

Technical Support Document:
Preparation of Emissions Inventories
for the Version 4, 2005-based Platform

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TABLE OF CONTENTS

ACRONYMS.....	III
LIST OF TABLES.....	V
LIST OF FIGURES.....	VI
LIST OF APPENDICES.....	VI
1 INTRODUCTION.....	1
2 2005 EMISSION INVENTORIES AND APPROACHES.....	2
2.1 2005 NEI POINT SOURCES (PTIPM AND PTNONIPM)	10
2.1.1 IPM sector (<i>ptipm</i>).....	12
2.1.2 Non-IPM sector (<i>ptnonipm</i>).....	14
2.2 2005 NONPOINT SOURCES (AFDUST, AG, NONPT).....	15
2.2.1 Area Fugitive dust sector (<i>afdust</i>).....	15
2.2.2 Agricultural Ammonia sector (<i>ag</i>).....	16
2.2.3 Other nonpoint sources (<i>nonpt</i>).....	19
2.3 FIRES (PTFIRE AND AVEFIRE).....	22
2.3.1 Day-specific point source fires (<i>ptfire</i>).....	22
2.3.2 Average fires (<i>avefire</i>).....	26
2.4 BIOGENIC SOURCES (BIOG).....	28
2.5 2005 MOBILE SOURCES (ON_NOADJ, ON_MOVES_RUNPM, ON_MOVES_STARTPM, NONROAD, ALM_NO_C3, SECA_C3).....	29
2.5.1 Onroad mobile MOVES cold-start exhaust sources requiring temperature adjustments (<i>on_moves_startpm</i>).....	31
2.5.2 Onroad mobile MOVES running exhaust sources requiring temperature adjustments (<i>on_moves_runpm</i>).....	33
2.5.3 Onroad no-adjustments mobile sources (<i>on_noadj</i>).....	34
2.5.4 Nonroad mobile sources –NMIM-based nonroad (<i>nonroad</i>)	35
2.5.5 Nonroad mobile sources: locomotive and non-C3 commercial marine (<i>alm_no_c3</i>)	36
2.5.6 Nonroad mobile sources: C3 commercial marine (<i>seca_c3</i>).....	38
2.6 EMISSIONS FROM CANADA, MEXICO AND OFFSHORE DRILLING PLATFORMS (OTHPT, OTHAR, OTHON)	42
2.7 SMOKE-READY NON-ANTHROPOGENIC INVENTORIES FOR MERCURY AND CHLORINE	44
2.7.1 Mercury	44
2.7.2 Chlorine	45
3 EMISSIONS MODELING SUMMARY.....	45
3.1 KEY EMISSIONS MODELING SETTINGS.....	46
3.1.1 Spatial configuration	47
3.1.2 Chemical speciation configuration	49
3.1.3 Temporal processing configuration.....	56
3.2 EMISSIONS MODELING ANCILLARY FILES.....	58
3.2.1 Spatial allocation ancillary files.....	58
3.2.2 Chemical speciation ancillary files.....	62
3.2.3 Temporal allocation ancillary files.....	66
4 DEVELOPMENT OF FUTURE YEAR EMISSION INVENTORIES.....	69
5 REFERENCES.....	70

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
IMO	International Marine Organization
IPM	Integrated Planning Model
ITN	Itinerant
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
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

List of Tables

Table 2-1. Platform sectors used in emissions modeling for the 2005 Platform	3
Table 2-2. Summary of significant changes between 2002 and 2005 Platforms by sector	6
Table 2-3. Summaries by sector of 2002 and 2005 Platform base year CAPs-only emissions for the continental United States (48 states + District of Columbia).....	9
Table 2-4. Summaries by sector for the other (“oth” –Canada, Mexico, and offshore- 2002 and 2005 Platform base year CAPs-only emissions within the 36km domain.....	10
Table 2-5. SCCs in the afdust platform sector	16
Table 2-6. Livestock SCCs extracted from the 2002 NEI to create the ag sector	17
Table 2-7. Fertilizer SCCs extracted from the 2002 NEI for inclusion in the “ag” sector	19
Table 2-8. Oil and gas production nonpoint emissions in WRAP states in 2002 and 2005 platforms. Emissions provided in short tons/year.....	20
Table 2-9. New SCCs from the Phase II WRAP Oil and Gas Inventory.....	20
Table 2-10. RWC Emissions Changes for CAPs between 2002 and 2005 platforms. Emissions values provided in short tons/year.	21
Table 2-11. 2005 NEI SCCs representing emissions in the ptfire and avefire modeling sectors	22
Table 2-12. SCCs in the ptfire sector	23
Table 2-13. Average fire VOC changes from 2002 to 2005 platform. Emissions provided in short tons/year	27
Table 2-14. HAP emission factors applied to avefire PM _{2.5} emissions	27
Table 2-15. Pollutants covered by the draft MOVES model in the 2005 Platform ¹	29
Table 2-16. SCCs in the 2005 alm_no_c3 inventory compared to the 2002 platform alm sector	36
Table 2-17. Regional growth factors used to project 2002 C3 emissions to 2005	40
Table 2-18. Contiguous U.S. C3 CMV emissions in 2002 and 2005 platforms.....	40
Table 2-19. HAP emission ratios for generation of HAP emissions from criteria emissions for C3 commercial marine vessels.....	41
Table 2-20. Summary of the othpt, othpt_hg, othar, othar_hg, and othon sectors in the 2005 Platform.....	43
Table 3-1. Key emissions modeling steps by sector	46
Table 3-2. Descriptions of the 2005-based Platform Grids	48
Table 3-3. Model Species produced by SMOKE for CB05 with SOA for CMAQ4.7	50
Table 3-4. Integration status of benzene, acetaldehyde, formaldehyde and methanol (BAFM) for each platform sector	53
Table 3-5. Source-category specific criteria for integrating nonpt SCCs for categories comprising 80% of the nonpoint VOC emissions.....	54
Table 3-6. Temporal Settings Used for the Platform Sectors in SMOKE	57
Table 3-7. U.S. Surrogates Available for the 2002 and 2005 Platforms	59
Table 3-8. Surrogate assignments to new mobile categories in the 2005 Platform	60
Table 3-9. Canadian Spatial Surrogates for 2005-based platform Canadian Emissions	61
Table 3-10. Differences between two profiles used for coal combustion.....	64
Table 3-11. Summary of VOC speciation profile approach by sector for 2005	65
Table 3-12. Temporal Profiles Assigned to New Onroad SCC from the Draft MOVES model: Parking Areas.....	68

