.
- Residential wood combustion (RWC) emissions were replaced with data for Oregon and New York. This update is consistent with the 2005 NEIv2 NEI.
- RWC VOC emissions were recalculated for all states except California to reflect an updated emissions factor for VOC from RWC sources. This update is consistent with the 2005 NEIv2 NEI.
- We utilized benzene, formaldehyde, acetaldehyde and methanol (BAFM) emissions from sources that met the HAP-CAP integration criteria discussed in Section 3.1.2.1 (i.e., the “integrate” sources). We removed BAFM from sources that did not meet the integration criteria (i.e., the “no-integrate” sources) so that BAFM would not be double counted with the BAFM generated via speciation of VOC.

Updates from 2005v4 platform used in creating the 2005v4.1 platform

- We changed the integration status for pesticide emissions from using the “integrate” case to using the “no-integrate” case. The main reason is that there were significant benzene emissions from this category in the NEI that was considered incorrect. The NEI benzene came from solvent utilization data (Fredonia) for "other markets" for the year 1998. Since benzene no longer allowed in pesticides, we chose to eliminate the use of these HAP data and use a VOC speciation profile that did not include benzene emissions to be more consistent with the changed regulations.
- We added oil and gas emissions for Texas and replaced oil and gas emissions with updated 2005 data from Oklahoma.

TCEQ Oil and Gas Emissions

The Texas Commission on Environmental Quality (TCEQ) provided 2005 oil and gas emissions which we added to the nonpt sector. The emissions were for a single SCC: 2310000220 Industrial Processes; Oil and Gas Exploration and Production; All Processes; Drill Rigs. The TCEQ indicated that these should replace emissions in the nonroad inventory from the NONROAD model (drill rigs: SCC=2270010010). Because the nonroad emissions are significantly less than the updated nonpt emissions, we did not remove the nonroad emissions. Both the TCEQ and related nonroad emissions from the 2005 NEI are summarized in Table 2-10.

Table 2-10. Additional TCEQ oil and gas emissions added to the 2005v2 NEI

Pollutant	TCEQ Emissions 2005, added to nonpt (tons/yr)	NEI 2005 Emissions (nonroad inventory), not subtracted (tons/yr)
CO	15,878	1,396
NH ₃		3
NO _x	42,854	4,704
PM ₁₀	3,036	275
PM _{2.5}	2,945	267
SO ₂	5,977	573
VOC	4,337	340

Oklahoma Oil and Gas Emissions

The state of Oklahoma provided and emissions replacement for their 2005 oil and gas sector emissions. These data added emissions for the SCCs shown in Table 2-11.

Table 2-11. SCCs provided with Oklahoma oil and gas sector emissions

SCC	SCC Description
31000103	Crude Oil Production;Wells: Rod Pumps*
31000122	Crude Oil Production;Drilling and Well Completion*
31000203	Natural Gas Production;Compressors*
31000215	Natural Gas Production;Flares Combusting Gases >1000 BTU/scf*
31000222	Natural Gas Production;Drilling and Well Completion*
31000227	Gas Production;Glycol Dehydrator Reboiler Still Stack*
31000228	Natural Gas Production;Glycol Dehydrator Reboiler Burner*
31000403	Industrial Processes;Oil and Gas Production;Process Heaters;Crude Oil
31000404	Industrial Processes;Oil and Gas Production;Process Heaters;Natural Gas
31088811	Industrial Processes;Oil and Gas Production;Fugitive Emissions;Fugitive Emissions

*These SCC descriptions start with the preface "Industrial Processes;Oil and Gas Production"

In addition, this update removed emissions for SCC 2310000000, which is "Industrial Processes;Oil and Gas Production: SIC 13;All Processes;Total: All Processes."

The resultant Oklahoma emissions are shown below in Table 2-12. Note that Oklahoma instructed that PM₁₀ emissions were size PM_{2.5}, and therefore no coarse PM (PMC) are generated and PM₁₀ is the same as PM_{2.5}

Table 2-12. Changes to Oklahoma oil and gas emissions

Pollutant	2005 Oklahoma Oil and gas emissions 2005, removed from nonpt (tons/yr)	2005 Oklahoma Oil and gas emissions, added to nonpt (tons/yr)
CO	11,251	32,821
VOC	104,193	155,908
NO _x	66,480	39,668
SO ₂	0	1,014
PM ₁₀ = PM _{2.5}	0	1,918

2.3 Fires (avefire)

This sector is unchanged from the 2005v4 platform; the documentation is repeated here for completeness.

The purpose of the avefire sector is to represent emissions for a typical year's fires for use in projection year inventories, since the location and degree of future year fires are not known. This approach keeps the fires information constant between the 2005 base case and future-year cases to eliminate large and uncertain differences between those cases that would be caused by changing the fires. Using an average of multiple years of data reduces the possibility that a single-year's high or low fire activity would unduly affect future year model-predicted concentrations.

The avefire sector contains wildfire and prescribed burning emissions. It excludes agricultural burning and other open burning sources, which are included in the nonpt sector. Generally, their year-to-year impacts are not as variable as wildfires and non-agricultural prescribed/managed burns.

We use this sector for the 2005 base case, and all future year cases. Emissions are annual and county-level. The same emissions are used in the v4 and v4.1 versions of the 2005-based platform.

We created the average-fires inventory based on the 2001 (1999 NEI-based) fire emissions data. The average fire sector is comprised of a 1996-2002 average fire inventory for wildfires and prescribed burning. We calculated the average wildfire and prescribed burning inventories using the following formula for all pollutants:

$$average\ fire = 2001\ fire \times \frac{average\ acres\ burned}{2001\ acres\ burned}$$

The average acres-burned was calculated base on 1996 through 2002 data; therefore, the average fire inventory represent average fires from 1996 through 2002, with the assumption of 2001 emissions rates and a spatial distribution of emissions to counties based on fires from 2001. This approach is the same as that used for our previous emissions modeling platforms used to model 2001 and 2002 base years, with some differences described here.

The 2005 platform avefire sector differs from the avefire sector in the 2002 platform in the following ways:

- a. We recomputed VOC as a function of CO: $VOC = CO * 0.229$ at the suggestion of EPA fire inventory expert who reviewed the VOC emissions and found them too high (Tom Pace, personal communication).
- b. We created HAP emissions records by applying emission ratios to $PM_{2.5}$.

Table 2-13 provides the VOC differences between the 2002 and 2005 platforms for each of the types of fires in the avefire sector. Emissions for CO and $PM_{2.5}$ are unchanged and are provided for reference.

Table 2-13. Average fire VOC changes from 2002 to 2005 platform.

SCC	SCC Description *	2002 VOC (tons/yr)	2005 VOC (tons/yr)	CO (tons/yr)	$PM_{2.5}$ (tons/yr)
2810001000	Forest Wildfires;Total	386,997	1,883,230	8,223,736	685,783
2810005000	Managed Burning, Slash (Logging Debris);Total	67,664	105,661	461,404	7,460
2810015000	Prescribed Burning for Forest Management;Total	84,784	399,880	1,746,208	147,298

* all SCC descriptions begin with "Miscellaneous Area Sources; Other Combustion"

The 2005 HAP emissions records were created by multiplying PM_{2.5} emissions by the emission factors in Table 2-14. The HAP factors are the same for all source types. Because we chose not to integrate criteria and HAP VOCs for the avefire sector, the HAPs contained in the avefire inventory were not used to generate air quality modeling inputs for the 2005 platform.

Table 2-14. HAP emission factors applied to avefire PM_{2.5} emissions

Pollutant Description	CAS	PM_{2.5} factor
1,3-butadiene	106990	0.0147
1-Methylpyrene	2381217	0.00033
Acetaldehyde	75070	0.0148
Acrolein	107028	0.0154
Antracene	120127	0.00018
Benz[a]Anthracene	56553	0.00022
Benzene	71432	0.041
Benzo(a)fluoranthene	203338	0.00009
Benzo(c)phenanthrene	195197	0.00014
Benzo[a]Pyrene	50328	0.00005
Benzo[e]Pyrene	192972	0.0001
Benzo[g,h,i]Perylene	191242	0.00018
Benzo[k]Fluoranthene	207089	0.00009
Carbonyl sulfide	463581	0.00002
Chrysene	218019	0.00022
Fluoranthene	206440	0.00024
Formaldehyde	50000	0.0936
Hexane	110543	0.00059
Indeno[1,2,3-c,d]Pyrene	193395	0.00012
Methyl chloride	74873	0.00464
Methylantracene	26914181	0.0003
Methylbenzopyrene	65357699	0.00011
Methylchrysene	41637905	0.00029
O-xylene	95476	0.001932554
M-xylene	108383	0.005392065
P-xylene	106423	0.00145538
Perylene	198550	0.00003
Phenanthrene	85018	0.00018
Pyrene	129000	0.00034
Toluene	108883	0.0206

2.4 Biogenic sources (biog)

This sector is unchanged from the 2005v4 platform; the documentation is repeated here for completeness.

The biogenic emissions were computed based on 2005 meteorology data using the BEIS3.14 model within SMOKE. The 2002 platform used the BEIS3.13 model; otherwise, all underlying land use data and parameters are unchanged for the 2005 platform.

The BEIS3.14 model creates gridded, hourly, model-species emissions from vegetation and soils. It estimates CO, VOC, and NO_x emissions for the U.S., Mexico, and Canada. The BEIS3.14 model is described further in:

http://www.cmascenter.org/conference/2008/slides/pouliot_tale_two_cmas08.ppt

The inputs to BEIS include:

- Temperature data at 2 meters which were obtained from the CMAQ meteorological input files,
- Land-use data from the Biogenic Emissions Landuse Database, version 3 (BELD3). BELD3 data provides data on the 230 vegetation classes at 1-km resolution over most of North America, which is the same land-use data were used for the 2002 platform.

2.5 2005 Mobile sources (on_noadj, on_moves_runpm, on_moves_startpm, nonroad, alm_no_c3, seca_c3)

For the 2005 platform, as indicated in Table 2-2, we separated the 2005 onroad emissions into three sectors: (1) “on_moves_startpm”; (2) “on_moves_runpm”; and (3) “on_noadj”. The aircraft, locomotive, and commercial marine emissions are divided into two nonroad sectors: “alm_no_c3” and “seca_c3”, and as previously mentioned, the aircraft emissions are in the non-EGU (ptnonipm) point inventory.

The major changes between v4.1 and v4 versions of the 2005-based platform are that (1) we used a final version of MOVES, MOVES2010, rather than a draft version of MOVES; (2) we used the MOVES emissions for all vehicle types and modes (as opposed to non-motorcycle gasoline exhaust vehicles only); (3) MOVES2010 emissions cover all criteria pollutants and criteria pollutant precursors (as opposed to only exhaust mode PM_{2.5}, VOC, NO_x and CO); (4) we used NH₃ from MOVES for California (as opposed to NH₃ from NMIM) since California-supplied emissions in the 2005v2 NEI do not include NH₃. It should also be noted that the exhaust PM_{2.5} from diesel vehicles, which had previously come from NMIM but in v4.1 come from MOVES, are not impacted by cold temperatures. In addition, PM brake wear and tire wear mode emissions are now provided in MOVES in v4.1; these emissions for both gasoline and diesel vehicles are also not impacted by cold temperatures.

The onroad emissions were primarily based on the 12/21/2009 version of the Motor Vehicle Emissions Simulator (MOVES2010) (<http://www.epa.gov/otaq/models/moves/>). MOVES was

run with a state/month aggregation using county-average fuels for each state, state/month-average temperatures, and national default vehicle age distributions. 2005 VMT, consistent with the 2005v2 NEI, were used.

Table 2-15 lists the pollutants in the onroad sector based on MOVES2010 versus NMIM. A full list of the NMIM HAPs (most of which are not used in the v4.1 platform) is provided in Appendix C.

Table 2-15. Pollutants covered by MOVES2010 as used in the 2005v4.1 platform¹

Used in the 2005v4.1 platform from MOVES2010	Available from MOVES2010, but not used in the 2005v4.1 platform	Used in the 2005v4.1 platform from NMIM
PM _{2.5} ; exhaust, partially speciated ²	Naphthalene	Elemental mercury
PM _{2.5} , brake and tirewear, unspiciated	1,3 butadiene	Divalent gaseous mercury
VOC; except refueling	Acrolein	Particulate Mercury
CO, NO _x , SO ₂ , NH ₃		
Benzene; except refueling		
Formaldehyde		
Acetaldehyde		

¹ MOVES data were not used for any California onroad emissions other than NH₃

² Exhaust mode PM_{2.5} species from MOVES consist of: PEC, PSO₄ and the difference between PM_{2.5} and PEC (named as “PM25OC”). Procedures to produce the species needed are provided in Appendix D. Diesel partially speciated emissions are not impacted by cold temperatures and do not need to be adjusted by gridded temperature as do the gasoline exhaust particulate emissions. Brake wear and tire wear PM_{2.5} emissions were not pre-speciated.

Similar to the v4 platform, we used the MOVES data to create emissions by state and month (and SCC) and then allocated to counties based on 2005 NMIM-based county-level data. The reason for using the state resolution was due to (a) run time issues that made a county run for the entire nation infeasible in the timeframe required and (b) incomplete efforts to create a national database of county-specific inputs to MOVES. The emissions that did not come from the MOVES model were obtained from the 2005 NMIM runs, which are consistent with the 2005v2 NEI.

The 2005v2 NEI does not contain the MOVES data that we use for the 2005 platform. Instead, it contains onroad and nonroad mobile emissions that we generated using NMIM (EPA, 2005b) for all of the U.S. except for California.⁶ The NMIM data was used for the mercury emissions, to allocate California-submitted data to road types, to allocate the state-month-SCC MOVES data to counties, and for some of the nonroad mobile sources. NMIM relies on calculations from the MOBILE6 and NONROAD2005 models as described below, and in the NEI documentation. Inputs to NMIM are posted with the 2005 Emission Inventory. The direct link is: ftp://ftp.epa.gov/EmisInventory/2005_nei/mobile_sector/ncd/ncd20080522.zip.

⁶ Although OTAQ generated emissions using NMIM for California, these were not used in the 2005 NEI version 2, but rather were replaced by state-submitted emissions. Since California did not submit NH₃, values from MOVES were used.

NMIM creates the onroad and nonroad emissions on a month-specific basis that accounts for temperature, fuel types, and other variables that vary by month. Inventory documentation for the 2005v2 NEI onroad and nonroad sectors is also posted with other 2005 NEI documentation; the direct link is:

ftp://ftp.epa.gov/EmisInventory/2005_nei/mobile/2005_mobile_nei_version_2_report.pdf

The residual fuel commercial marine vessel (CMV), also referred to as Category 3 (C3) from the 2002 platform have been replaced with a new set of approximately 4-km resolution point source format emissions; these were modeled separately as point sources in the “seca_c3” sector for the 2005 platform. They were updated for v4.1 by using revised 2005 emissions from the category 3 commercial marine sector to reflect the final projections from 2002 developed for the category 3 commercial marine Emissions Control Area (ECA) proposal to the International Maritime Organization (EPA-420-F-10-041, August 2010). Unlike for the v4 platform, we projected Canada as part of the ECA, using region-specific growth rates; thus the v4.1 seca_c3 inventories contain Canadian province codes for near shore emissions.

The nonroad sector, based on NMIM did not change for the v4.1 platform other than for California, for which missing PM_{2.5} emissions for 7 counties was discovered. We corrected these PM_{2.5} emissions by using an earlier version of the 2005 submittal which California had provided values for the 7 counties.

The mobile sectors are compiled at a county and SCC resolution, with the exception of the seca_c3 sector that uses point sources to map the pre-gridded data to the modeling domain. Similar to v4, in v4.1, tribal data from the alm_no_c3 sector have been dropped because we do not have spatial surrogate data, and the emissions are small; these data were removed from the SMOKE input inventories for 2005.

Most mobile sectors use the HAP portion on the inventory to provide benzene, acetaldehyde, formaldehyde and/or methanol to the modeling inputs through HAP VOC “integration”, as described in Section 3.1.2.1. A few categories of nonroad sources (CNG and LPG-fueled equipment) do not have the BAFM pollutants in the inventory and therefore utilize the “no-integrate”, “no-hap-use” case, which means VOC from these sources is speciated to provide BAFM.

2.5.1 Onroad mobile MOVES cold-start exhaust sources requiring temperature adjustments (on_moves_startpm)

This sector contains MOVES2010 emissions for PM and naphthalene⁷ for non-California onroad gasoline cold-start exhaust. These emissions (and the on_moves_runpm sector discussed in the next section) are processed separately from the remainder of the onroad mobile emissions because they are subject to hourly temperature adjustments, and these temperature adjustments are different for cold-start and running exhaust modes.

⁷ Naphthalene is not used in the 2005v4 CAP-BAFM platform, but it is contained in the MOVES emissions.

Temperature adjustments were applied to account for the strong sensitivity of PM and naphthalene exhaust emissions to temperatures below 72°F. Because it was not feasible to run MOVES directly for all of the gridded, hourly temperatures needed for modeling, we created emissions of PM and naphthalene exhaust at 72°F and applied temperature adjustments after the emissions were spatially and temporally allocated. The PM_{2.5} (and naphthalene) adjustment factors were different for starting and running exhaust because these two processes respond differently to temperature as shown in Figure 2-1 which shows how these emissions increase with colder temperatures. The temperature adjustment factor in this figure is defined in terms of primary elemental carbon (PEC) as follows:

$$PEC = Adjustment\ Factor \times PEC_{72}$$

Where:

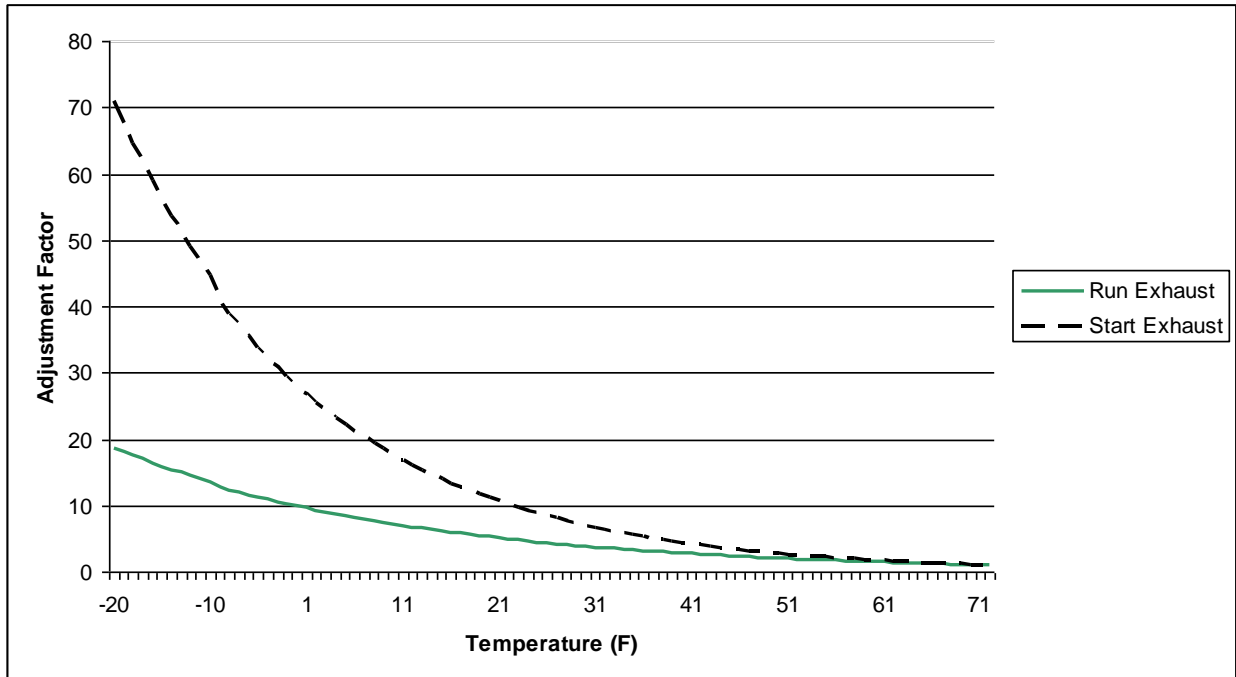
PEC = PEC at Temperatures below 72°F

PEC₇₂ = PEC at 72°F or higher

As seen in the figure, start exhaust emissions increase more than running exhaust emissions as temperatures decrease from 72°F.

Figure 2-1 also shows that the actual adjustments are different for start exhaust and running exhaust emissions. The method for applying these adjustments was the same for both start and running exhaust sectors: They were applied to SMOKE gridded, hourly intermediate files, based upon the gridded hourly temperature data (these same data are also input to the air quality model). One result of this approach is that inventory summaries based on the raw SMOKE inputs for the on_moves_startpm and on_moves_runpm sectors will not be valid because they will not include the temperature adjustments. As a result, the post-processing for temperature adjustments included computing the emissions totals at state, county, and month resolution to use for summaries.

Figure 2-1. MOVES exhaust temperature adjustment functions.



The MOVES output data required pre-processing to develop county-level monthly ORL files for input to SMOKE. As stated earlier, the resolution of the MOVES data was state-SCC totals, and the state level data were allocated to county level prior to input into SMOKE. An additional pre-processing step was for the exhaust $PM_{2.5}$, for which emissions from MOVES were partially speciated. To retain the speciated elemental carbon and sulfate emissions from MOVES, the speciation step that is usually done in SMOKE was performed prior to SMOKE, and it was modified to allow the temperature adjustments to be applied to only the species affected by temperature as described in the list below. Finally, because the start exhaust emissions were broken out separately from running exhaust emissions, they were assigned to new SCCs (urban and rural parking areas) that allowed for the appropriate spatial and temporal profiles to be applied in SMOKE.

A list of the procedures performed to prepare the MOVES data for input into SMOKE is provided here.

- i. We allocated state-level emissions to counties using state-county emission ratios by SCC, pollutant, month, and emissions mode (e.g., evaporative, exhaust, brake wear, and tire wear) for each month. The ratios were computed using NMIM 2005 data (same data included in the 2005v2 NEI).
- ii. We assigned these start exhaust emissions to urban and rural SCCs based on the county-level ratio of emissions from urban versus rural local roads from the NMIM onroad gasoline exhaust mode data. For example, we split light duty gasoline vehicle (LDGV) start emissions in the state-total MOVES data (assigned SCC 2201001000) into urban (2201001370) and rural (2201001350) based on the ratio of LDGV urban (2201001330) and rural (2201001210) local roads.

- iii. We converted MOVES-based PM_{2.5} species at 72°F to SMOKE-ready PM species. The SMOKE-ready species are listed below and the speciation technique used to obtain the SMOKE-ready species is further discussed in Appendix D.
- NAPHTH_72: unchanged from MOVES-based file, subject to temperature adjustment below 72°F.
 - PEC_72: unchanged from MOVES-based PM25EC, subject to temperature adjustment below 72°F.
 - POC_72: modified MOVES-based PM25OC to remove metals, PNO3 (computed from MOVES-based PM25EC), NH₄ (computed from MOVES-based PM25SO₄ and PNO3), and MOVES-based PM25SO₄. Subject to temperature adjustment below 72°F.
 - PSO4: unchanged from MOVES-based PM25SO₄, not subject to temperature adjustment.
 - PNO3: computed from MOVES-based PM25EC, not subject to temperature adjustment.
 - OTHER: sum of computed metals (fraction of MOVES-based PM25EC) and NH₄ (computed from PNO3 and PSO4), not subject to temperature adjustment.
 - PMFINE_72: Computed from OTHER and fraction of POC_72. Subject to temperature adjustment below 72 °F.
 - PMC_72: Computed as fraction of sum of PMFINE_72, PEC_72, POC_72, PSO4, and PNO3 –described in Appendix D. Subject to temperature adjustment below 72 °F.

The result of these preprocessing steps is SMOKE-ready PM emissions that do not exactly match what MOVES provides. The emissions are conserved during allocation from the state to county and from the generic total “start” SCCs to the two new parking SCCs that end in “350” and “370”. PEC and PSO4 components of PM_{2.5} emissions are also conserved as they are simply renamed from the MOVES species “PM25EC” and “PM25SO₄”. However, as seen above, POC, PNO3, and PMFINE components involve multiplying the MOVES PM species by components of an onroad gasoline exhaust speciation profile described in Appendix D.

2.5.2 Onroad mobile MOVES running exhaust sources requiring temperature adjustments (on_moves_runpm)

This sector is identical to the on_moves_startpm sector discussed in Section 2.5.1, but contains running exhaust emissions instead of cold-start exhaust emissions. The same pollutants are in this sector, and allocation from the MOVES state-level to county-level inventory is a simple match by SCC and month to NMIM state-county ratios. The only reason this sector is separated from on_moves_startpm is because the temperature adjustments are less extreme for these running emissions at colder temperatures when compared to the curve for cold-start emissions (Figure 2-1).

2.5.3 Onroad no-adjustments mobile sources (on_noadj)

This sector consists of the bulk of the onroad mobile emissions, which are not covered by the on_moves_startpm and on_moves_runpm sectors. These emissions did not receive any temperature adjustments in our processing. There are four sources of data that are pre-processed to create three sets of monthly inventories for this sector.

1. MOVES-based onroad gasoline and diesel: These are the monthly (does not include gasoline exhaust mode PM and naphthalene) MOVES-based emissions from three MOVES inventories:
 - a. Gasoline Exhaust: VOC, NO_x, CO, SO₂, NH₃, 1,3-butadiene (106990), acetaldehyde (75070), acrolein (107028), benzene (71432), formaldehyde (50000), and brake and tire wear PM_{2.5};
 - b. Diesel Exhaust: Partially-speciated PM_{2.5} (that were fully speciated prior to input into SMOKE (via Appendix D), VOC, NO_x, CO, SO₂, NH₃, 1,3-butadiene (106990), acetaldehyde (75070), acrolein (107028), benzene (71432), formaldehyde (50000), and brake and tire wear PM_{2.5}. Because diesel exhaust PM does not require the same intermediate temperature adjustments as gasoline exhaust PM, diesel exhaust PM can therefore be processed with the remaining onroad mobile emissions.
 - c. Evaporative: Non-refueling VOC, benzene, and naphthalene (91203).

For the pollutants listed, these non-California MOVES emissions encompass the same sources as the on_moves_startpm and on_moves_runpm sectors: light duty gasoline vehicles, light duty gasoline trucks (1 & 2), and heavy duty gasoline vehicles, but they do not require the same intermediate temperature adjustments and can therefore be processed with the remaining onroad mobile emissions. These emissions contain both running and parking sources and are pre-processed from state-level to county-level much like the on_moves_startpm and on_moves_runpm sectors already discussed. The preprocessing for the non-PM emissions did not require species calculations because the raw MOVES emissions translated directly to SMOKE inventory species.

2. California onroad inventory: California 2005v2 NEI complete CAP/HAP onroad inventory. California monthly onroad emissions are year 2005 and are based on September 2007 California Air Resources Board (CARB) data from Chris Nguyen. NH₃ emissions are from MOVES2010 runs for California. We retained only those HAPs that are also estimated by NMIM for onroad mobile sources; all other HAPs provided by California were dropped. The California onroad inventory does not use the SCCs for Heavy Duty Diesel Vehicles (HDDV) class 6 & 7 (2230073XXX) emissions. California does not specify road types, so we used NMIM-based California ratios to break out vehicle emissions to the match the more detailed NMIM level.
3. Remaining NMIM-based onroad inventory: The remainder of the non-California onroad inventory that was not replaced by MOVES. This includes monthly emissions the three species of mercury (divalent gas, elemental and particulate) as well as a number of other HAPs not used by the platform. The NMIM county database is NCD20080522; this is an update of NCD20070912 in which state/local and tribal inputs replace EPA default inputs

where provided. These emissions are identical to those in the v4 platform and are not described further here.

2.5.4 Nonroad mobile sources – NMIM-based nonroad (nonroad)

This sector includes monthly exhaust, evaporative and refueling emissions from nonroad engines (not including commercial marine, aircraft, and locomotives) derived from NMIM for all states except California, which were corrected due to an inadvertent omission of PM_{2.5} from 7 counties. Thus, except for California, emissions from this sector did not change between the v4 and v4.1 platform versions, and we repeat the documentation here for completeness.

The NMIM relied on the version of the NONROAD2005 model (NR05c-BondBase) used for the marine spark ignited (SI) and small SI engine proposed rule, published May 18, 2007 (EPA, 2007c). For 2005, the NONROAD2005 model (NR05c-BondBase) is equivalent to NONROAD2008a, since it incorporated Bond rule revisions to some of the base case inputs and the Bond rule controls did not take effect until future years. As with the onroad emissions, NMIM provides nonroad emissions for VOC by three emission modes: exhaust, evaporative and refueling. Unlike the onroad sector, refueling emissions nonroad sources are not dropped from processing for this sector.

Similar to the on_noadj pre-processing for evaporative emissions, we also reassigned NMIM evaporative and refueling xylene to the various isomers of xylene. We use the same percentages for refueling as for evaporative emissions as follows: we converted compound XYL or CAS=EVP__1330207, RFL__1330207) into MXYL (CAS=EVP__108383, RFL__108383) and OXYL (CAS=EVP__95476, RFL__95476) using a 68% and 32% ratio to both evaporative and refueling XYL, respectively. We also split NMIM exhaust xylene (CAS=EXH__1330207) into MXYL (CAS=EXH__108383) and OXYL (CAS=EXH__95476) using a 74% and 26% ratio to XYL, respectively.

EPA/OTAQ ran NMIM to create county-SCC emissions for the NEI 2005v2 nonroad mobile CAP/HAP inventory, and similar to on_noadj, we removed California NMIM emissions that were submitted separately by California. Emissions were converted from monthly totals to monthly average-day based on the number of days in each month. Similar to onroad NMIM emissions, EPA default inputs were replaced by state inputs where provided. The NMIM inventory documentation describes this and all other details of the NMIM nonroad emissions development:

ftp://ftp.epa.gov/EmisInventory/2005_nei/mobile/2005_mobile_nei_version_2_report.pdf

California nonroad

California monthly nonroad emissions are year 2005 and are based on September 2007 California Air Resources Board (CARB) data from Chris Nguyen, other than for the PM_{2.5} missing from 7 counties, which used the March 2007 version. In addition, NH₃ emissions are from NMIM runs for California because these were not included in the California NEI submittal. HAP emissions were estimated by applying HAP-to-CAP ratios computed from California data in the NEI 2005 v2 submittal. We retained only those HAPs that are also estimated by NMIM for nonroad mobile sources; all other HAPs were dropped.

The CARB-based nonroad data did not have mode-specific data for VOC (exhaust, evaporative, and refueling). To address this inconsistency with other states, we split the annual total California data into monthly, mode-specific nonroad emissions for California using the NMIM results. Details on this process are documented separately (Strum, 2007). Nonroad refueling emissions for California were computed as Gasoline Transport (SCC=2505000120) emissions multiplied by a factor of 0.46 (to avoid double counting with portable fuel container (PFC) emissions in the nonpt sector) and were allocated to the gasoline equipment types based on ratios of evaporative-mode VOC. The factor of 0.46 was computed by dividing the NMIM-derived California refueling for 2005 by the sum of portable fuel container emissions and NMIM-derived refueling for 2005.

2.5.5 Nonroad mobile sources: locomotive and non-C3 commercial marine (alm_no_c3)

The alm_no_c3 sector contains CAP and HAP emissions from locomotive and commercial marine sources, except for category 3/residual-fuel (C3) commercial marine vessels and railway maintenance. In modeling platforms prior to the 2005v4 platform, this sector also contained aircraft emissions. Point-source airports were included in the non-EGU point sector (ptnonipm) through the 2005v2 NEI point source inventory. The C3 commercial marine vessel emissions are in the seca_c3 sector. We note that the “a” in the “alm_no_c3” sector name is now misleading because aircraft are no longer in this sector. This sector is unchanged from the v4 platform; we repeat the documentation for completeness.

The remaining emissions in the alm_no_c3 sector are year 2002 emissions unchanged from the 2002 platform. The SCCs in the alm_no_c3 sector are listed in Table 2-16.

Table 2-16. SCCs in the 2005 alm_no_c3 inventory compared to the 2002 platform alm sector

SCC	Action	SCC Description
2275000000	Emissions removed and replaced by aircraft in ptnonipm sector for 2005 platform	Mobile Sources; Aircraft: All Aircraft Types and Operations: Total
2275001000	Emissions removed and replaced by aircraft in ptnonipm sector for 2005 platform	Mobile Sources; Aircraft: Military Aircraft: Total
2275020000	Emissions removed and replaced by aircraft in ptnonipm sector for 2005 platform	Mobile Sources; Aircraft: Commercial Aircraft: Total: All Types
2275050000	Emissions removed and replaced by aircraft in ptnonipm sector for 2005 platform	Mobile Sources; Aircraft: General Aviation: Total
2275060000	Emissions removed and replaced by aircraft in ptnonipm sector for 2005 platform	Mobile Sources; Aircraft: Air Taxi: Total
2280002100	Retained from 2002 platform	Mobile Sources;Marine Vessels, Commercial;Diesel;Port emissions
2280002200	Retained from 2002 platform	Mobile Sources;Marine Vessels, Commercial;Diesel;Underway emissions
2280003100	Emissions removed and replaced by seca_c3 inventories for 2005 platform	Mobile Sources;Marine Vessels, Commercial;Residual;Port emissions
2280003200	Emissions removed and replaced by seca_c3 inventories for 2005 platform	Mobile Sources;Marine Vessels, Commercial;Residual;Underway emissions
2280004000	Retained from 2002 platform	Mobile Sources;Marine Vessels, Commercial;Gasoline;Total, All Vessel Types
2285002006	Retained from 2002 platform	Mobile Sources;Railroad Equipment;Diesel;Line Haul Locomotives: Class I Operations
2285002007	Retained from 2002 platform	Mobile Sources;Railroad Equipment;Diesel;Line Haul Locomotives: Class II / III Operations
2285002008	Retained from 2002 platform	Mobile Sources;Railroad Equipment;Diesel;Line Haul Locomotives: Passenger Trains (Amtrak)
2285002009	Retained from 2002 platform	Mobile Sources;Railroad Equipment;Diesel;Line Haul Locomotives: Commuter Lines
2285002010	Retained from 2002 platform	Mobile Sources;Railroad Equipment;Diesel;Yard Locomotives

The documentation of the 2002 NEI for the category 1 and 2 (C1/C2) commercial marine and locomotive emissions is available at:

<http://www.epa.gov/ttn/chief/net/2002inventory.html#documentation>

For modeling purposes, the following additional changes were made to the NEI data for the 2005 platform:

- For the 2005 platform, we removed C3 CMV SCCs (residual fuel) and aircraft SCCs.