List of Figures

Figure 2-1. SMARTFIRE System	24
Figure 2-2. MOVES exhaust temperature adjustment functions.	32
Figure 3-1. CMAQ modeling domains	48
Figure 3-2. Process of integrating BAFM with VOC for use in VOC Speciation.....	52
Figure 3-3. Diurnal Profiles are based only on road type (use local for “start”) and whether the road is urban versus rural.....	69

List of Appendices

Appendix A. Methodology to Revise VOC from Residential Wood Combustion	
Appendix B. Methodology to Speciate Partially-Speciated MOVES PM2.5 Emissions	

1 Introduction

The U.S. Environmental Protection Agency (EPA), hereto referred to as “we,” has developed a 2005-based air quality modeling platform. This document describes the emissions inventory and emissions modeling for a version of the platform consisting of Criteria Air Pollutants (CAPs) and the following select Hazardous Air Pollutants (HAPs: mercury (Hg), chlorine (Cl), hydrochloric acid (HCl) and benzene, acetaldehyde, formaldehyde and methanol. The latter four are also denoted BAFM. This platform is called the “CAP-BAFM 2005-Based Platform, Version 4” platform, since it is primarily a CAP platform, with BAFM and Hg included. The reason it is “Version 4” is that it has been updated from the 2002-based platform, version 3. It is based on the 2005 National Emission Inventory (NEI), version 2 (<http://www.epa.gov/ttn/chief/net/2005inventory.html>). From this point on, we refer to it simply as the “2005 Platform.” This document describes the approach and data used to produce the emission inputs to the air quality models used in the 2005 Platform. A version of the 2005-based platform that contains additional HAPs is documented as part of the Revised Annual Renewable Fuel Standard (RFS2) rule (EPA, 2010).

Emissions preparation for the 2005 Platform supports two air quality models: (1) the Community Multiscale Air Quality (CMAQ) model (<http://www.epa.gov/AMD/CMAQ/>) and (2) the Comprehensive Air Quality Model, with extensions (CAMx) (<http://www.camx.com/>). Both models support modeling ozone (O₃) and particulate matter (PM) 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), and individual component species for particulate matter less than or equal to 2.5 microns (PM_{2.5}). In addition, the CMAQ CB05 with chlorine chemistry, which is part of the “base” version of CMAQ, allows explicit treatment of BAFM and includes anthropogenic HAP emissions of HCl and Cl. Readers may note that the base version of CMAQ targeted by the 2005 Platform described here does not support Hg, but that this modeling platform does include Hg for 2005.

The effort to create the emission inputs for the 2005 Platform included

- (1) development of emission inventories for a 2005 model evaluation case,
- (2) development of emission inventories for a 2005 base case and projected years consistent with that base,
- (3) updates to the emissions modeling tools,
- (4) updates to the emissions modeling ancillary files used with the tools, and
- (5) application of the tools.

The primary emissions modeling tool used to create the CMAQ model-ready emissions was the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system. We used this tool to create emissions files for a 36-km national grid, a 12-km Eastern grid and a 12-km Western grid for the following cases:

- 2005 evaluation (also known as the “2005ak” case): The purpose of this case is to compare the air quality model results to ambient air observations to assess the ability of the air quality model to estimate ambient air concentrations of ozone and PM_{2.5} levels.

For regulatory applications, this case is not included in the relative response factor (RRF) calculations.

- 2005 base case (also known as the “2005ck” case): 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 RRF calculations.

A final version of this documentation will also contain sections on the development of the 2020 (2020ck) base case.

Other 2005 and future-year base case emissions have been developed but are associated with specific regulatory actions and are therefore documented as part of those rules (e.g., RFS2, Light Duty Greenhouse Gas Rule).

There are two differences between the 2005 evaluation and the 2005 base case. The evaluation case uses 2005-specific fire emissions and 2005 hour-specific continuous emission monitoring (CEM) data for electric generating units (EGUs). The 2005 base case includes an “average year” scenario for fires, described in Section 2.3.2. For EGUs, the base case allocates the 2005 emissions to days and hours using a different approach; this method is also used when creating the future-year emissions.