- Removed railway maintenance emissions (SCCs 2285002015, 2285004015, and 2285006015) because these are included in the nonroad NMIM monthly inventories. This change was made for the 2002 platform and is retained here in the 2005 platform.
- For the purpose of CAP-HAP VOC integration as discussed in Section 3.1.2.1, we removed benzene, formaldehyde, and acetaldehyde for all sources that we did not integrate these HAPs with VOC. As discussed in Section 3.1.2.1, sources are considered no-integrate when the source of data between VOC and VOC HAPs is inconsistent or VOC analysis of VOC and VOC HAPs indicates the source is not integrated. Although our CAP-HAP integration approach also required the removal of methanol for no-integrate sources, the only sources in this sector that included methanol were in California, where we used the integrate approach for all sources and therefore did not need to remove it.

The 2002 platform documentation goes into greater detail on the locomotives and C1/C2 CMV emissions in this sector.

2.5.6 Nonroad mobile sources: C3 commercial marine (seca_c3)

The raw seca_c3 sector emissions data were developed in an ASCII raster format used since the Emissions Control Area-International Marine Organization (ECA-IMO) project began in 2005, then known as the Sulfur Emissions Control Area (SECA). These emissions consist of large marine diesel engines (at or above 30 liters/cylinder) that until very recently, were allowed to meet relatively modest emission requirements, often burning residual fuel. The emissions in this sector are comprised of primarily foreign-flagged ocean-going vessels, referred to as Category 3 (C3) ships. The seca_c3 (ECA) inventory includes these ships in several intra-port modes (cruising, hoteling, reduced speed zone, maneuvering, and idling) and underway mode and includes near-port auxiliary engines. An overview of the ECA-IMO project and future year goals for reduction of NO_x, SO₂, and PM C3 emissions can be found at:

<http://www.epa.gov/oms/regs/nonroad/marine/ci/420f09015.htm>

The resulting coordinated strategy, including emission standards under the Clean Air Act for new marine diesel engines with per-cylinder displacement at or above 30 liters, and the establishment of Emission Control Areas is at: <http://www.epa.gov/oms/oceanvessels.htm>

The base year ECA inventory is 2002 and consists of these CAPs: PM₁₀, CO, CO₂, NH₃, NO_x, SO_x (assumed to be SO₂), and Hydrocarbons (assumed to be VOC). EPA developed regional growth (activity-based) factors that we applied to create the v4.1 platform 2005 inventory from the 2002 data.

These region-specific and pollutant-specific growth factors were updated for the v4.1 platform as compared to the v4 platform to be consistent with the final projections from 2002, developed for the C3 ECA proposal to the International Maritime Organization (EPA-420-F-10-041, August 2010).

The updated factors that we used to project from 2002 to 2005 are presented in Table 2-17.

Table 2-17. Adjustment factors to update the 2005 seca_c3 sector emissions for the v4.1 platform.

Region	2005 Adjustments Relative to 2002					
	NO _x	PM ₁₀	PM _{2.5}	VOC (HC)	CO	SO ₂
Alaska East (AE)	1.08561	1.10440	1.10350	1.10453	1.10411	1.10438
Alaska West (AW)	1.04671	1.06382	1.06404	1.06389	1.06391	1.06386
East Coast (EC)	1.10524	1.15242	1.15383	1.15256	1.15238	1.15244
Gulf Coast (GC)	1.04056	1.08521	1.08269	1.08467	1.08536	1.08530
Hawaii East (HE)	1.09054	1.13429	1.13258	1.13352	1.13429	1.13422
Hawaii West (HW)	1.09108	1.13402	1.13289	1.13443	1.13399	1.13428
North Pacific (NP)	1.07254	1.11354	1.09817	1.11358	1.11318	1.11339
South Pacific (SP)	1.12539	1.17416	1.17257	1.17055	1.17012	1.17565
Great Lakes (GL)	1.04397	1.06264	1.06241	1.06341	1.06280	1.06251
Outside ECA	1.08654	1.13186	1.13186	1.13186	1.13186	1.13186

In addition to the updated values, near-shore Canadian emissions are now assigned to regions whereas previously Canadian sources used the “Outside ECA” factors. Canada uses North Pacific, Great Lakes and East Coast depending on where the emissions are. For example, near-shore emissions around Vancouver British Columbia are projected from 2002 using North Pacific (NP) factors rather than “Outside ECA” factors.

The raw ECA inventory started as a set of ASCII raster datasets at approximately 4-km resolution that we converted to SMOKE point-source ORL input format as described in <http://www.epa.gov/ttn/chief/conference/ei17/session6/mason.pdf>.

In summary, this paper describes how the ASCII raster dataset was converted to latitude-longitude, mapped to state/county FIPS codes that extend up to 200 nautical miles (nm) from the coast, assigned stack parameters, and how the monthly ASCII raster dataset emissions were used to create monthly temporal profiles. Counties were assigned as extending up to 200nm from the coast because of this was the distance through the Exclusive Economic Zone (EEZ), a distance that would be used to define the outer limits of ECA-IMO controls for these vessels.

The 2005 ECA-based C3 inventory also does not delineate between ports and underway (or other C3 modes such as hoteling, maneuvering, reduced-speed zone, and idling) emissions; therefore, we assigned these emissions to the broad (“total”) SCC for C3 CMV (2280003000). This has no effect on temporal allocation or speciation compared to existing profiles for underway and port C3 emissions (2280003100 and 2280003200). The C3 CMV emissions in the 2002 and 2005 platforms are shown in Table 2-18.

Table 2-18. Contiguous U.S. C3 CMV emissions in 2002 and 2005 platforms

Pollutant	2002 platform (tons/yr)	2005v4 platform (tons/yr)	2005v4.1 platform (tons/yr)
CO	28,195	53,746	54,049
NH ₃	131	0	0
NO _x	244,988	642,089	647,884
PM ₁₀	13,687	53,581	53,918
PM _{2.5}	12,620	49,294	49,541
SO ₂	150,532	417,307	420,110
VOC	7,377	22,367	44,990

For the v4.1 platform, we chose only to include some HAPs in the seca_c3 sector: benzene, formaldehyde, and acetaldehyde. We projected these HAPs using the following VOC factors:

Benzene = VOC * 9.795E-06
 Acetaldehyde = VOC * 2.286E-04
 Formaldehyde = VOC * 1.5672E-03

Because we computed HAPs directly from the CAP inventory and the calculations are therefore consistent, the entire seca_c3 sector utilizes CAP-HAP VOC integration to use the VOC HAP species directly, rather than VOC speciation profiles.

Mercury was not included due to uncertainties in the emissions.

We converted the emissions to SMOKE point source ORL format, allowing for the emissions to be allocated to modeling layers above the surface layer. We also corrected FIPS code assignments for one county in Rhode Island. All non-US emissions (i.e., in waters considered outside of the 200nm EEZ, and hence out of the U.S. territory) are simply assigned a dummy state/county FIPS code=98001. Due the huge size of these data, the CAP emissions are in one ORL file and the HAP emissions are split into 6 separate ORL files. The SMOKE-ready data have also been cropped from the original ECA-IMO data to cover only the 36-km air quality model domain, which is the largest domain used for this effort.

2.6 Emissions from Canada, Mexico and Offshore Drilling Platforms (othpt, othar, othon, othpt_hg, and othar_hg)

These sectors are unchanged from the 2005v4 platform; the documentation is included here for completeness.

The emissions from Canada, Mexico, and Offshore Drilling platforms are included as part of five sectors: othpt, othpt_hg, othar, other_hg, and othon.

The “oth” refers to the fact that these emissions are “other” than those in the 2005 NEI, and the third and fourth characters provide the SMOKE source types: “pt” for point, “ar” for “area and

nonroad mobile”, and “on” for onroad mobile. The othpt_hg and othar_hg sectors contain year 2000 Canadian speciated mercury emissions for point and area inventories. They were used with the EPA’s 2002v3 multi-pollutant platform posted at <http://www.epa.gov/ttn/chief/emch/index.html#2002> (see “CAP and HAP 2002-Based Platform, Version 3”). All other “oth” emissions are CAP-only inventories. Mexico’s emissions are unchanged from the 2002 platform with one exception –one stack diameter was updated (recomputed from stack velocity and flowrate) in the Mexico border states point inventory.

For Canada we updated the emissions from the 2002 platform, migrating the non-Hg data from year 2000 inventories to year 2006 inventories for the 2005 platform. We migrated to these 2006 Canadian emissions despite not receiving future year emissions, as we were advised by Canada that the improvement in the 2006 inventory over the 2000 inventory was more significant than the undesirable effect of retaining these 2006 emissions for all future year modeling. We applied several modifications to the 2006 Canadian inventories:

- i. We did not include wildfires, or prescribed burning because Canada does not include these inventory data in their modeling.
- ii. We did not include in-flight aircraft emissions because we do not include these for the U.S. and we do not have an appropriate approach to include in our modeling.
- iii. We applied a 75% reduction (“transport fraction”) to PM for the road dust, agricultural, and construction emissions in the Canadian “afdust” inventory. This approach is more simplistic than the county-specific approach used for the U.S., but a comparable approach was not available for Canada.
- iv. We did not include speciated VOC emissions from the ADOM chemical mechanism.
- v. Residual fuel CMV (C3) SCCs (22800030X0) were removed because these emissions are included in the seca_c3 sector, which covers not only emissions close to Canada but also emissions far at sea. Canada was involved in the inventory development of the seca_c3 sector emissions.
- vi. Wind erosion (SCC=2730100000) and cigarette smoke (SCC=2810060000) emissions were removed from the nonpoint (nonpt) inventory; these emissions are also absent from our U.S. inventory.
- vii. Quebec PM_{2.5} emissions (2,000 tons/yr) were removed for one SCC (2305070000) for Industrial Processes, Mineral Processes, Gypsum, Plaster Products due to corrupt fields after conversion to SMOKE input format. This error should be corrected in a future inventory.
- viii. Excessively high CO emissions were removed from Babine Forest Products Ltd (British Columbia SMOKE plantid=’5188’) in the point inventory. This change was made at our discretion because the value of the emissions was impossibly large.
- ix. The county part of the state/county FIPS code field in the SMOKE inputs were modified in the point inventory from “000” to “001” to enable matching to existing temporal profiles.
- x. Fixed coordinates for facility “ON105803” in the othpt_hg inventory to match those in the National Pollutant Release Inventory (NPRI) othpt sector.

- xi. Nonpoint speciated mercury emissions duplicate emissions summed and state/county FIPS code field changed from Nunavut (62) to NW Territories (61) to match surrogates.

For Mexico we continued to use emissions for 1999 (Eastern Research Group Inc., 2006) which were developed as part of a partnership between Mexico's Secretariat of the Environment and Natural Resources (Secretaría de Medio Ambiente y Recursos Naturales-SEMARNAT) and National Institute of Ecology (Instituto Nacional de Ecología-INE), the U.S. EPA, the Western Governors' Association (WGA), and the North American Commission for Environmental Cooperation (CEC). This inventory includes emissions from all states in Mexico.

The offshore emissions include point source offshore oil and gas drilling platforms. We used updated emissions from the 2005v2 NEI point source inventory. The offshore sources were provided by the Mineral Management Services (MMS).

Table 2-19 summarizes the data in the “oth” sectors and indicates where these emissions have been updated from the 2002 platform.

Table 2-19. Summary of the othpt, othpt_hg, othar, othar_hg, and othon sectors changes from the 2002 platform

Sector	Components	Changes from 2002 platform
othpt	Mexico, 1999, point	None
	Canada, 2006, point	Uses emissions from 2006 National Pollutant Release Inventory (NPRI), 3 components: <ol style="list-style-type: none"> 1) upstream oil and gas sector emissions for all CAPs except VOC; 2) VOC sources pre-speciated to CB05 speciation except for benzene; 3) Remaining point source emissions.
	Offshore, 2005, point	Uses emissions from 2005 v2 point inventory
othpt_hg	Canada, 2000, mercury point	Uses speciated mercury point source year 2000 inventory.
othar	Mexico, 1999, nonpoint	None
	Mexico, 1999, nonroad	None
	Canada, 2006, nonpoint	Uses 2006 Canadian aircraft (landing and take-offs only), agricultural NH ₃ , fugitive dust, and remaining nonpoint inventories.
	Canada, 2006, nonroad	Uses 2006 Canadian nonroad mobile, non-C3 marine, and locomotives inventories.
othar_hg	Canada, 2000, mercury nonpoint	Uses speciated mercury nonpoint source year 2000 inventory.
othon	Mexico, 1999, onroad	None
	Canada, 2006, onroad	Uses 2006 Canadian onroad inventory. Emissions are given at vehicle type resolution only (i.e., does not include road types).

2.7 SMOKE-ready non-anthropogenic inventories for mercury and chlorine

We generated elemental mercury from natural (**N**), recycled (**R**) and volcanic (**V**) emissions, which we added to anthropogenic (**A**) elemental mercury processed from the inventories discussed above, to provide the elemental mercury species “HG**NRVA**” required by the multi-pollutant version of CMAQ. This model species is intended to include the sum of elemental mercury emissions from these sources. For the ocean chlorine, we used the same data as in the CAP and HAP 2002-based platform. See <ftp://ftp.epa.gov/EmisInventory/2002v3CAPHAP/documentation> for details.

A new recycled mercury file was developed for 2005 since the scaling factors applied to temporally allocate the annual natural and recycled emissions from oceans and land are based on solar radiation and skin temperature from the 2005 meteorology files. The *annual* files (prior to temporal allocation) differed from those of the 2002 platform only in that we reduced emissions of the natural emissions from land by 90% based on literature (Gustin, et. al., 2008), which indicated that the emissions are 10-12 tons per year as opposed to the 120 tons we had been using previously.

2.7.1 Mercury

As discussed in the CAP and HAP 2002v3-based platform documentation (<ftp://ftp.epa.gov/EmisInventory/2002v3CAPHAP/documentation>), the initial data for natural mercury, provided by Atmospheric and Environmental Research, Incorporated (AER), consisted of three existing global inventories containing annual flux rates of elemental mercury, gridded to 1 degree by 1 degree resolution:

- mercury emissions from oceans—direct + recycled
- mercury emissions from land—direct + recycled
- mercury emissions from volcanoes – direct

As indicated earlier, we reduced the direct land mercury emissions by 90%, based on literature (Gustin, et. all, 2008) indicating that the emissions are 10-12 tons per year as opposed to the 120 tons we had been using previously.

Annual fluxes of recycled elemental mercury for 2001 were created using the deposition results from a CMAQ 4.5.1 run. The approaches assumed that all recycled mercury emissions are in the form of elemental mercury gas. It is necessary to treat these recycled emissions whenever a version of CMAQ is used that also treats dry deposition of elemental mercury gas. The total deposition (wet plus dry) of all forms of mercury was used as the basis for the recycled emission estimates. A fraction equal to one-half the total deposition flux was used as the estimate for recycled emissions based on previous model calibrations done by AER.

Natural and recycled emissions from oceans and land (but not volcanic emissions) were allocated to hourly values based on the meteorological variables of solar radiation and temperature, which are shown to be positively correlated with the evasion of elemental mercury from water surfaces soils and vegetation. While the correlation is widely variable for each of these surfaces, simple

scaling functions for land and ocean developed for the 2001 applications were used for the 2002 and were repeated again for the 2005v4 and v4.1 platforms, but using 2005-specific factors:

$$\text{Ocean: } \frac{SOLRAD_{hr} * (SFCTMP_{hr} - 273)}{\sum_{allhrs} [SOLRAD * (SFCTMP - 273)]} \quad \text{or exactly zero for } SFCTMP < 273 \text{ K}$$

$$\text{Land: } \frac{SOLRAD_{hr} * (SFCTMP_{hr} - 253)}{\sum_{allhrs} [SOLRAD * (SFCTMP - 253)]} \quad \text{or exactly zero for } SFCTMP < 253 \text{ K}$$

where SOLRAD is the solar radiation in W/m² and SFCTMP is the skin temperature (Kelvin), both from the 2-dimensional meteorology file from the Meteorology Chemistry Interface Processor (MCIP) output.

The same sequence of steps were performed apply the hourly gridded scaling factors to create hourly gridded files for recycled and natural mercury based on 2005 meteorological data. No changes were made to the 2002 volcano mercury data

2.7.2 Chlorine

The oceanic chlorine gas emission estimates were the same as those used in the CAP and HAP 2002 platform.

3 Emissions modeling summary

The CMAQ and CAM_X models require hourly emissions of specific gas and particle species for the horizontal and vertical grid cells contained within the modeled region (i.e., modeling domain). To provide emissions in the form and format required by the model, it is necessary to “pre-process” the “raw” emissions (i.e., emissions input to SMOKE) for the sectors described above in Section 2. In brief, this processing step transforms these emissions from their original temporal resolution, pollutant resolution, and spatial resolution into the data required by the air quality model. As seen in Section 2, the temporal resolution of the emissions input to SMOKE for the 2005 platform varies across sectors, and may be hourly, monthly, or annual total emissions. The spatial resolution, which also can be different for different sectors, may be individual point sources or county totals (province totals for Canada, municipio totals for Mexico). The pre-processing steps involving temporal allocation, spatial allocation, pollutant speciation, and vertical allocation of point sources are referred to as emissions modeling. This section provides some basic information about the tools and data files used for emissions modeling as part of the 2005 platform. Since we devoted Section 2 to describing the emissions inventories, we have limited this section’s descriptions of data to the ancillary data SMOKE uses to perform the emissions modeling steps

All SMOKE inputs for the 2005v4.1 platform emissions are available at the 2005v4.1 website (see the end of Section 1).

We used SMOKE version 2.6 to pre-process the raw emissions to create the emissions inputs for CMAQ and CAM_X. The emissions processing steps and ancillary data for v4.1 were very

similar to those done for v4. A summary of the revisions is as follows:

- We updated the ancillary files to handle additional MOVES SCCs related to parking area emissions and to make some changes to the temporal and spatial approaches that were originally assigned to parking area SCCs.
- We changed speciation profiles for headspace vapor (VOC).
- We changed the PM_{2.5} speciation profile for category 3 commercial marine vessels burning residual oil.
- We used an updated county-to-cell spatial surrogate for U.S. oil and gas emissions.
- We changed the temporal allocation approach to use profiles that vary by day of week and to use new temporal profiles for the afdust sector.

We also utilized the feature in SMOKE (updated in version 2.5) to create combination speciation profiles that could vary by state/county FIPS code and by month; we used this approach for some mobile sources as described in Section 3.1.2. As with the v4 platform, we used the CMAQ and CAM_x in-line emissions capability to create source-based emissions files rather than the 3-dimensional files for sectors that have plume rise. When CAM_x was used, the emissions were first created in a form appropriate for CMAQ, and were converted to a form usable by CMAQ using a Fortran convertor called ‘inline2camx’. In addition to generating the gridded surface level 2-dimensional emissions and elevated point source files necessary for CAM_x, the program renames certain emissions species to the names needed by CAM_x. Emissions totals by specie for the entire model domain are output as reports that are then compared to reports generated by SMOKE to ensure mass is not lost or gained during this conversion process.

3.1 Key emissions modeling settings

Each sector is processed separately through SMOKE, up until the final merge program (Mrggrid), which combines the model-ready, sector-specific emissions across sectors. The SMOKE settings in the run scripts and the data in the SMOKE ancillary files control the approaches used for the individual SMOKE programs for each sector. Table 3-1 summarizes the major processing steps of each platform sector. The “Spatial” column shows the spatial approach: “point” indicates that SMOKE maps the source from a point (i.e., latitude and longitude) location to a grid cell, “surrogates” indicates that some or all of the sources use spatial surrogates to allocate county emissions to grid cells, and “area-to-point” indicates that some of the sources use the SMOKE area-to-point feature to grid the emissions (further described in Section 3.2.1.2). The “Speciation” column indicates that all sectors use the SMOKE speciation step, though biogenics speciation is done within BEIS3 and not as a separate SMOKE step. The “Inventory resolution” column shows the inventory temporal resolution from which SMOKE needs to calculate hourly emissions.

Finally, the “plume rise” column indicates the sectors for which the in-line approach is used. These sectors are the only ones which will have emissions in aloft layers, based on plume rise. For the 2005v4 and v4.1 platforms, we did not have SMOKE compute vertical plume rise; this was done in the air quality model using stack data found in the SMOKE output files for each model-ready sector. The one sector with “in-line” only, *seca_c3*, was processed so that the entire emissions would be in aloft layers. Thus, there were no *seca_c3* emissions in the 2-dimensional,

layer-1 files created by SMOKE. Rather, the speciated and hourly source-based CMAQ and CAM_x inputs for seca_c3 were used for the vertical allocation.

Table 3-1. Key emissions modeling steps by sector.

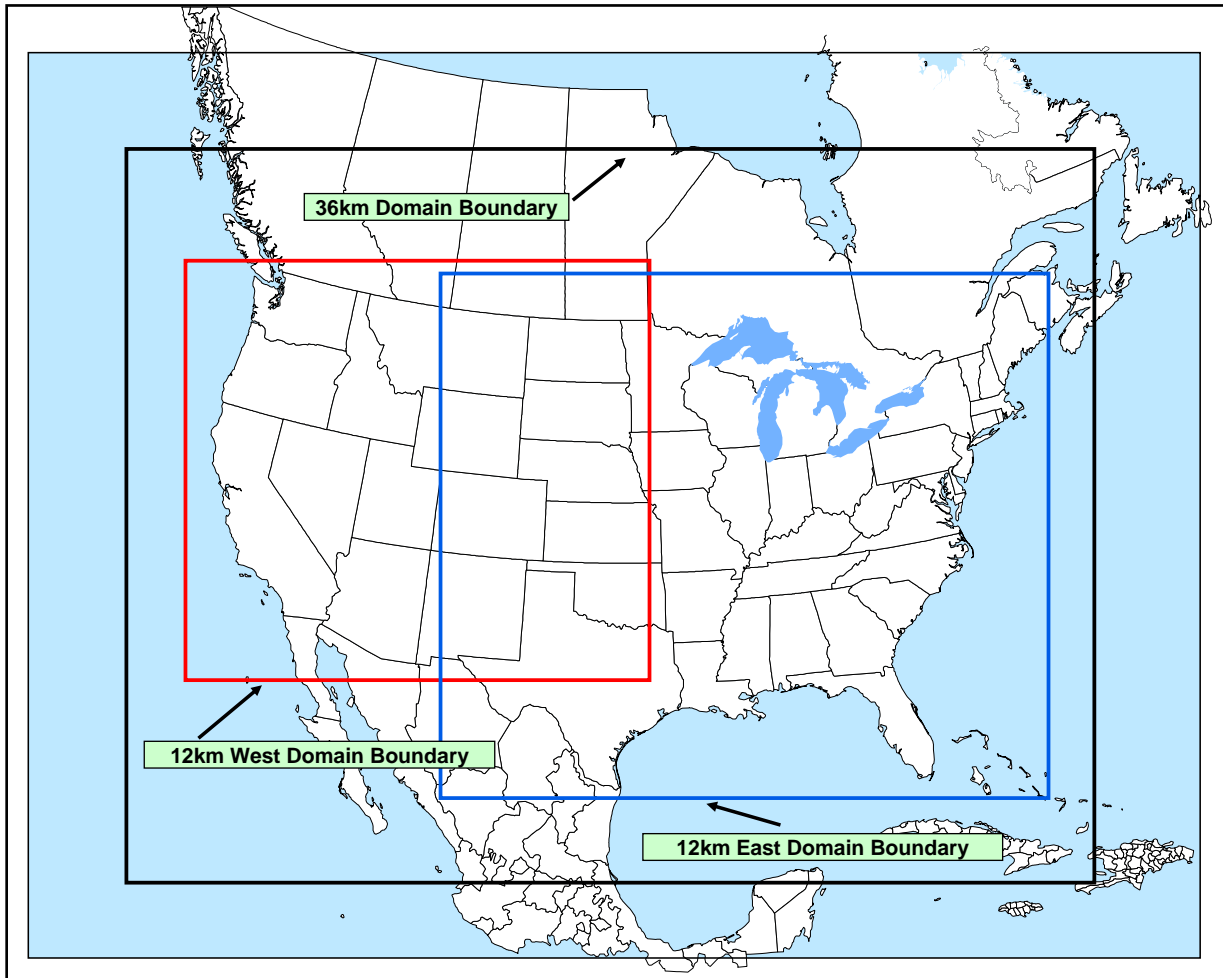
Platform sector	Spatial	Speciation	Inventory resolution	Plume rise
ptipm	point	Yes	daily & hourly	in-line
ptnonipm	point	Yes	annual	in-line
othpt	point	Yes	annual	in-line
othpt_hg	point	Yes	annual	in-line
nonroad	surrogates & area-to-point	Yes	monthly	
othar	surrogates	Yes	annual	
seca_c3	point	Yes	annual	in-line
alm_no_c3	surrogates & area-to-point	Yes	annual	
on_noadj	surrogates	Yes	monthly	
on_noadj	surrogates	Yes	monthly	
on_moves_startpm	surrogates	Yes	monthly	
on_moves_runpm	surrogates	Yes	monthly	
othon	surrogates	Yes	annual	
nonpt	surrogates & area-to-point	Yes	annual	
ag	surrogates	Yes	annual	
afdust	surrogates	Yes	annual	
biog	pre-gridded landuse	in BEIS3.14	hourly	
avefire	surrogates	Yes	annual	

In addition to the above settings, we used the PELVCONFIG file, which can be optionally used to group sources so that they would be treated as a single stack by SMOKE when computing plume rise. For the 2005v4.1 platform we chose to have no grouping, which is a difference the 2005v4 platform. We changed this because grouping done for “in-line” processing will not give identical results as “offline” (i.e., processing whereby SMOKE creates 3-dimensional files). The only way to get the same results between in-line and offline is to choose to have no grouping.

3.1.1 Spatial configuration

For the 2005v4.1 platform, we ran SMOKE and CMAQ or CAM_x (depending on the application) for modeling domains with 36-km and 12-km spatial resolution. These are the same domains as were used for the 2005v4 and 2002 platform. Figure 3-1 shows the 36-km CONTinental United States “CONUS” modeling domain, the 12-km eastern domain (EUS), and the 12-km western domain (WUS).

Figure 3-1. CMAQ modeling domains



All three grids use a Lambert-Conformal projection, with Alpha = 33°, Beta = 45° and Gamma = -97°, with a center of X = -97° and Y = 40°. Table 3-2 describes the grids for the three domains.

Table 3-2. Descriptions of the 2005-based platform grids

Common Name	Grid Cell Size	Description (see Figure 3-1)	Grid name	Parameters listed in SMOKE grid description (GRIDDESC) file: projection name, xorig, yorig, xcell, ycell, ncols, nrows, nthik
US 36 km or CONUS-36	36 km	Entire conterminous US plus some of Mexico/Canada	US36KM_148X112	'LAM_40N97W', -2736.D3, -2088.D3, 36.D3, 36.D3, 148, 112, 1
Big East 12 km	12 km	Goes west to Colorado, covers some Mexico/Canada	EUS12_279X240	'LAM_40N97W', -1008.D3, -1620.D3, 12.D3, 12.D3, 279, 240, 1
West 12 km	12 km	Goes east to Oklahoma, covers some of Mexico/Canada	US12_213X192	'LAM_40N97W', -2412.D3, -972.D3, 12.D3, 12.D3, 213, 192, 1

Section 3.2.1 provides the details on the spatial surrogates and area-to-point data used to accomplish spatial allocation with SMOKE.

3.1.2 Chemical speciation configuration

The emissions modeling step for chemical speciation creates “model species” needed by the air quality model for a specific chemical mechanism. These model species are either individual chemical compounds or groups of species, called “model species.” The chemical mechanism used for the 2005 platform is the CB05 mechanism (Yarwood, 2005). The same base chemical mechanism is used with CMAQ and CAM_x, but the implementation differs slightly between the two models. For details of the chemical mechanism as it is implemented in CAM_x, see the CAM_x 5.2 user’s guide available from <http://www.camx.com>. The specific version of CMAQ used included secondary organic aerosol (SOA) and HONO enhancements as described in http://www.cmascenter.org/help/model_docs/cmaq/4.7/RELEASE_NOTES.txt. This is unchanged from the CMAQ applications of the v4 platform.

From the perspective of emissions preparation, the CMAQ CB05 mechanism is the same as was used in the 2002 platform except that additional input model species are needed to support the nitrous acid (HONO) chemistry enhancements and additional input model species are needed to support SOA. Table 3-3 lists the model species produced by SMOKE for use in CMAQ and CAM_x; the only three input species that were not in the CAP 2002-Based platform described in 2002 “CAP-only” platform

(http://www.epa.gov/scram001/reports/Emissions%20TSD%20Vol1_02-28-08.pdf) are nitrous acid (HONO), BENZENE and sesquiterpenes (SESQ). It should be noted that the BENZENE model species is not part of CB05 in that the concentrations of BENZENE do not provide any feedback into the chemical reactions (i.e., it is not “inside” the chemical mechanism). Rather, benzene is used as a reactive tracer and as such is impacted by the CB05 chemistry. BENZENE, along with several reactive CBO5 species (such as TOL and XYL) plays a role in SOA formation in CMAQ4.7.

Table 3-3. Model species produced by SMOKE for CB05 with SOA for CMAQ4.7 and CAM_x*

Inventory Pollutant	Model Species	Model species description
CL2	CL2	Atomic gas-phase chlorine
HCL	HCL	Hydrogen Chloride (hydrochloric acid) gas
CO	CO	Carbon monoxide
NO _x	NO	Nitrogen oxide
	NO2	Nitrogen dioxide
	HONO	Nitrous acid
SO ₂	SO2	Sulfur dioxide
	SULF	Sulfuric acid vapor
NH ₃	NH3	Ammonia
VOC	ALD2	Acetaldehyde
	ALDX	Propionaldehyde and higher aldehydes
	BENZENE	Benzene (not part of CB05)
	ETH	Ethene
	ETHA	Ethane
	ETOH	Ethanol
	FORM	Formaldehyde
	IOLE	Internal olefin carbon bond (R-C=C-R)
	ISOP	Isoprene
	MEOH	Methanol
	OLE	Terminal olefin carbon bond (R-C=C)
	PAR	Paraffin carbon bond
	TOL	Toluene and other monoalkyl aromatics
XYL	Xylene and other polyalkyl aromatics	
Various additional VOC species from the biogenics model which do not map to the above model species	SESQ	Sesquiterpenes
	TERP	Terpenes
PM ₁₀	PMC	Coarse PM > 2.5 microns and ≤ 10 microns
PM _{2.5}	PEC	Particulate elemental carbon ≤ 2.5 microns
	PNO3	Particulate nitrate ≤ 2.5 microns
	POC	Particulate organic carbon (carbon only) ≤ 2.5 microns
	PSO4	Particulate Sulfate ≤ 2.5 microns
	PMFINE	Other particulate matter ≤ 2.5 microns
Sea-salt species (non –anthropogenic emissions)	PCL	Particulate chloride
	PNA	Particulate sodium
*The same species names are used for the CAM _x model with exceptions as follows:		
1. CL2 is not used in CAM _x		
2. CAM _x mercury species are HG0 (gaseous elemental), HG2 (divalent gas) and HGP (particulate mercury)		
3. CAM _x particulate sodium is NA (in CMAQ it is PNA)		

4. CAM_x uses different names for species that are both in CBO5 and SOA for the following: TOLA=TOL, XYLA=XYL, ISP=ISOP, TRP=TERP. They are duplicate species in CAM_x that are used in the SOA chemistry. CMAQ uses the same names in CBO5 and SOA for these species.
5. CAM_x uses a different name for sesquiterpenes: CMAQ SESQ = CAM_x SQT
6. CAM_x uses particulate species uses different names for organic carbon, coarse particulate matter and other particulate mass as follows: CMAQ POC = CAM_x POA, CMAQ PMC = CAM_x CPRM, and CMAQ PMFINE= CAM_x FPRM

The approach for speciating PM_{2.5} emissions in v4.1 is the same as v4 except that in addition to the on_moves_startpm and on_moves_runpm sectors, exhaust PM from diesel is provided to SMOKE as speciated emissions. Thus, the only PM species requiring speciation in SMOKE from the onroad sector are the brake and tirewear PM_{2.5}. Canada point sources have an SCC of 3999999999 and all use the Speciation profile '92037' which is the "Industry Manufacturing Avge profile." While this had not changed between v4 and v4.1, the documentation for v4 incorrectly stated that the Canadian point inventory (othpt sector) was pre-speciated. The Canadian point source inventory is pre-speciated for VOC but not for PM_{2.5}. One other difference in PM_{2.5} speciation is that we used a new profile ('92200') called "simplified profile - Marine Vessel – Main Boiler - Heavy Fuel Oil – Simplified." At the time that this profile was used, we anticipated its release with SPECIATE4.3.