The version 4 2005-based Platform builds upon the concepts, tools and emissions modeling data from EPA’s version 3 2002-based Platform, documented by:

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

A summary of the key differences between the 2005 Platform and the 2002 Platform are provided in Table 2-1.

This document contains five sections and two 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. Section 4, to be added in a future version of this document, describes the development of the 2020 inventory (projected from 2005). Section 5 provides references. Appendices A and B 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-BAFM 2005-Based Platform”. This is referred to as the “2005v4 website” throughout this document.

2 2005 emission inventories and approaches

This section describes the 2005 emissions data created for input to SMOKE. The primary basis for the 2005 emission inputs for the version 4 Platform 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 2005 platform utilizes select HAPs: the base version includes chlorine, HCl, Hg, benzene, acetaldehyde, formaldehyde, and methanol. The RFS2

version of the platform (EPA, 2010) utilized the following additional HAPs: acrolein, 1,3-butadiene, naphthalene, toluene and xylenes (m,o,p and mixed).

Documentation for the 2005 NEI can be found at:

<http://www.epa.gov/ttn/chief/net/2005inventory.html#documentation>. Version 2 of the 2005 NEI was used for the 2005 Platform. 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. The fires portion of the inventory includes emissions from wildfires and prescribed burning computed as hour-specific point sources. For purposes of preparing the CMAQ-ready emissions, we split the 2005 emissions inventory into several additional “platform” sectors for use in emissions modeling, and we added biogenic emissions, emissions from the Canadian and Mexican inventories, and augmented with other emissions data to be explained below. 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 temporalized emissions together to create the CMAQ or CAMx emission inputs.

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. We did not use all sectors for all modeling cases; in particular, we used the ptfire platform sector only for the 2005 model performance evaluation. We used the avefire platform sector for all modeling cases except for the model performance evaluation. The rationale for using average fires in the 2005 base case and future-year cases rather than the 2005 year-specific fires (ptfire) is described in Section 2.3.2. Updates from the 2002 platform are discussed in Table 2-2.

Table 2-1. Platform sectors used in emissions modeling for the 2005 Platform

Platform Sector	2005 NEI Sector	Description and resolution of the data input to SMOKE
IPM sector: <i>ptipm</i>	Point	2005v2 NEI point source EGUs mapped to the Integrated Planning Model (IPM) model using the National Electric Energy Database System (NEEDS, 2006 version 3.02) database. Hourly files for continuous emission monitoring (CEM) sources are included only for the 2005 evaluation case. Day-specific emissions for non-CEM sources created for input into SMOKE.
Non-IPM sector: <i>ptnonipm</i>	Point	All 2005v2 NEI point source records not matched to the ptipm sector, annual resolution. Includes all aircraft emissions.
Point source fire sector: <i>ptfire</i>	Fires	Point source day-specific wildfires and prescribed fires for 2005. This sector used only for the 2005 evaluation case.
Average-fire sector: <i>avefire</i>	N/A	Average-year wildfire and prescribed fire emissions derived from the 2002 Platform avefire sector, county and annual resolution. Used for the 2005 base year and the future base model runs, but not for the model evaluation case.

Platform Sector	2005 NEI Sector	Description and resolution of the data input to SMOKE
Agricultural sector: <i>ag</i>	Nonpoint	NH ₃ emissions from NEI nonpoint livestock and fertilizer application, county and annual resolution.
Area fugitive dust sector: <i>afdust</i>	Nonpoint	PM ₁₀ and PM _{2.5} from fugitive dust sources from the NEI nonpoint inventory (e.g., 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 and year 2005 non-California Western Regional Air Partnership (WRAP) oil and gas “Phase II” inventory.
Nonroad sector: <i>nonroad</i>	Mobile: Nonroad	Monthly nonroad emissions from the National Mobile Inventory Model (NMIM) using NONROAD2005 version nr05c-BondBase 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	Year 2002 non-rail maintenance locomotives, and category 1 and category 2 commercial marine vessel (CMV) emissions sources, county and annual resolution. Unlike prior platforms, aircraft emissions are now included in the ptnonipm sector and category 3 CMV emissions are now contained in the seca_c3 sector
C3 commercial marine: <i>seca_c3</i>	Mobile : Nonroad	Annual point source formatted year 2005 category 3 (C3) CMV emissions, developed for the EPA rule called “Control of Emissions from New Marine Compression-Ignition Engines at or Above 30 Liters per Cylinder”, usually described as the Emission Control Area (ECA) study, originally called SO ₂ (“S”) ECA.
Onroad California, NMIM-based, and MOVES sources not subject to temperature adjustments: <i>on_noadj</i>	Mobile: onroad	Three, monthly, county-level components: 1) Onroad emissions from NMIM using MOBILE6.2, other than for California. 2) California onroad, created using annual emissions submitted by CARB for the 2005v2 NEI. 3) Onroad gasoline non-motorcycle vehicle emissions from draft MOVES not subject to temperature adjustments: exhaust CO, NO_x, VOC, some VOC HAPs, and evaporative VOC and some VOC Hazardous Air Pollutants (HAPs).
Onroad cold-start gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: <i>on_moves_startpm</i>	Mobile: onroad	Monthly, county-level draft MOVES-based onroad non-motorcycle 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 on_moves_runpm sector).
Onroad running gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: <i>on_moves_runpm</i>	Mobile: onroad	Monthly, county-level draft MOVES-based onroad non-motorcycle 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 on_moves_startpm sector).