The approach for speciating VOC emissions from non-biogenic sources is the same for the v4.1 platform as for the v4 platform, though there are some differences in the data files used. The approach is that:

1. For some sources, HAP emissions are used in the speciation process to allow integration of VOC and HAP emissions in the NEI. This has the result of modifying the speciation profiles based on the HAP emission estimates which are presumed to be more accurate than the speciated VOC results for the HAPs; and,
2. For some mobile sources, "combination" profiles are specified by county and month and emission mode (e.g., exhaust, evaporative). SMOKE computes the resultant profile using the fraction of each specific profile assigned by county, month and emission mode. A new feature and new profile file in SMOKE (the GSPRO_COMBO file) allowed the use of this approach for the 2005v4 platform, and its use continues here.

The VOC speciation data files are different because we added another part of the nonpt sector to exclude from HAP VOC integration: the category of pesticide application. Additionally, the v4.1 platform used a new headspace profile representative of E0 gasoline, profile code 8762: "Gasoline Headspace Vapor using 0% Ethanol - Composite Profile". This profile is part of SPECIATE4.3 and was used in place of the SPECIATE4.0 profile 8737 (Composite Profile - Non-oxygenated Gasoline Headspace Vapor), which was used in the v4 platform. The new headspace profile was used for the same sources as was the previous headspace profile: year 2005 refueling and other ambient temperature evaporative gasoline processes (portable fuel containers and any evaporation of gasoline associated with gasoline storage and distribution sources).

The below subsections provide a further description of the HAP/CAP integration and use of combination profiles. Section 3.2.2 provides the details about the data files used to accomplish these speciation processing steps.

3.1.2.1 The Combination of HAP BAFM (benzene, acetaldehyde, formaldehyde and methanol) and VOC for VOC Speciation

The VOC speciation approach for the 2005v4.1 platform differed from the 2002 platform in that we included, for some of the U.S. platform sectors, HAP emissions from the NEI in the speciation process. That is, instead of speciating VOC to generate all of the species listed in Table 3-3 as we did for the 2002 platform, we integrated emissions of the 4 HAPs, benzene, acetaldehyde, formaldehyde and methanol (BAFM) from the NEI with the NEI VOC. The integration process (described in more detail below) combines the BAFM HAPs with the VOC in a way that does not double count emissions and uses the BAFM directly in the speciation process. We believe that generally, the HAP emissions from the NEI are more representative of emissions of these compounds than their generation via VOC speciation.

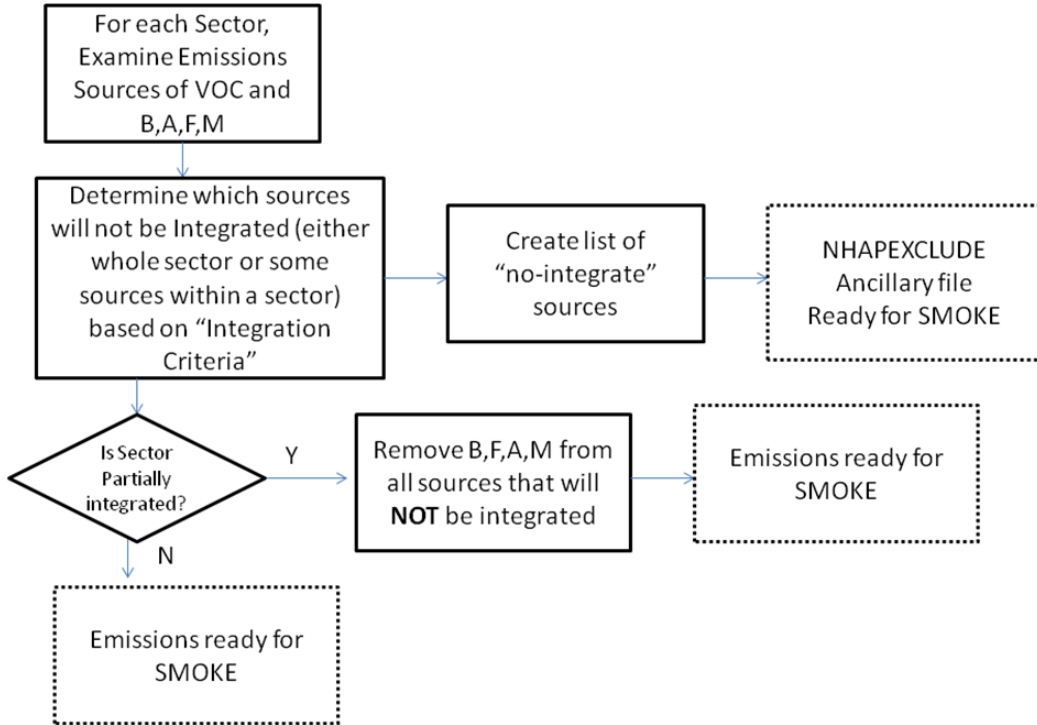
We chose these HAPs because, with the exception of BENZENE, they are the only explicit VOC HAPs in the base version of CMAQ 4.7 (CAPs only with chlorine chemistry) model. By “explicit VOC HAPs,” we mean model species that participate in the modeled chemistry using the CB05 chemical mechanism. We denote the use of these HAP emission estimates along with VOC as “HAP-CAP integration”. BENZENE was chosen because it was added as a model species in the base version of CMAQ 4.7, and there was a desire to keep its emissions consistent between multi-pollutant and base versions of CMAQ.

The integration of HAP VOC with VOC is a feature available in SMOKE for all inventory formats other than PTDAY (the format used for the ptfire sector). SMOKE allows the user to specify the particular HAPs to integrate and the particular sources to integrate. The particular HAPs to integrate are specified in the INVTABLE file, and the particular sources to integrate are based on the NHAPEXCLUDE file (which actually provides the sources that are *excluded* from integration⁸). For the “integrate” sources, SMOKE subtracts the “integrate” HAPs from the VOC (at the source level) to compute emissions for the new pollutant “NONHAPVOC.” The user provides NONHAPVOC-to-NONHAPTOG factors and NONHAPTOG speciation profiles. SMOKE computes NONHAPTOG and then applies the speciation profiles to allocate the NONHAPTOG to the other air quality model VOC species not including the integrated HAPs. This process is illustrated in Figure 3-2. Note that we did not need to remove BAFM from no-integrate sources in a sector where all sources are no-integrate because this is accomplished by through use of a SMOKE ancillary “INVTABLE” which essentially drops all BAFM in that sector.

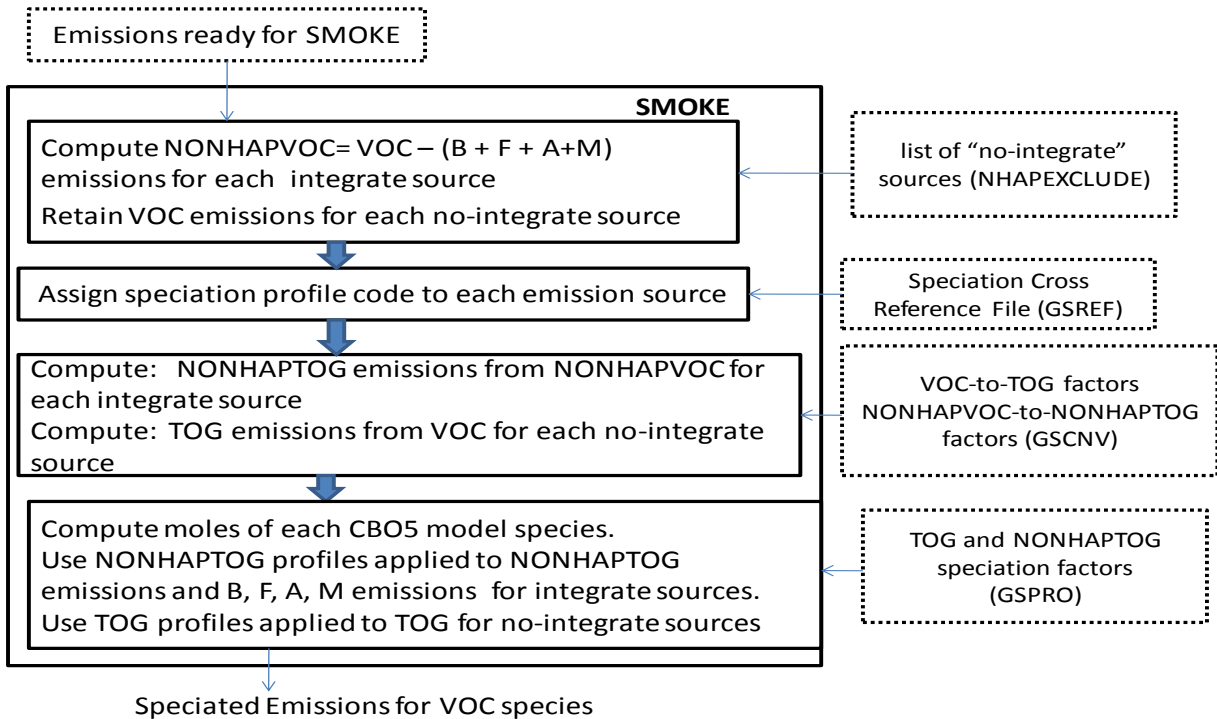
⁸ In SMOKE version 2.6 the options to specify sources for integration are expanded so that a user can specify the particular sources to include or exclude from integration, and there are settings to include or exclude all sources within a sector. We did not take advantage of this new flexibility in processing v4.1 emissions or v4 emissions, but the user will now have the ability for easier inclusion of specific sources to get the same result.

Figure 3-2. Process of integrating BAFM with VOC for use in VOC Speciation

Step 1: Analyze Inventory to determine which sources will be “integrate” sources



Step 2: Run SMOKE



We considered CAP-HAP integration for all sectors and developed “integration criteria” for some of those. Table 3-4 summarizes the integration approach for each platform sector used in Step 1 of Figure 3-2.

Table 3-4. Integration status of benzene, acetaldehyde, formaldehyde and methanol (BAFM) for each platform sector

Platform Sector	Approach for Integrating NEI emissions of Benzene (B), Acetaldehyde (A), Formaldehyde (F) and Methanol (M)
ptipm	No integration because emissions of BAFM are relatively small for this sector
ptnonipm	No integration because emissions of BAFM are relatively small for this sector and it is not expected that criteria for integration would be met by a significant number of sources
avefire	No integration
ag	N/A – sector contains no VOC
afdust	N/A – sector contains no VOC
nonpt	Partial integration; details provided below table
nonroad	For other than California: Partial integration – did not integrate CNG or LPG sources (SCC beginning with 2268 or 2267) because NMIM computed only VOC and not any HAPs for these SCCs. For California: Full integration
alm_no_c3	Partial integration; details provided below table
seca_c3	Full integration
onroad	Full integration
biog	N/A – sector contains no inventory pollutant "VOC"; but rather specific VOC species
othpt	No integration – not the NEI
othar	No integration – not the NEI
othon	No integration – not the NEI

For the nonpt sector, we used the following integration criteria to determine the sources to integrate (Step 1):

1. Any source for which BAFM emissions were from the 1996 NEI were not integrated (data source code contains a “96”).
2. Any source for which the sum of BAFM is greater than the VOC was not integrated, since this clearly identifies sources for which there is an inconsistency between VOC and VOC HAPs. This includes some cases in which VOC for a source is zero.
3. For certain source categories (those that comprised 80% of the VOC emissions), we chose to integrate sources in the category per the criteria specified in the first column in Table 3-5. For most of these source categories, we allow sources to be integrated if they had the minimum combination of BAFM specified in the first column. For a few source categories, we designated all sources as “no-integrate”. The one change we made from Table 3-5 for the v4.1 platform is highlighted: we changed pesticides application to “no-integrate.”
4. For source categories not covered in Table 3-5 (i.e., that do not comprise the top 80% of VOC emissions), then as long as the source has emissions of one of the BFAM pollutants, then it can be integrated.

Table 3-5. Source-category specific criteria for integrating nonpt SCCs for categories comprising 80% of the nonpoint VOC emissions

minimum HAP(s) needed	SCC Tier 3	SCC Tier 3 Description	Comments
BFA	2104008000	Stationary Source Fuel Combustion;Residential;Wood	
B	2501060000	Storage and Transport;Petroleum and Petroleum Product Storage;Gasoline Service Stations	
BM	2440000000	Solvent Utilization;Miscellaneous Industrial;All Processes	Speciation profile: 3144 has no benzene but most records have it and they're from EPA (and Calif)
FAM	2401001000	Solvent Utilization;Surface Coating;Architectural Coatings	
B	2310001000	Industrial Processes;Oil and Gas Production: SIC 13;All Processes : On-shore	
M	2460000000	Solvent Utilization;Miscellaneous Non-industrial: Consumer and Commercial;All Processes	
B	2501011000	Storage and Transport;Petroleum and Petroleum Product Storage;Residential Portable Gas Cans	
M	2425000000	Solvent Utilization;Graphic Arts;All Processes	
M	2465000000	Solvent Utilization;Miscellaneous Non-industrial: Consumer;All Products/Processes	3144 is profile, and it does have methanol (but no BFA).
BFA	2801500000	Miscellaneous Area Sources;Agriculture Production - Crops;Agricultural Field Burning - whole field set on fire	8746 is speciation profile and has BFA
M	2440020000	Solvent Utilization;Miscellaneous Industrial;Adhesive (Industrial) Application	3142 is speciation profile which has methanol (.32%) and 0 form (and no acetald, benz)
B	2501050000	Storage and Transport;Petroleum and Petroleum Product Storage;Bulk Terminals: All Evaporative Losses	
B	2310000000	Industrial Processes;Oil and Gas Production: SIC 13;All Processes	
M	2465400000	Solvent Utilization;Miscellaneous Non-industrial: Consumer;Automotive Aftermarket Products	8520 is speciation profile which doesn't have benz but does have methanol. OR is only state with benzene which is negligible
No-integrate (change from v4 platform)	2461850000	Solvent Utilization;Miscellaneous Non-industrial: Commercial;Pesticide Application: Agricultural	Profile has no benzene. Inventory benzene came from solvent utilization data (Fredonia) for "other markets" for the year 1998. Since benzene no longer allowed in pesticides, use of a no-benzene profile would give more accurate results. Note that this is a change from the v4 platform, where this sector was "integrate."
BFA	2630020000	Waste Disposal, Treatment, and Recovery;Wastewater Treatment;Public Owned	profile BFA 2002 (wastewater treatment plants). No methanol in profile. No methanol mentioned in POTW NESHAP (nor were A,F). Methanol in NEI documentation.
no-integrate	2461021000	Solvent Utilization;Miscellaneous Non-industrial: Commercial;Cutback Asphalt	profile 1007 has none of these HAP. Only Minnesota has a tiny amount.
no-integrate	2401005000	Solvent Utilization;Surface Coating;Auto Refinishing: SIC 7532	Only NY has benzene. Spec. profile is 2402 and has none of these HAP. Documentation for NEI does not estimate this HAP.
use Integrate case	2301030000	Industrial Processes;Chemical Manufacturing: SIC 28;Process Emissions from Pharmaceutical Manuf (NAPAP cat. 106)	profile 2462 - has nearly 8% benzene. Will create a LOT of benzene with "no HAP use" case.
M	2460200000	Solvent Utilization;Miscellaneous Non-industrial: Consumer and Commercial;All Household Products	profile is 3146 contains only nonzero methanol.

minimum HAP(s) needed	SCC Tier 3	SCC Tier 3 Description	Comments
any 1 HAP	2415000000	Solvent Utilization;Degreasing;All Processes/All Industries	profile 8745 (non legacy but composite made up of a bunch of E-rated profiles)has M, B.
M	2401002000	Solvent Utilization;Surface Coating;Architectural Coatings - Solvent-based	profile 3139 has only M
no-integrate	2401020000	Solvent Utilization;Surface Coating;Wood Furniture: SIC 25	profile 2405 has no HAP
B	2505040000	Storage and Transport;Petroleum and Petroleum Product Transport;Pipeline	
any 1 HAP	2610030000	Waste Disposal, Treatment, and Recovery;Open Burning;Residential	profile 0121 is old and has only hexane.
any 1 HAP	2610000000	Waste Disposal, Treatment, and Recovery;Open Burning;All Categories	profile 0121 is old and has only hexane.
FAM	2401003000	Solvent Utilization;Surface Coating;Architectural Coatings - Water-based	profile 3140 has FAM
M	2460100000	Solvent Utilization;Miscellaneous Non-industrial: Consumer and Commercial;All Personal Care Products	profile (3247, nonlegacy based on CARB 1997 survey) has no M or B. However, Freedomia was used for M.
M	2465200000	Solvent Utilization;Miscellaneous Non-industrial: Consumer;Household Products	
M	2415300000	Solvent Utilization;Degreasing;All Industries: Cold Cleaning	profile 8745 (non legacy but composite made up of a bunch of E-rated profiles)has M, B.
any 1 HAP	2401040000	Solvent Utilization;Surface Coating;Metal Cans: SIC 341	profile 2408 has none. - no HAPs in NEI so this SCC will not have any integrated sources
any 1 HAP	2401050000	Solvent Utilization;Surface Coating;Miscellaneous Finished Metals: SIC 34 - (341 + 3498)	SPEC PROFILE 3127 has none - no HAPs in NEI so this SCC will not have any integrated sources
any 1 HAP	2401200000	Solvent Utilization;Surface Coating;Other Special Purpose Coatings	profile 3138 has methanol. Not legacy. 0.11% aerosol coatings.
B	2461800000	Solvent Utilization;Miscellaneous Non-industrial: Commercial;Pesticide Application: All Processes	3001 is speciation profile (not legacy) "D" rating 2004. Calif. Testing for speciation profile from 2000. Has NO benzene! Benzene came from solvent utilization data (Freedomia) for "other markets" for the year 1998.
M	2460800000	Solvent Utilization;Miscellaneous Non-industrial: Consumer and Commercial;All FIFRA Related Products	3145 has M only and just a 0.01%

For the alm_no_c3 sector, the integration criteria were (1) that the source had to have at least one of the 4 HAPs and (2) that the sum of BAFM could not exceed the VOC emissions. The criteria for this sector were less complex than the nonpt sector because it has much fewer source categories.