Platform Sector	2005 NEI Sector	Description and resolution of the data input to SMOKE
Biogenic: <i>biog</i>	N/A	Hour-specific, grid cell-specific emissions generated from the BEIS3.14 model -includes emissions in Canada and Mexico.
Other point sources not from the NEI: <i>othpt</i>	N/A	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.
Other point sources not from the NEI, Hg only: <i>othpt_hg</i>	N/A	Annual year 2000 Canada speciated mercury point source emissions.
Other nonpoint and nonroad not from the NEI: <i>othar</i>	N/A	Annual year 2006 Canada (province resolution) and year 1999 Mexico Phase III (municipio resolution) nonpoint and nonroad mobile inventories, annual resolution.
Other nonpoint sources not from the NEI, Hg only: <i>othar_hg</i>	N/A	Annual year 2000 Canada speciated mercury from nonpoint sources.
Other onroad sources not from the NEI: <i>othon</i>	N/A	Year 2006 Canada (province resolution) and year 1999 Mexico Phase III (municipio resolution) onroad mobile inventories, annual resolution.

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

Before discussing the specific components of the 2005 emissions platform, we provide a summary of the significant differences between the 2002 V3 emissions platform and this 2005 platform. Table 2-2 shows the emissions inventory updates from 2002 V3 to this 2005 platform. New sectors appear in the 2005 platform and some sources migrate to different sectors. Table 2-2 does not discuss the modifications to these inventories for emissions modeling; these details are provided in the sections that follow.

Table 2-2. Summary of significant changes between 2002 and 2005 Platforms by sector

Platform Sector	Summary of Significant Inventory Differences in 2005 Platform
IPM sector: <i>ptipm</i>	– Updated from 2002 NEI version 3 to 2005 NEI version 2 point inventory. – Updated hourly CEM data from 2002 to 2005. – Updated day-specific CEM and non-CEM data using temporal information based on years 2004 through 2006, rather than 2001 through 2003. – Updated NEEDS database to NEEDS 2006, version 3.02. – EGUs from 2002 platform assigned to ptnonipm sector have been reassigned to the ptipm sector.
Non-IPM sector: <i>ptnonipm</i>	– Updated from 2002 NEI version 3 to 2005 NEI version 2 point inventory. – Now includes all aircraft emissions (no longer in alm_no_c3 sector). – EGUs from 2002 platform assigned to ptnonipm sector have been reassigned to the ptipm sector.
Point source fire sector: <i>ptfire</i>	– Updated to include all wildfire and prescribed burning emissions for 2005. The 2002 platform contained some county-level monthly prescribed burning emissions that were included in the nonptfire sector. In contrast, all 2005 fires data used for modeling are resolved as point sources at day-specific temporal resolution. Therefore, there is no nonptfire sector in the 2005 platform. – This sector uses BAFM emissions from the inventory for BAFM model species as part of VOC speciation (as opposed to getting BAFM model species from solely speciating VOC as was done in the 2002 CAP-only platform)
Average-fire sector: <i>avefire</i>	Same as 2002 Platform with the following exceptions: 1) VOC revised higher, now as a factor of CO; 2) Avefire inventory data contains HAPs, computed as factor from PM_{2.5}; however, these data were not used during processing of the emissions (they are provided in the inventory files)
Agricultural sector: <i>ag</i>	Unchanged from 2002 Platform.
Area fugitive dust sector: <i>afdust</i>	Transport fraction for PM _{2.5} , inadvertently not applied in the original 2002 platform, is correctly applied in 2005 platform.
Remaining nonpoint sector: <i>nonpt</i>	Similar to the 2002 Platform except for the following: 1) Replaced non-California WRAP oil and gas emissions with WRAP Phase II oil and gas emissions; 2) Residential Wood Combustion (RWC) emissions updated for PM and VOC for Oregon and New York, VOC emissions factor corrected for all states except California, and, VOC HAPs computed; 3) HCl corrections made to GA, UT, and VA for Industrial and Commercial/Institutional coal-fueled boilers; 4) Use BAFM emissions from the inventory as part of VOC speciation for some sources in this sector.¹
Nonroad sector: <i>nonroad</i>	2002 platform emissions replaced with 2005 NEI version 2 emissions. 1) California 2002v3 emissions replaced with CARB-submitted 2005v2 emissions with NH₃ and some HAPs computed separately. 2) The remaining states emissions simply replaced with 2005v2 NMIM. Use BAFM as part of VOC speciation for the nearly the entire sector¹ (only LPG and CNG fueled sources did not have BAFM emissions; these were the only sources for which we did not use BAFM.)

Platform Sector	Summary of Significant Inventory Differences in 2005 Platform
locomotive, and non-C3 commercial marine: <i>alm_no_c3</i>	Locomotives, and Category 1 and Category 2 CMV emissions are the same as 2002 Platform alm sector. 2005 Platform does not include these emissions in this sector: 1) aircraft –these are in the 2005 ptnonipm sector; 2) Category 3 CMV –these are replaced by 2005 seca_c3 sector inventory; 3) Tribal data removed due to lack of spatial surrogates. Use BAFM emissions from the inventory as part of VOC speciation for some sources in this sector. ¹
C3 commercial marine: <i>seca_c3</i>	New sector for 2005 Platform. These point source C3 CMV emissions replace a subset of the 2002 Platform alm sector emissions, specifically, port and underway residual fuel C3 county-level emissions. Use BAFM emissions from the inventory as part of VOC speciation for all sources in this sector. ¹
Onroad California, NMIM-based, and MOVES sources not subject to temperature adjustments: <i>on_noadj</i>	2002 platform emissions replaced with updated 2005 emissions as follows: 1) California –2005 CAP and HAP emissions. Supplied by CARB, gap-filled with NMIM NH ₃ and allocated to road types using NMIM –based ratios. 2) Draft MOVES (except for California) onroad gasoline emissions for exhaust and evaporative mode for all vehicle types except motorcycles for the pollutants NO _x , VOC, CO, benzene, acetaldehyde, formaldehyde, 1,3-butadiene, acrolein, and naphthalene. 3) All other emissions not covered by (1) and (2) above used the 2005 NEI version 2 emissions, except for PM ₁₀ and PM _{2.5} emissions included in the on_moves_startpm and on_moves_runpm sectors, as described below. Use BAFM emissions from the inventory as part of VOC speciation for all sources in this sector. ¹
Onroad cold-start gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: <i>on_moves_startpm</i>	For the 2005 platform, this new sector includes the draft MOVES onroad gasoline, non-motorcycle PM and naphthalene cold start mode emissions subject to grid cell and hourly temperature adjustments. Temperature adjustments for cold starts (here) are different than running mode emissions, hence the need to separate these emissions into these new sectors, on_moves_startpm and on_moves_runpm.
Onroad running gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: <i>on_moves_runpm</i>	For the 2005 platform, this new sector includes the draft MOVES onroad gasoline, non-motorcycle PM and naphthalene running mode emissions subject to grid cell and hourly temperature adjustments. Temperature adjustments for running mode (here) are different than cold start mode emissions, hence the need to separate these emissions into these new sectors, on_moves_startpm and on_moves_runpm.
Biogenic: <i>biog</i>	Updated from BEIS3.13 in the 2002 platform to BEIS3.14 in the 2005 platform. Underlying land use data was not updated. Domains in both 2002 and 2005 platforms are the same: U.S., Canada, and Mexico.
Other point sources not from the NEI: <i>othpt</i>	New offshore oil emissions from 2005 NEI version 2 point inventory. Canadian emissions updated from year 2000 to 2006, and using point-specific speciated emissions and facility-specific temporal allocation.
Other point sources not from the NEI, Hg only: <i>othpt_hg</i>	This sector was not in the “CAP-only” version of the 2002 Platform, but it was in the multi-pollutant version. It contains the same data as in the 2002 multi-pollutant platform: year 2000 Canadian point source mercury emissions.

Platform Sector	Summary of Significant Inventory Differences in 2005 Platform
Other nonpoint and nonroad not from the NEI: <i>othar</i>	Canadian emissions updated from year 2000 to 2006.
Other nonpoint sources not from the NEI, Hg only: <i>othar_hg</i>	New sector in the 2005 platform, contains year 2000 Canadian point source mercury emissions.
Other onroad sources not from the NEI: <i>othon</i>	Canadian emissions updated from year 2000 to 2006.

¹ Section 3.1.2.1 details the use of BAFM emissions from the inventory as part of VOC speciation; this is one of the changes between the 2005 Platform and the 2002 Platform for several sectors.

Annual emission summaries for 2005, with comparisons to 2002 CAPs emissions by emissions modeling sector are provided in Table 2-3. VOC totals are before BAFM speciation; they are inventory VOC emissions, and not the sum of VOC emissions after BAFM speciation. Table 2-4 provides a summary of emission changes for CAPs only for Canada and off shore oil between the 2002 and 2005 platforms. The Mexico emissions are unchanged from 2002 platform.

The emission inventories for input to SMOKE for the 2005 base and evaluation 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 provided indicates the particular zipped files associated with each platform sector.

Table 2-3. Summaries by sector of 2002 and 2005 Platform base year CAPs-only emissions for the continental United States (48 states + District of Columbia)