We used the SMOKE feature to compute speciation profiles from mixtures of other profiles in user-specified proportions. The combinations are specified in the GSPRO_COMBO ancillary file by pollutant (including pollutant mode, e.g., EXH__VOC), state and county (i.e., state/county FIPS code) and time period (i.e., month).

We used this feature for onroad and nonroad mobile and gasoline-related related stationary sources whereby the emission sources use fuels with varying ethanol content, and therefore the speciation profiles require different combinations of gasoline, E10 and E85 profiles. Since the ethanol content varies spatially (e.g., by state or county), temporally (e.g., by month) and by modeling year (future years have more ethanol) the feature allows combinations to be specified at various levels for different years.

3.1.2.2 Creation of model-ready mercury species

As part of 2005 platform, we created model-ready mercury species by speciating any of the mercury in the NEI that was not provided as divalent gaseous, elemental or divalent particulate mercury. The same speciation approach was used in the CAP and HAP 2002v3 platform.

For the EGU sector (ptipm), all emissions except for 0.97 tons of the 52.9 tons of total 2005 Hg was provided in the inventory as speciated emissions. The unspicated Hg are primarily associated with oil-fired units. The speciation of the coal units was retained from the 2002 inventory, since 2005 EGU emissions were based on applying a 2005-to-2002 heat input ratio to the 2002 EGU emissions.

3.1.3 Temporal processing configuration

Table 3-6 summarizes the temporal aspect of the emissions processing configuration. It compares the key approaches we used for temporal processing across the sectors. We control the temporal aspect of SMOKE processing through (a) the scripts L_TYPE (temporal type) and M_TYPE (merge type) settings and (b) the ancillary data files described in Section 3.2.3. The one change made from the v4 to the v4.1 platform is the treatment of the afdust sector. In the v4 platform we used “aveday” settings and no use of holidays such that every day in a specific month had the same emissions. In the v4.1 platform, we used “week” settings and holidays and used profiles which were day-of-week dependent for some categories, such as road dust and tilling, where non-uniform profiles were being used for other pollutants associated with these processes.

Table 3-6. Temporal settings used for the platform sectors in SMOKE, v4.1 platform

Platform sector	Inventory resolution	Monthly profiles used?	Daily temporal approach ^{1,2}	Merge processing approach ^{1,3}	Process Holidays as separate days?
ptipm	daily & hourly		all	all	yes
ptnonipm	annual	yes	mwdss	all	yes
othpt	annual	yes	mwdss	all	
othpt_hg	annual	yes	mwdss	all	
nonroad	monthly		mwdss	mwdss	yes
othar	annual	yes	mwdss	mwdss	
alm_no_c3	annual	yes	mwdss	mwdss	
seca_c3	annual	yes	mwdss	mwdss	
on_noadj	monthly		week	week	yes
on_moves_startpm	monthly		week	week	yes
on_moves_runpm	monthly		week	week	yes
othon	annual	yes	week	week	
nonpt	annual	yes	mwdss	mwdss	yes
ag	annual	yes	aveday	aveday	
afdust	annual	yes	week	week	yes
biog	hourly		n/a	n/a	
avefire	annual	yes	aveday	aveday	

¹ **Definitions for processing resolution:**

all = hourly emissions computed for every day of the year, inventory is already daily
week = hourly emissions computed for all days in one “representative” week, representing all weeks for each month, which means emissions have day-of-week variation, but not week-to-week variation within the month
mwdss= hourly emissions for one representative Monday, representative weekday, representative Saturday and representative Sunday for each month, which means emissions have variation between Mondays, other weekdays, Saturdays and Sundays within the month, but not week-to-week variation within the month. Also Tuesdays, Wednesdays and Thursdays are treated the same.
aveday = hourly emissions computed for one representative day of each month, which means emissions for all days of each month are the same.

² **Daily temporal approach** refers to the temporal approach for getting daily emissions from the inventory using the Temporal program. The values given are the values of the L_TYPE setting.

³ **Merge processing approach** refers to the days used to represent other days in the month for the merge step. If not “all”, then the SMOKE merge step just run for representative days, which could include holidays as indicated by the rightmost column. The values given are the values of the M_TYPE setting.

In addition to the resolution, temporal processing includes a ramp-up period for several days prior to January 1, 2005, which is intended to mitigate the effects of initial condition concentrations. The same procedures were used for all grids, but with different ramp-up periods for each grid:

- 36 km: 10 days (Dec 22 - Dec 31)
- 12 km (East): 3 days (Dec 29 - Dec 31)
- 12 km (West): 3 days (Dec 29 - Dec 31)

For most sectors, our approach used the emissions from December 2005 to fill in surrogate emissions for the end of December 2004. In particular, we used December 2005 emissions (representative days) for December 2004. For biogenic emissions, we processed December 2004 emissions using 2004 meteorology.

3.2 Emissions modeling ancillary files

In this section we summarize the ancillary data that SMOKE used to perform spatial allocation, chemical speciation, and temporal allocation for the 2005v4.1 platform. The ancillary data files, particularly the cross-reference files, provide the specific inventory resolution at which spatial, speciation, and temporal factors are applied. For the 2005v4.1 platform, we generally applied spatial factors by country/SCC, speciation factors by pollutant/SCC or (for combination profiles) state/county FIPS code and month, and temporal factors by some combination of country, state, county, SCC, and pollutant.

For the v4.1 platform, we updated the 2005v4 ancillary files in two major areas:

1. We used new data for spatially allocating oil and gas emission sources
2. We assigned spatial, temporal and speciation profiles to parking area emissions for additional vehicle types (new data from MOVES2010) and updated previous assignments for some vehicle types (summarized in Table 3-15 and Table 3-16).
3. We updated the headspace VOC speciation profile we used for refueling.
4. We used a new profile for speciating PM_{2.5} from C3 marine emissions.

3.2.1 Spatial Allocation Data

As described in Section 3.1.1, we performed spatial allocation for a national 36-km domain, an Eastern 12-km domain, and a Western 12-km domain. To do this, SMOKE used national 36-km and 12-km spatial surrogates and a SMOKE area-to-point data file. For the U.S. and Mexico, we used the same spatial surrogates as were used for the 2002v3 platform. For Canada we used a new set of Canadian surrogates provided by Environment Canada. The spatial data files we used can be obtained from the files listed below; these are available from the 2002v3CAP (for US and Mexico) and 2005v4CAP-BAFM (for Canada) platform websites (see the end of Section 1). The oil and natural gas surrogate files are posted at the 2005v4.1 website. The following list of seven files provides descriptions of each of their contents and intended uses for the v4.1 platform.

- **36km_surg_2002v3mpCAP_smokeformat.zip:** U.S. and Mexican surrogate files for 36-km spatial resolution (Canadian data contained in this zip file was not used for the 2005-based platform except for the year 2000 mercury data which is contained in the sector othpt)
- **12km_surg_2002v3mpCAP_smokeformat.zip:** U.S. and Mexican surrogate files for 12 km spatial resolution (Canadian data contained in this zip file was not used for the 2005-based platform except for the year 2000 mercury data which is contained in the sector othar)
- **new36km_surg_2005v4_smokeformat.zip:** Canadian surrogate files for 36-km spatial resolution for Canadian surrogates

- **new12km_surg_2005v4_smokeformat.zip:** Canadian surrogate files for 12-km spatial resolution for Canadian surrogates
- **new_oilgas_surg_2005v4_1_smokeformat.zip:** Oil and gas surrogate files for 36-km spatial resolution and 12-km spatial resolution for the new oil and gas surrogate (US)
- **ancillary_2005v4.1_smokeformat.zip:** spatial related data included are the grid description (GRIDDESC), surrogate description (SRGDESC), surrogate cross reference file (AGREF), and area-to-point (ARTOPNT) file

The U.S., Mexican, and Canadian 12-km surrogates cover the entire CONUS domain, though they are used directly as inputs for the two separate Eastern and Western Domains shown in Figure 3-1. The SMOKE model windowed the Eastern and Western grids while it created these emissions. The remainder of this subsection provides further detail on the origin of the data used for the spatial surrogates and the area-to-point data.

3.2.1.1 Surrogates for U.S. Emissions

There are 67 spatial surrogates available for spatially allocating U.S. county-level emissions to the 36-km and 12-km grid cells used by the air quality model; 66 are the same as for the v4 platform, and one new surrogate, “Oil & Gas Wells, IHS Energy, Inc. and USGS” was added for v4.1 which is discussed below. As described in Section 3.2.1.2, an area-to-point approach overrides the use of surrogates for some sources. Table 3-7 lists the codes and descriptions of the surrogates.

Table 3-7. U.S. Surrogates available for the 2005v4.1 platform.

Code	Surrogate Description	Code	Surrogate Description
N/A	Area-to-point approach (see 3.3.1.2)	515	Commercial plus Institutional Land
100	Population	520	Commercial plus Industrial plus Institutional
110	Housing	525	Golf Courses + Institutional +Industrial + Commercial
120	Urban Population	527	Single Family Residential
130	Rural Population	530	Residential - High Density
137	Housing Change	535	Residential + Commercial + Industrial + Institutional + Government
140	Housing Change and Population	540	Retail Trade
150	Residential Heating - Natural Gas	545	Personal Repair
160	Residential Heating - Wood	550	Retail Trade plus Personal Repair
165	0.5 Residential Heating - Wood plus 0.5 Low Intensity Residential	555	Professional/Technical plus General Government
170	Residential Heating - Distillate Oil	560	Hospital
180	Residential Heating - Coal	565	Medical Office/Clinic
190	Residential Heating - LP Gas	570	Heavy and High Tech Industrial
200	Urban Primary Road Miles	575	Light and High Tech Industrial
210	Rural Primary Road Miles	580	Food, Drug, Chemical Industrial
220	Urban Secondary Road Miles	585	Metals and Minerals Industrial
230	Rural Secondary Road Miles	590	Heavy Industrial
240	Total Road Miles	595	Light Industrial
250	Urban Primary plus Rural Primary	596	Industrial plus Institutional plus Hospitals

Code	Surrogate Description	Code	Surrogate Description
255	0.75 Total Roadway Miles plus 0.25 Population	600	Gas Stations
260	Total Railroad Miles	650	Refineries and Tank Farms
270	Class 1 Railroad Miles	675	Refineries and Tank Farms and Gas Stations
280	Class 2 and 3 Railroad Miles	680	Oil & Gas Wells, IHS Energy, Inc. and USGS
300	Low Intensity Residential	700	Airport Areas
310	Total Agriculture	710	Airport Points
312	Orchards/Vineyards	720	Military Airports
320	Forest Land	800	Marine Ports
330	Strip Mines/Quarries	807	Navigable Waterway Miles
340	Land	810	Navigable Waterway Activity
350	Water	850	Golf Courses
400	Rural Land Area	860	Mines
500	Commercial Land	870	Wastewater Treatment Facilities
505	Industrial Land	880	Drycleaners
510	Commercial plus Industrial	890	Commercial Timber

We did not use all of the available surrogates to spatially allocate sources in the v4.1 platform; that is, some surrogates in Table 3-7 were not assigned to any SCCs.

The creation of surrogates and shapefiles for the U.S. via the Surrogate Tool was discussed in the 2002v3 platform documentation and is not repeated here. The tool and updated documentation for it is available at <http://www.ie.unc.edu/cempd/projects/mims/spatial/> and http://www.cmascenter.org/help/documentation.cfm?MODEL=spatial_allocator&VERSION=3.6&temp_id=99999. This same tool was used for the new surrogate 680, “Oil & Gas Wells, IHS Energy, Inc. and USGS”

The new surrogate “Oil & Gas Wells, IHS Energy, Inc. and USGS” was developed for oil and gas SCCs, which had previously (in the v4 platform) used surrogate 585. The data reflect data through 10/1/2005. The underlying data for this surrogate is a grid of one-quarter square mile cells containing an attribute to indicate whether the wells within the cell are predominantly oil-producing, gas-producing, both oil- and gas-producing, or the wells are dry or their production status is unknown. The well information was initially retrieved from IHS Inc.'s PI/Dwights PLUS Well Data on CD-ROM, which is a proprietary commercial database containing information for most oil and gas wells in the U.S. Cells were developed as a graphic solution to overcome the problem of displaying proprietary well data. No proprietary data are displayed or included in the cell maps. More information can be obtained from <http://pubs.usgs.gov/dds/dds-069/dds-069-q/text/layer.htm> and http://certmapper.cr.usgs.gov/rooms/utilities/layer_info.jsp?docId={A90AF432-612F-41F9-A315-7329FD933FB3}&type=download&docURL=http://certmapper.cr.usgs.gov/data/noga00/natl/spatial/doc/uscells05g.htm

The spatial cross-reference file was also updated to assign onroad off-network (parking area) emissions from the MOVES2010 model, new to the 2005v4 platform, were allocated as shown in Table 3-8.

Table 3-8. Surrogate assignments to new mobile categories in the 2005v4 platform

SCC & Description	Surrogate
2201001350 Light Duty Gas Vehicles- parking areas rural 2201002350 Light Duty Gas Trucks 1&2- parking areas rural 2201004350 Light Duty Gas Trucks 3&4- parking areas rural	Rural population (same as rural local roads), code= 130
2201001370 Light Duty Gas Vehicles- parking areas urban 2201002370 Light Duty Gas Trucks 1&2- parking areas urban 2201004370 Light Duty Gas Trucks 3&4- parking areas urban	Urban population (same as urban local roads), code =120
2201070350 Heavy Duty Gasoline Vehicles 2B through 8B & Buses (HDGV)- parking areas rural 2201070370 Heavy Duty Gasoline Vehicles 2B through 8B & Buses (HDGV)- parking areas urban	Commercial plus Industrial plus Institutional, code = 520

3.2.1.2 Allocation Method for Airport-Related Sources in the U.S.

There are numerous airport-related emission sources in the 2005 NEI, such as aircraft, airport ground support equipment, and jet refueling. Unlike the 2002v3 platform in which most of these emissions were contained in sectors with county-level resolution – alm (aircraft), nonroad (airport ground support) and nonpt (jet refueling), the 2005 platform includes the aircraft emissions as point sources. As shown in Table 2-1, aircraft emissions are part of the ptnonipm sector, since the 2005v2 inventory included them as point sources.

Thus, for the 2005 platform, we used the SMOKE “area-to-point” approach for only airport ground support equipment (nonroad sector), and jet refueling (nonpt sector). The approach is described in detail in the 2002 platform documentation:

http://www.epa.gov/scram001/reports/Emissions%20TSD%20Vol1_02-28-08.pdf.

We used nearly the same ARTOPNT file to implement the area-to-point approach as was used for the CAP and HAP-2002-Based platform. This was slightly updated from the CAP-only 2002 platform by further allocating the Detroit-area airports into multiple sets of geographic coordinates to support finer scale modeling that was done under a different project. We chose to retain the updated file for the 2005 platform. This approach is the same in the v4.1 and v4 platforms.

3.2.1.3 Surrogates for Canada and Mexico Emission Inventories

We used an updated set of surrogates for Canada to spatially allocate the 2006 Canadian emissions for the 2005v4 platform with the exception of the nonpoint Canadian mercury emissions. The updated set completely replaced the 2002v3 platform surrogates for allocating the 2006 province-level Canadian emissions. The 2002v3 platform surrogates for Canada were used for the mercury data in the sector other_hg because Canada did not provide updated mercury data with its 2006 inventory.

The updated surrogate data provided in the 2005v4 zip files and described in Table 3-9 came from Environment Canada. They provided the surrogates and cross references; the surrogates they provided were outputs from the Surrogate Tool (previously referenced). Per Environment Canada, the surrogates are based on 2001 Canadian census data. We changed the cross-references that Canada originally provided as follows: all assignments to surrogate '978' (manufacturing industries) were changed to '906' (manufacturing services), and all assignments to '985' (construction and mining) and '984' (construction industries) were changed to '907' (construction services) because the surrogate fractions in 984, 978 and 985 did not sum to 1. We also changed codes for surrogates other than population that did not begin with the digit "9". The same surrogates were used for the 12-km domains as were used for the 36-km domain.

Table 3-9. Canadian Spatial Surrogates for 2005-based platform Canadian Emissions (v4.1 unchanged from v4)

Surrogate description	Filename of 2005 Platform Surrogate	Surrogate description	Filename of 2005 Platform Surrogate
Population	CA_100_NOFILL.txt	asphalt	CA_951_NOFILL.txt
Total dwelling	CA_901_NOFILL.txt	cement	CA_952_NOFILL.txt
Agriculture and Forestry and Fishing	CA_902_NOFILL.txt	chemical	CA_953_NOFILL.txt
Waste Management Service	CA_903_NOFILL.txt	commfuelcomb	CA_954_NOFILL.txt
Upstream Oil and Gas (UOG)	CA_904_NOFILL.txt	downstream_petroleum	CA_955_NOFILL.txt
Mining and Oil and Gas services	CA_905_NOFILL.txt	egu	CA_956_NOFILL.txt
Manufacturing services	CA_906_NOFILL.txt	grain	CA_957_NOFILL.txt
Construction services	CA_907_NOFILL.txt	manufacturing	CA_958_NOFILL.txt
Transportation of Passengers and goods	CA_908_NOFILL.txt	mining	CA_959_NOFILL.txt
Electric and Gas and Water utilities	CA_909_NOFILL.txt	oilgas_distribution	CA_960_NOFILL.txt
Wholesaling Merchandise services	CA_910_NOFILL.txt	smelting	CA_961_NOFILL.txt
Retailing Merchandise services	CA_911_NOFILL.txt	waste	CA_962_NOFILL.txt
Government Services	CA_915_NOFILL.txt	wood	CA_963_NOFILL.txt
All Sales	CA_920_NOFILL.txt	asphalt industries	CA_971_NOFILL.txt
Intersection of AGRFORFISH and MANUFACT	CA_921_NOFILL.txt	cement industries	CA_972_FILL.txt
Intersection of Forest and Housing	CA_922_NOFILL.txt	chemical industries	CA_973_FILL.txt
Intersection of MININGOILG and MANUFACT	CA_923_NOFILL.txt	commercial fuel combustion	CA_974_FILL.txt
Intersection of UTILITIES and DWELLING	CA_924_NOFILL.txt	downstream petroleum industries	CA_975_FILL.txt
Intersection of CONSTRUCTION and	CA_925_NOFILL.txt	Electric utilities	CA_976_FILL.txt

Surrogate description	Filename of 2005 Platform Surrogate	Surrogate description	Filename of 2005 Platform Surrogate
DWELLING			
Intersection of PUBADMIN and DWELLING	CA_926_NOFILL.txt	grain industries	CA_977_FILL.txt
Commercial Marine Vessels	CA_928_NOFILL.txt	manufacturing industries ¹	CA_978_FILL.txt
HIGHJET	CA_929_NOFILL.txt	mining industries	CA_979_FILL.txt
LOWMEDJET	CA_930_NOFILL.txt	smelting industries	CA_981_FILL.txt
OTHERJET	CA_931_NOFILL.txt	waste management	CA_982_NOFILL.txt
CANRAIL	CA_932_NOFILL.txt	construction industries ¹	CA_984_NOFILL.txt
LDGV	CA_934_NOFILL.txt	construction and mining ¹	CA_985_NOFILL.txt
PAVED ROADS	CA_941_NOFILL.txt	TOTALBEEF ²	CA_986_NOFILL.txt ²
UNPAVED ROADS	CA_942_NOFILL.txt	TOTALPOUL ²	CA_987_NOFILL.txt ²
Oil Sands	CA_950_NOFILL.txt	TOTALSWIN ²	CA_988_NOFILL.txt ²
		TOTALFERT ²	CA_989_NOFILL.txt ²
1: Not used because fractions did not sum to 1;			
2: Surrogates 986, 987, 988 and 989 were originally numbered by Canada as 611, 615, 620 and 65, respectively. We changed the numbers so that all Canadian surrogates would begin with "9".			

The Mexican emissions and single surrogate (population) are the same in the v4.1 platform as were used in the 2005v4 and 2002 platforms.

3.2.2 Chemical speciation ancillary files

The following data files, provided at the 2005v4 website (see the end of Section 1), contain the SMOKE inputs used for chemical speciation of the inventory species to the CMAQ model species. SMOKE environmental variable names, used in the file names, are shown using capital letters in parentheses:

- **ancillary_2005v4.1_smokeformat.zip:** inventory table (INVTABLE), NONHAPVOC emissions calculation exclusions file (NHAPEXCLUDE), speciation cross references (GSREF), speciation VOC-to-TOG conversion factors (GSCNV), speciation profiles (GSPRO), and combined, monthly speciation profiles (GSPRO_COMBO).
- **ancillary_2005v4.1_futureyear_smokeformat.zip:** speciation-related files associated with the future year speciation changes.

The following subsections explain these SMOKE input files.

3.2.2.1 INVABLE and NHAPEXCLUDE

The INVTABLE and NHAPEXCLUDE SMOKE input files have a critical function in the VOC speciation process for emissions modeling cases utilizing HAP-CAP integration, as is done for the 2005v4.1 platform.

We prepared two different INVTABLE files to use with different sectors of the platform. For sectors in which we chose no integration across the entire sector (see Table 3-5), we created a “no HAP use” INVTABLE that set the “KEEP” flag to “N” for BAFM pollutants. Thus, any BAFM pollutants in the inventory input into SMOKE would be dropped. This approach both

avoids double-counting of these species and assumes that the VOC speciation is the best available approach for these species for the sectors using the approach. The second INVTABLE, used for sectors in which one or more sources are integrated, causes SMOKE to keep the BAFM pollutants and indicates that they are to be integrated with VOC (by setting the “VOC or TOG component” field to “V” for all four HAP pollutants).

We also prepared sector-specific NHAPEXCLUDE files that provide the specific sources that are excluded from integration (see Table 3-5).

3.2.2.2 GSPRO, GSPRO_COMBO, GSREF and GSCNV,

For VOC speciation, we generated the following SMOKE-ready profiles for the CB05 chemical mechanism using the Speciation Tool (Eyth, 2006):

- TOG-to-model species (used only for no-integrate sources)
- NONHAPTOG-to-model species (used only for the integrate sources)
- TOG-to-BENZENE (used only for no-integrate sources)

We added speciation profile entries that simply map NEI emissions of benzene, acetaldehyde, formaldehyde and methanol to the model species BENZENE, ALD2, FORM and METHANOL, respectively. These profiles were used only for the integrate sources. Note that we process the integrate and no-integrate sources using the same GSREF and GSPRO files. Thus, to avoid double counting of these HAP species, we removed BAFM pollutants for all no-integrate sources in the inventory. If the entire sector was no-integrate, then we were able to remove these in SMOKE (by using “N” in the INVTABLE) but if a sector was partially integrated, then we needed to remove these HAPS from the actual inventory input to SMOKE, but only for the no HAP use, no-integrate sources.

In addition to the speciation profiles, the Speciation Tool generates the SMOKE-ready speciation conversion files (GSCNV). We generated two of these: one containing profile-specific VOC-to-TOG conversion factors and the other containing profile-specific NONHAPVOC-to-NONHAPTOG conversion factors.

The TOG and PM_{2.5} speciation factors that are the basis of the chemical speciation approach were developed from the SPECIATE4.2 database (<http://www.epa.gov/ttn/chief/software/speciate/index.html>) which is EPA's repository of TOG and PM speciation profiles of air pollution sources. However, a few of the profiles we used in the v4.1 platform will be published in SPECIATE4.3 after the release of this documentation.

The SPECIATE database development and maintenance is a collaboration involving EPA's ORD, OTAQ, and EPA's Office of Air Quality Planning and Standards (OAQPS), and Environment Canada (EPA, 2006c). The SPECIATE database contains speciation profiles for TOG, speciated into individual chemical compounds, VOC-to-TOG conversion factors associated with the TOG profiles, and speciation profiles for PM_{2.5}. The database also contains the PM_{2.5} speciated into both individual chemical compounds (e.g., zinc, potassium, manganese, lead), and into the “simplified” PM_{2.5} components used in the air quality model. These simplified components are:

- PSO4 : primary particulate sulfate
- PNO3: primary particulate nitrate
- PEC: primary particulate elemental carbon
- POC: primary particulate organic carbon
- PMFINE: other primary particulate, less than 2.5 micrograms in diameter

As discussed earlier, for the v4.1 platform we updated the PM_{2.5} profile used for category 3 marine vessels burning residual oil to use the profile: Marine Vessel - Main Engine - Heavy Fuel Oil which will be published in SPECIATE4.3. This profile was compiled from data published in Emission Measurements from a Crude Oil Tanker at Sea, Environ. Sci. Technol. 2008, 42, 7098–7103. Previously the Draft Residual Oil Combustion – Simplified (92072) was used. The SCCs affected were:

2280003000 Mobile Sources;Marine Vessels, Commercial;Residual;Total, All Vessel Types
 2280003010 Mobile Sources;Marine Vessels, Commercial;Residual;Ocean-going Vessels
 2280003100 Mobile Sources;Marine Vessels, Commercial;Residual;Port emissions
 2280003200 Mobile Sources;Marine Vessels, Commercial;Residual;Underway emissions

The difference between the two profiles is provided in Table 3-10, and shows that the new profile produces much more organic carbon and less elemental carbon, sulfate, and other PM_{2.5}.

Table 3-10. Differences between two profiles used for commercial marine residual oil

Pollutant	Species	Split factors new c3 profile 92200 used for v4.1	Split factors residual oil combustion 92072, used for v4
PM2_5	PEC	0.005	0.01
PM2_5	PMFINE	0.5022	0.54
PM2_5	PNO3	0	0
PM2_5	POC	0.1125	0.01
PM2_5	PSO4	0.3803	0.44

We also updated the bituminous coal profile, 92095, which we had previously used for only a single nonpoint SCC (2101002000) with the sub-bituminous profile 92084, which was used for all other coal combustion SCCs. We replaced profile 92095 with 92084 for consistency. Table 3-11 shows the differences are shown below, though these are quite small and represent only a minor change to the SMOKE results:

Table 3-11. Differences between two profiles used for coal combustion

Pollutant	Species	Split factors sub-bituminous 92084	Split factors bituminous 92095
PM2_5	PEC	0.0188	0.01696
PM2_5	PMFINE	0.8266	0.827928
PM2_5	PNO3	0.0016	0.00208
PM2_5	POC	0.0263	0.026307
PM2_5	PSO4	0.1267	0.126725

We made other updates to profile assignments for the SCCs shown in Table 3-12 below as compared to the 2002 platform. These updates were kept for the v4.1 platform.

Table 3-12: PM_{2.5} speciation profile updates assignments for the v4 platform

SCC	New Profile Code	Pollutant	Profile Name
39900501	92025	PM2_5	Distillate Oil Combustion Source Type: Distillate Oil Combustion
49090021	92025	PM2_5	Distillate Oil Combustion Source Type: Distillate Oil Combustion
30890002	92072	PM2_5	Residential Oil Combustion Source Type: Residential Oil Combustion
10100912	92091	PM2_5	Wood Fired Boiler Source Type: Wood/Bark Combustion
10102018	92057	PM2_5	PM/SO2 controlled lignite combustion: Waste Coal Combustion
50410563	92082	PM2_5	Solid Waste Combustion Source Type: Solid Waste Combustion
10100692	92048	PM2_5	Natural Gas Combustion Source Type: Natural Gas Combustion
50100511	92086	PM2_5	Tire Burning Source Type: Tire Burning
50100512	92082	PM2_5	Solid Waste Combustion: Solid Waste Combustion
2810040000	92035	PM2_5	HDDV Source Type: Aircraft Engines

Key changes to the TOG profiles for the v4.1 platform from the 2005v4 platform are as follows:

- Used new headspace profiles for E0 (no ethanol gasoline) and E10 (10% ethanol gasoline), which will be published in SPECIATE4.3. Profile 8762 is Gasoline Headspace Vapor using 0% Ethanol - Composite Profile and Profile 8763 is Gasoline Headspace Vapor using 10% Ethanol - Composite Profile. In 2005, only the E0 profile is used. This was an oversight since we could have used the same combinations of profiles of E0 exhaust E10 exhaust (which are also the same combinations of E10 evaporative and E10 evaporative) that we used for 2005. We did, however use consistent combinations (E0/E10) in future year modeling for the headspace profiles as the evaporative and exhaust combinations.
- Added the fuel-specific VOC profiles for the new parking area SCCs generated due to the fact that MOVES2010 was used for all vehicle types in the v4.1 platform. A summary of the assignments of all profiles (speciation, temporal and spatial surrogates) is provided in Table 3-15 for gasoline vehicles and Table 3-16 for diesel vehicles.

Table 3-13 provides a summary of the 2005 speciation approach for mobile and other fuel-related sources. It shows the updated profiles that form the 2005 combinations. The headspace

profile, 8762 is a new profile for the v4.1 platform, and is used for other nonroad refueling and other fuel-related stationary source emission categories in 2005.

Table 3-13. Summary of VOC speciation profile approach by sector for 2005

Inventory type and mode	VOC speciation approach for fuels	VOC Profile Codes	2005 sectors
Mobile onroad and nonroad Exhaust	E0 and E10 combinations (excludes Tier 2)	8750 8751	on_noadj nonroad
Mobile onroad and nonroad Evaporative	E0 and E10 combinations	8753 8754	on_noadj nonroad
Mobile nonroad Refueling Stationary (no mode assigned to VOC): Portable Fuel Containers, bulk plant -to-pump, refinery-to-bulk terminal	E0	8762	Nonroad nonpt

In future years, different profile combinations and a different headspace profile is used, due to the influx of greater quantities of ethanol in fuels. Changes to the above profiles for future-year scenarios will be discussed in more detail in the documentation of future year emissions development for the rule or application of interest. In summary, we utilized additional profiles in the combinations that is appropriate. The profiles we added were Tier 2 profiles for E0 and E10 and an E10 headspace profile.

Mercury speciation was done for sources that were not already provided as elemental (HG NRVA), divalent gas (HG IIGAS) and particulate (PHGI). The vast majority of the IPM sector was pre-speciated in the 2005 NATA inventory, and thus did not require the application of profiles. Mercury emissions from NMIM were also pre-speciated. Table 3-14 shows the data profiles we used to speciate any inventory mercury reported as unspicated mercury. These are the same profiles as were used in the CAP and HAP 2002-based platform, Version 3 (<http://www.epa.gov/ttn/chief/emch/index.html#2002>) . The actual speciation profiles used also converted the mass of gaseous mercury to moles by dividing by the molecular weight of mercury. Profiles were assigned to the inventory on the basis of MACT code, SCC code and/or SIC code. The cross reference file is provided in the ancillary files (ancillary_2005v4.1_smokeformat.zip).

Table 3-14. Speciation of Mercury

Source Category	Particulate Divalent %	Gaseous Divalent %	Elemental Gaseous %	Profile code
Portland Cement	12	13	75	HGCEM
Mercury Cell Chlor-Alkali Plants	0	5	95	HGCHL
combustion or default	20	30	50	HGCMB

Source Category	Particulate Divalent %	Gaseous Divalent %	Elemental Gaseous %	Profile code
all other nonpoint categories; gold mining	0	0	100	HGGLD
Incineration/ - waste disposal	20	58	22	HGINC
Industrial Processes non combustion/incin	10	10	80	HGIND
mobile diesel (onroad and nonroad)	15	29	56	HGMD
mobile gasoline (onroad and nonroad)	0.4	8.6	91	HGMG
Medical Waste Incineration	20	75	5	HGMWI

Speciation profiles for use with BEIS are not included in SPECIATE. The 2005 platform uses BEIS3.14, which includes a new species (SESQ) that was not in BEIS3.13 (the version used for the 2002 platform). Thus we added this species (it is mapped to the CMAQ species SESQT) to the set of profiles that we had been using in the 2002 platform. The profile code associated with BEIS3.14 profiles for use with CB05 uses the same as in the 2002 platform: “B10C5.”

3.2.3 Temporal allocation ancillary files

The emissions modeling step for temporal allocation creates the 2005 hourly emission inputs for the air quality model by adjusting the emissions from the inventory resolution (annual, monthly, daily or hourly) that are input into SMOKE. The temporal resolution of each of the platform sectors prior to their input into SMOKE is included in the sector descriptions from Table 2-1 and repeated in the discussion of temporal settings in Table 3-6.

The monthly, weekly, and diurnal temporal profiles and associated cross references used to create the 2005 hourly emissions inputs for the air quality model were generally based on the temporal allocation data used for the 2002v3 platform. For the v4 and v4.1 platforms, we added new profile assignments for SCCs in the 2005 inventory that were not in the 2002 inventory, and we updated the profiles used for ptipm sources without CEM data to represent the year 2005.