Year	Sector	[tons/yr] VOC	[tons/yr] NO _x	[tons/yr] CO	[tons/yr] SO ₂	[tons/yr] NH ₃	[tons/yr] PM ₁₀	[tons/yr] PM _{2.5}
2002	afdust						8,858,989	1,830,273
	ag					3,251,990		
	alm ^{1,2}	123,458	2,258,985	806,170	312,180	904	96,981	86,719
	nonpt	7,929,917	1,531,603	7,526,721	1,250,266	135,542	1,377,055	1,100,884
	nonroad	2,873,623	2,176,159	21,386,058	187,284	1,859	227,875	216,658
	onroad ³	4,847,990	7,786,709	59,810,864	242,379	290,708	200,686	146,003
	ptipm	42,378	4,618,946	605,147	10,359,117	29,991	608,708	501,999
	ptnonipm	1,425,158	2,368,988	3,195,465	2,249,548	154,180	600,355	372,330
	avefire	1,958,992	189,428	8,554,551	49,094	36,777	796,229	684,035
	ptfire+nonptfire ⁴	1,825,284	82,613	8,039,286	67,229	123,414	742,980	629,635
2002 non-fires Total		17,242,523	20,741,388	93,330,425	14,600,775	3,865,173	11,970,649	4,254,865
2005	afdust						8,858,992	1,030,391
	ag					3,251,990		
	alm_no_c3 ^{1,2}	67,690	1,924,925	270,007	154,016	773	59,366	56,687
	seca_c3 ^{1,2,5}	22,336	641,228	53,677	416,793		53,519	49,237
	nonpt	7,474,512	1,683,490	7,376,314	1,252,645	134,080	1,349,685	1,076,954
	nonroad	3,480,959	2,115,408	19,502,718	197,341	1,972	209,100	198,734
	on_noadj ³	3,123,642	7,203,876	41,647,066	144,216	295,203	170,554	115,991
	on_moves_runpm ³						46,430	42,753
	on_moves_startpm ³						23,607	21,738
	ptipm	40,950	3,728,190	601,564	10,381,411	21,684	615,095	508,903
	ptnonipm ²	1,310,085	2,247,228	3,222,221	2,117,649	159,003	653,957	442,656
	avefire	451,127	189,428	8,554,551	49,094	36,777	796,229	684,035
	ptfire	2,962,421	193,371	12,529,792	101,012	206,081	1,294,651	1,097,162
2005 non-fires Total		15,520,175	19,544,345	72,673,566	14,664,071	3,864,706	12,040,304	3,544,046
% Difference (2005 - 2002) /2002 Emiss- ions	afdust						0%	-44%
	ag					0%		
	alm ^{1,2}	-27%	14%	-60%	83%	-14%	16%	22%
	nonpt	-6%	10%	-2%	0%	-1%	-2%	-2%
	nonroad	21%	-3%	-9%	5%	6%	-8%	-8%
	onroad ³	-36%	-7%	-30%	-40%	2%	20%	24%
	ptipm	-3%	-19%	-1%	0%	-28%	1%	1%
	ptnonipm ²	-8%	-5%	1%	-6%	3%	9%	19%
	avefire	-77%	0%	0%	0%	0%	0%	0%
% Difference non-fires Total		-10%	-6%	-22%	0%	0%	1%	-17%

1 –alm sector in % Difference calculation consists of alm from 2002 platform and aggregated alm_no_c3 and seca_c3 from the 2005 platform.

2- Note: aircraft in 2005 platform is contained in the ptnonipm sector.

3 –onroad sector in % Difference calculation consists of onroad from 2002 platform and aggregates on_noadj, on_moves_runpm, and on_moves_startpm from the 2005 platform.

4 – nonptfire emissions are in the 2002 platform only; these are covered by the ptfire sector in the 2005 platform.

5 – only U.S. state/county seca_c3 emissions are included here; emissions outside the (up to) 200nm offshore boundary and international boundaries, while included in our modeling, are not included in these summaries.

Table 2-4. Summaries by sector for the other (“oth” –Canada, Mexico, and offshore- 2002 and 2005 Platform base year CAPs-only emissions within the 36km domain.

Year	Sector	[tons/yr] VOC	[tons/yr] NO _x	[tons/yr] CO	[tons/yr] SO ₂	[tons/yr] NH ₃	[tons/yr] PM ₁₀	[tons/yr] PM _{2.5}
2002	Canada othar	1,878,996	1,060,097	4,282,782	227,942	569,738	1,462,643	400,493
	Canada othon	410,981	874,564	5,810,763	26,376	18,332	19,692	18,071
	Canada othpt	308,286	654,803	1,155,470	2,115,572	23,866	241,081	129,342
	Canada Subtotal	2,598,262	2,589,464	11,249,016	2,369,890	611,937	1,723,417	547,906
	Mexico othar	586,842	249,045	644,733	101,047	486,484	143,816	92,861
	Mexico othon	183,429	147,419	1,455,121	8,270	2,547	6,955	6,372
	Mexico othpt	113,044	258,510	88,957	980,359	0	125,385	88,132
	Mexico Subtotal	883,314	654,974	2,188,811	1,089,676	489,031	276,156	187,366
	Off-shore othpt	70,329	26,628	6,205	0	0	0	0
2002 Total		3,551,905	3,271,066	13,444,032	3,459,566	1,100,967	1,999,573	735,271
2005	Canada othar ¹	1,281,095	734,587	3,789,362	95,086	546,034	1,666,188	432,402
	Canada othon	270,872	524,837	4,403,745	5,309	21,312	14,665	10,395
	Canada othpt	447,313	857,977	1,270,438	1,664,040	21,268	117,669	68,689
	Canada Subtotal	1,999,279	2,117,402	9,463,544	1,764,434	588,614	1,798,523	511,486
	Mexico othar	586,842	249,045	644,733	101,047	486,484	143,816	92,861
	Mexico othon	183,429	147,419	1,455,121	8,270	2,547	6,955	6,372
	Mexico othpt	113,044	258,510	88,957	980,359	0	125,385	88,132
	Mexico Subtotal	883,314	654,974	2,188,811	1,089,676	489,031	276,156	187,366
	Off-shore othpt	51,240	82,581	89,812	1,961	0	839	837
2005 Total		2,933,833	2,854,957	11,742,168	2,856,070	1,077,645	2,075,518	699,688
Percent Difference (2005 – 2002)/2002 emissions	Canada othar ¹	-32%	-31%	-12%	-58%	-4%	14%	8%
	Canada othon	-34%	-40%	-24%	-80%	16%	-26%	-42%
	Canada othpt	45%	31%	10%	-21%	-11%	-51%	-47%
	Canada Subtotal	-23%	-18%	-16%	-26%	-4%	4%	-7%
	Mexico othar	0%	0%	0%	0%	0%	0%	0%
	Mexico othon	0%	0%	0%	0%	0%	0%	0%
	Mexico othpt	0%	0%	0%	0%		0%	0%
	Mexico Subtotal	0%	0%	0%	0%	0%	0%	0%
	Off-shore othpt	-27%	210%	1348%				
% Difference Total		-17%	-13%	-13%	-17%	-2%	4%	-5%