The following data file, provided at the 2005v4 website (see the end of Section 1) contains the SMOKE inputs used for chemical speciation of the inventory species to the air quality model species. SMOKE environmental variable names, used in the file names, are shown in capital letters in parentheses:

- **ancillary_2005v4.1_smokeformat.zip:** includes temporal cross reference files used across all inventory sectors (ATREF, MTREF, and PTREF) and for ptipm sector (used for electric generating units) for the evaluation case (PTREF) and, temporal profiles (ATPRO, MTPRO, and PTPRO)

The starting point for our temporal profiles was the 2002 platform. The remainder of this section discusses the development of the new temporal profiles or profile assignments used in the 2005v4 platform.

Canadian emissions

The profiles assignments for the Canadian 2006 inventory were provided by Environment Canada along with the inventory. They provided profile assignments that rely on the existing set of temporal profiles in the 2002 platform. For point sources, they provided profile assignments by PLANTID.

WRAP Oil and Gas Inventory Profiles

The WRAP 2005 oil and gas inventory SCCs utilized uniform monthly and day of week profiles (codes 262 and 7, respectively) and an hourly profile (code 26) that put emissions in every hour, but weighted towards the day light hours.

Diurnal Profiles for Electric Generating Units (ptipm)

We updated the state-specific and pollutant-specific diurnal profiles for use in allocating the day-specific emissions for non-CEM sources in the ptipm sector. We used the 2005 CEM data to create state-specific, day-to-hour factors, averaged over the whole year and all units in each state. We calculated the diurnal factors using CEM SO₂ and NO_x emissions and heat input. We computed SO₂ and NO_x-specific factors from the CEM data for these pollutants. All other pollutants used factors created from the hourly heat input data. We assigned the resulting profiles by state and pollutant.

Onroad Parking Area Profiles

The SCCs and descriptions, along with the assignments chosen are shown in Table 3-15 (gasoline vehicles) and Table 3-16 (diesel vehicles). Figure 3-3 and Figure 3-4 show the diurnal profiles referred to in the tables.

Figure 3-3. Diurnal Profiles based on road type (use local for “start”) and whether the road is urban versus rural

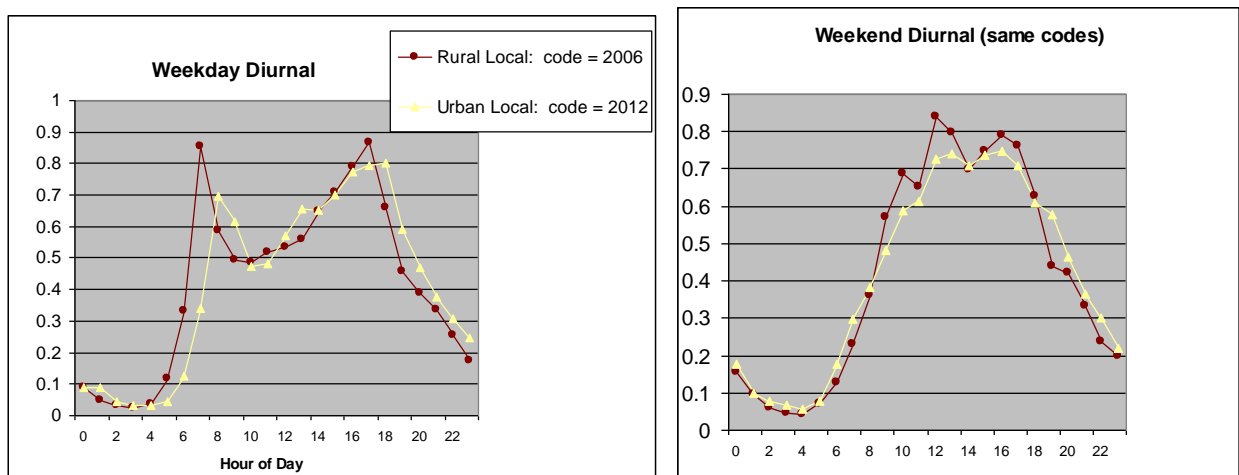


Figure 3-4. Diurnal temporal profile for HDDV 2B through 8B at Parking areas

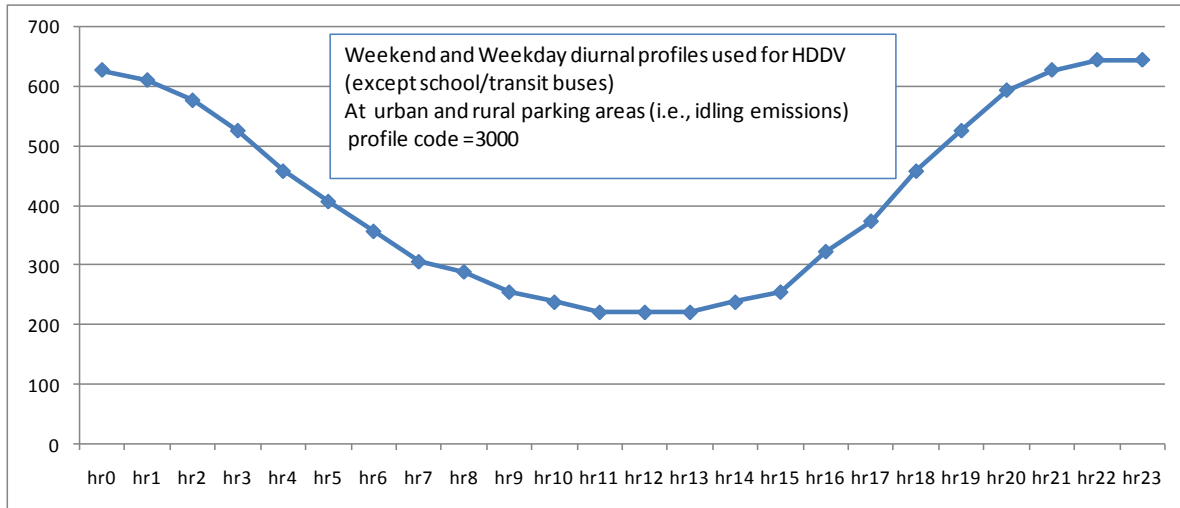


Table 3-15. Summary of spatial surrogates, temporal profiles, and speciation profiles used by gasoline vehicle types for the onroad parking area-related SCCs.

GASOLINE VEHICLE TYPES					
SCC&Description	Surrogate	Temporal Profile: Monthly Variation	Temporal Profile: Day of Week Variation	Temporal Profile: Diurnal variation	Speciation Profile
2201001350 Light Duty Gas Vehicles- parking areas rural 2201020350 Light Duty Gas Trucks 1&2- parking areas rural 2201040350 Light Duty Gas Trucks 3&4- parking areas rural 2201080370 Motorcycles (MC) - parking areas rural	Rural Population (same as rural local roads) 130	Not applicable – inventory contains monthly emissions	RURAL LD values are: Mon –Fri 12.1% 12.1% 12.1% 12.1% 18.3% Sat/Sun: 15.3% 18.3% Weekly_code (for SMOKE) =20021	Use same as profile as rural local roads (Rdtype=210) . Code = 2006 (see Figure 3-3, reddish curve)	Use same speciation profiles as what is used for LD GAS vehicles on the other roadway types. * i.e.: EVP_VOC: COMBO of 8753 (Gasoline Vehicle - Evaporative emission - Reformulated gasoline) & 8754 (Gasoline Vehicle - Evaporative emission - E10 ethanol gasoline) Note that these are the combinations used in 2005. In some cases future year profiles may also include 8755 (Gasoline Vehicle - Evaporative emission - E85) EXH_VOC: COMBO of 8750&8751 These combinations are used in 2005. In some cases future year profiles may also include combinations of 8752 (E85) , 8756 (tier 2 exhaust, E0), 8757 (tier 2 exhaust, E10) EXH_PM2.5 not needed because OTAQ supplies pre-specified emissions BRK_PM2.5 and TIR_PM2.5 use same as other roadways (92009 and 92087, respectively)
2201001370 Light Duty Gas Vehicles- parking areas urban 2201020370 Light Duty Gas Trucks 1&2- parking areas urban 2201040370 Light Duty Gas Trucks 3&4- parking areas urban 2201080370	Urban Population (same as urban local roads) 120	Not applicable – inventory contains monthly emissions	URBAN LD values are: Mon-Fri 14.8% 14.8% 14.8% 14.8% 16.0% Sat Sun 13.4% and 11.6% Weekly_code (for SMOKE) =20031	Use same as profile as urban local roads. (Rdtype=330) . Code = 2012 (see Figure 3-3, yellow curve)	Same as above

GASOLINE VEHICLE TYPES					
SCC&Description	Surrogate	Temporal Profile: Monthly Variation	Temporal Profile: Day of Week Variation	Temporal Profile: Diurnal variation	Speciation Profile
Motorcycles (MC) - parking areas rural					
2201070350 Heavy Duty Gasoline Vehicles 2B through 8B & Buses (HDGV)- parking areas rural	Commercial plus Industrial plus Institutional (code = 520)	Not applicable – inventory contains monthly emissions	RURAL HD values are: Mon-Fri 16.8% 16.8% 16.8% 16.8% 15.9% Sat Sun 8.8% and 8.8% Weekly_code (for SMOKE) =20022	Use same as profile rural local roads . Code = 2006 (see Figure 3-3, reddish curve)	Same as above
2201070370 Heavy Duty Gasoline Vehicles 2B through 8B & Buses (HDGV)- parking areas urban	Same as above	Not applicable – inventory contains monthly emissions	URBAN HD values are: Mon-Fri 17.7% 17.7% 17.7% 17.7% 17.7% Sat Sun 7% and 5% Weekly_code (for SMOKE) =20032	Use same as profile on urban local roads . Code = 2012 (see Figure 3-3, yellow curve)	Same as above

Table 3-16. Summary of spatial surrogates, temporal profiles, and speciation profiles used by diesel vehicle types for the onroad parking area-related SCCs from MOVES2010.

DIESEL VEHICLE TYPES					
SCC&Description	Surrogate	Temporal Profile: Monthly Variation	Temporal Profile: Day of Week Variation	Temporal Profile: Diurnal variation	Speciation Profile
<p>2230001350 Light Duty Diesel Vehicles (LDDV)- parking areas rural</p> <p>2230060350 Light Duty Diesel Trucks 1 through 4 (M6) (LDDT) - parking areas rural</p>	<p>Rural Population (same as rural local roads) 130</p>	<p>Not applicable – inventory contains monthly emissions</p>	<p>RURAL LD values are: Mon –Fri 12.1% 12.1% 12.1% 12.1% 18.3% Sat/Sun: 15.3% 18.3%</p> <p>Weekly_code (for SMOKE) =20021</p> <p>Rationale: choose same weekend/weekday variation for all Light Duty Vehicles on all rural road types</p>	<p>Use same as profile as rural local roads (Rdtype=210). Code = 2006 (see Figure 3-3, reddish curve)</p> <p>Rationale: choose same diurnal profile for all vehicles (except HDDV 2B to 8B) for all rural parking areas (which is the profile used for rural local roads)</p>	<p>Use same speciation profiles as what is used for LD DIESEL vehicles, irrespective of road type. i.e.: EVP_VOC: ZERO emissions (placeholder profile is required by SMOKE: 4547 (Gasoline Headspace Vapor - Circle K Diesel - adjusted for oxygenates) EXH_VOC: 4674 (Diesel Exhaust - Medium Duty Trucks)</p> <p>PM2.5 : ZERO emissions →not needed since OTAQ supplies pre-speciated emissions. Placeholder profile is required by SMOKE: 92042 (LDDV Exhaust – Simplified)</p> <p>BRK_PM2.5 and TIR_PM2.5 use same as other roadways (92009 and 92087, respectively)</p>
<p>2230001370 Light Duty Diesel Vehicles (LDDV)- parking areas urban</p> <p>2230060370 Light Duty Diesel Trucks 1 through 4 (M6) (LDDT) - parking areas urban</p>	<p>URBAN Population (same as urban local roads) 120</p>	<p>Not applicable – inventory contains monthly emissions</p>	<p>URBAN LD values are: Mon-Fri 14.8% 14.8% 14.8% 14.8% 16.0% Sat Sun 13.4% and 11.6%</p> <p>Weekly_code (for SMOKE) =20031</p> <p>Rationale: choose same weekend/weekday variation for all Light Duty Vehicles on urban road types</p>	<p>Use same as profile as urban local roads. (Rdtype=330).</p> <p>Code = 2012 (see Figure 3-3, yellow curve)</p> <p>Rationale: choose same diurnal profile for all vehicles (except HDDV 2B to 8B) for all rural parking areas (which is the profile used for rural local roads)</p>	<p>Same as above</p>

DIESEL VEHICLE TYPES					
SCC&Description	Surrogate	Temporal Profile: Monthly Variation	Temporal Profile: Day of Week Variation	Temporal Profile: Diurnal variation	Speciation Profile
<p>2230071350 Heavy Duty Diesel Vehicles (HDDV) Class 2B- parking areas rural</p> <p>2230072350 Heavy Duty Diesel Vehicles (HDDV) Class 3, 4, & 5- parking areas rural</p> <p>2230073350 Heavy Duty Diesel Vehicles (HDDV) Class 6 & 7- parking areas rural</p> <p>2230074350 Heavy Duty Diesel Vehicles (HDDV) Class 8A & 8B- parking areas rural</p>	<p>Rural primary roads code=210</p> <p>Rationale: most idling will occur at truckstops</p>	<p>Not applicable – inventory contains monthly emissions</p>	<p>RURAL HD values are: Mon-Fri 16.8% 16.8% 16.8% 16.8% 15.9% Sat Sun 8.8% and 8.8%</p> <p>Weekly_code (for SMOKE) =20022</p>	<p>Construct new profile CODE=3000 which is low at daytime and high at night-time (11pm to 2am) See Figure 3-4</p>	<p>Use same speciation profiles as what is used for HD DIESEL vehicles, irrespective of road type. i.e.: EVP_VOC: ZERO emissions (placeholder profile is required by SMOKE: 4547 (Gasoline Headspace Vapor - Circle K Diesel - adjusted for oxygenates) EXH_VOC: 4674 (Diesel Exhaust - Medium Duty Trucks)</p> <p>PM2.5: ZERO emissions →not needed since OTAQ supplies pre-speciated emissions. Placeholder profile is required by SMOKE: 92035 (HDDV Exhaust – Simplified)</p> <p>BRK_PM2.5 and TIR_PM2.5 use same as other roadways (92009 and 92087, respectively)</p>
<p>2230071370 Heavy Duty Diesel Vehicles (HDDV) Class 2B- parking areas urban</p> <p>2230072370 Heavy Duty Diesel Vehicles (HDDV) Class 3, 4, & 5- parking areas urban</p> <p>2230073370 Heavy Duty Diesel Vehicles (HDDV) Class 6 & 7- parking areas urban</p> <p>2230074370 Heavy Duty Diesel Vehicles (HDDV) Class 8A & 8B- parking areas urban</p>	<p>URBAN primary roads code=200</p> <p>Rationale: most idling will occur at truckstops</p>	<p>Not applicable – inventory contains monthly emissions</p>	<p>URBAN LD values are: Mon-Fri 14.8% 14.8% 14.8% 14.8% 16.0% Sat Sun 13.4% and 11.6%</p> <p>Weekly_code (for SMOKE) =20031</p>	<p>Construct new profile CODE=3000 which is low at daytime and high at night-time (11pm to 2am) See Figure 3-4</p>	<p>Same as above</p>

DIESEL VEHICLE TYPES					
SCC&Description	Surrogate	Temporal Profile: Monthly Variation	Temporal Profile: Day of Week Variation	Temporal Profile: Diurnal variation	Speciation Profile
2230075350 Heavy Duty Diesel Buses (School & Transit) - parking areas rural	Rural Population (same as rural local roads) 130	Not applicable – inventory contains monthly emissions	USE URBAN LD values: Mon-Fri 14.8% 14.8% 14.8% 14.8% 16.0% Sat Sun 13.4% and 11.6% Weekly_code (for SMOKE) =20031 Rationale: these vehicles follow profile of LD vehicles better than HD; day of week variation should more closely follow urban (higher weekday than weekend)	Use same as profile as rural local roads (Rdtype=210) . Code = 2006 (see Figure 3-3, reddish curve) Rationale: choose same diurnal profile for all vehicles (except HDDV 2B to 8B) for all rural parking areas (which is the profile used for rural local roads)	Same as above
2230075370 Heavy Duty Diesel Buses (School & Transit) - parking areas urban	URBAN Population (same as urban local roads) 120	Not applicable – inventory contains monthly emissions	USE URBAN LD values: Mon-Fri 14.8% 14.8% 14.8% 14.8% 16.0% Sat Sun 13.4% and 11.6% Weekly_code (for SMOKE) =20031	Use same as profile as urban local roads. (Rdtype=330) . Code = 2012 (see Figure 3-3, yellow curve) Rationale: choose same diurnal profile for all vehicles (except HDDV 2B to 8B) for all rural parking areas (which is the profile used for rural local roads)	Same as above

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