1- Canada provided year 2006 fires but we did not include them in our 2005 platform.

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 these 2005 platform emissions changed appreciably since the previously-documented 2002 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 contiguous

U.S. NEI point sources. The offshore oil platform (othpt sector) and category 3 CMV emissions (seca_c3 sector) are point source formatted inventories, but they are discussed later in Section 2.

After removing offshore oil platforms (othpt sector), we created two platform sectors from the remaining 2005 point source NEI, v2 for input into SMOKE: the Integrated Planning Model (IPM) sector (ptipm) and the non-IPM sector (ptnonipm). This split facilitates the use of different SMOKE temporal processing and future year projection techniques for 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, Hg and Cl. We did not utilize BAFM from these sectors as we chose to speciate VOC without any integration of VOC HAP (integration is discussed in detail in Section 3.1.2.1).

The ptnonipm emissions were provided to SMOKE as annual emissions. The ptipm emissions used in 2005 were different for the model evaluation case and for the base case. For the model evaluation case, those ptipm sector sources with CEM data (that we could match to the NEI) used hourly SO₂ and NO_x emissions and annual emissions of all other pollutants. The hourly data also contained heat input, which was used to allocate the annual emissions to hourly values. For the non-CEM sources, we created daily emissions using an approach described in Section 2.1.1, and applied state-specific diurnal profiles to create hourly emissions. Finally, for the base case, all sources (both CEM and non-CEM) used the daily emissions and diurnal profiles approach.

Full 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. 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 2002 NEI v3 emissions to obtain 2005 estimates.
2. Non-EGU Stationary Source enhancements 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 NEI point sources 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 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 for 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.

2.1.1 IPM sector (ptipm)

The ptipm sector contains emissions from EGUs in the 2005 NEI version 2 point inventory that we were able to match to the units found in the 2006 NEEDS database, version 3.02 (<http://www.epa.gov/airmarkets/progsregs/epa-ipm/index.html>), which is used by the IPM, version 3.02. 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 in order 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 2005 NEI point source inventory contains emissions estimates for both EGU and non-EGU sources. The IPM is used to predict the future year emissions for the EGU sources. The remaining non-EGU point sources are projected by applying projection and control factors to the base year emissions. It was therefore necessary to identify and separate into two sectors: (1) all sources that are projected via the IPM and (2) those that are not. This procedure prevents double-counting or dropping significant emissions when creating the future-year emissions. The matching process relies on imperfect data; consequently, we experienced a small degree of dropped and/or double-counted emissions for sources that we could not match. We believe that the unmatched units are small emissions sources because we have reviewed both the NEI and the NEEDS database to ensure that all significant EGUs have been captured in the matching process.

The methodology that follows describes how we split the point inventory into the ptipm and ptnonipm sectors. The approach started with the splits identified for the 2002 NEI (step 1) and then included additional steps to apply these to the 2005 NEI.

Methodology to split the EGU from the non-EGU sources

Step 1: Obtain facilities and units identified as EGUs from the 2002 NEI

We identified 2002 NEI units as IPM units using the 2006 NEEDS 3.0 database. This methodology is described in the 2002 Platform documentation previously referenced. Since some source identifiers are held constant between the 2002 and 2005 NEI, particularly “NEI

Unique ID”, we were able to more easily compare the two inventories to ensure that we made improvements in the 2005 matching rather than inadvertent omissions.

Step 2: Create the 2005 NEI v2 point modeling inventory from the 2005v2 NEI and impacts on EGU matching

We further enhanced the published 2005 NEI v2 point inventory to improve the ptipm and ptnonipm splits and make other updates. What follows are the issues and how we resolved them, and these represent differences between the published 2005 v2 NEI and what we used for modeling.

- 1) We identified facilities added with HAP emissions records that were clearly EGUs, but had not been flagged as “IPM” sources. These facilities had facility identifiers (i.e., plant IDs) beginning with “EGU”. We further confirmed that these records were EGU emissions; and therefore, we moved these units to the ptipm sector.
- 2) We found one additional unit with HAP emissions records not flagged as an EGU, but that we confirmed were representing emissions from a facility for which we had identified CAP records as ptipm sector records. We moved this unit (South Mississippi Electric Power, plantid = 2807300021, unitid = 012, NEI_UNIQUE_ID=NEI409) into the ptipm inventory.
- 3) Several facilities and units closed between 2002 and 2005 and had not initially been removed in the development of the 2005v2 NEI; we removed these based on a list from the NEI developers.
- 4) Inspection of CEM and 2005 NEI v2 point inventory revealed some duplication of sources with state and non-state reported data. This can occur because EPA created the EGU records in the 2005 NEI, but the states sometimes still submitted these emissions records. We removed these duplicates.
- 5) ORIS facility and boiler codes (used to match to the CEM hourly data) were unintentionally dropped between a preliminary and final 2005 NEI v2 point dataset. We completely repopulated these ORIS facility and boiler codes based on what we had in hand.

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. The ptipm sector uses the available hourly CEM data via a method first implemented in the 2002 platform that was also used for the 2005 platform. For sources with CEMs, we used the actual hourly CEM data for the 2005 evaluation case. The hourly CEM data were obtained from the CAMD Data and Maps website². The SMOKE modeling system matches the ORIS Facility and Boiler IDs in the NEI SMOKE-ready file to the same fields in the CEM data. This allowed us to use the hourly SO₂ and NO_x CEM emissions directly from the CEM data file. We used the heat input from the hourly CEM

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

data to allocate the NEI annual values for all other pollutants from CEM sources, because hourly data for these other pollutants are not available with the hourly CEM data.

For sources not matching the CEM data (“non-CEM” sources), we computed daily emissions from the NEI annual emissions using a structured query language (SQL) program and state-average CEM data. To allocate annual emissions to each month, we created state-specific, three-year averages of 2004-2006 CEM data. These average annual-to-month factors were assigned to non-CEM 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 in 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.

For the 2005 base case, we do not use year-specific CEM data, and for future-year scenarios, there are no CEM data available for specific units. Thus, for the base and future-year cases, we used the same procedures as for “non-CEM” sources to compute daily emissions for input to SMOKE for all ptipm sources.

2.1.2 Non-IPM sector (ptnonipm)

The non-IPM (ptnonipm) sector contains all 2005 NEI v2 point sources that we did not include in the IPM (ptipm) sector³. The ptnonipm sector contains fugitive dust PM emissions from vehicular traffic on paved or unpaved roads at industrial facilities or coal handling at coal mines⁴. Prior to input to SMOKE, we reduced the fugitive dust PM emissions to estimate the emissions 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 most significant changes we made to the ptnonipm emissions involved moving some HAP records that should have been flagged as IPM into the ptipm sector (discussed in section 2.1.1). The other modifications are listed here and represent differences between the published 2005 NEI v2 and the 2005 inventory we used for modeling:

- 1) Removed duplicate annual records. We correctly did not delete sub-annual, non-repeating records.

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.

⁴Point 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.

- 2) 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.
- 3) Dropped sources with coordinates located well into the oceans or lakes.
- 4) 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 NO_x, 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.

2.2 2005 Nonpoint sources (*afdust*, *ag*, *nonpt*)

The 2005 NEI v2 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 as 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 costly 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 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 (2002) platform afdust sector (which are a subset of the SCCs in the web link) are provided in Table 2-5.

Table 2-5. 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 the approach 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 2005 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)

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 2-6, and the fertilizer SCCs are listed in Table 2-7.

Table 2-6. 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 399999999 (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. This will be discussed further in Section 4 in the final version of this documentation.

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

Table 2-7. 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. This sector is similar to the nonpt sector in the 2002 Platform, which uses the 2002 NEI v3 emissions. The differences are that:

- The 2005 platform replaces 2002 NEI v3 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.
- 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.
- 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.

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 2005 platform.

2005 Phase II WRAP oil and gas inventory

NEI 2002 Industrial Processes, Oil and Gas Production emissions (SCC=2310000000) were removed from all non-California WRAP states and the WRAP 2005 Phase II oil and gas emissions were added. As seen in Table 2-8, the 2002 NEI nonpt inventory contains a very small amount of emissions for this category. The 2002 NEI oil and gas nonpt emissions were limited to VOC in Arizona, Montana, Nevada, New Mexico, North and South Dakota, and Wyoming, and negligible CO and NO_x emissions in New Mexico. In contrast, the 2005 WRAP oil and gas inventory contains much higher emissions, reflecting greatly improved information on the activity and equipment and emission factors for this sector for all WRAP states except for California (and Washington): AK, AZ, CO, MT, NV, NM, ND, OR, SD, UT, WY. The motivation and development of the Phase II WRAP oil and gas emissions is described in this report:

[http://www.wrapair.org/forums/ogwg/documents/2007-10_Phase_II_O&G_Final\)Report\(v10-07%20rev.s\).pdf](http://www.wrapair.org/forums/ogwg/documents/2007-10_Phase_II_O&G_Final)Report(v10-07%20rev.s).pdf)

Table 2-8. Oil and gas production nonpoint emissions in WRAP states in 2002 and 2005 platforms. Emissions provided in short tons/year.

Pollutant	2002	2005
CO	1	53,784
NO _x	31	155,133
SO ₂	0	2,842
VOC	2,184	480,252

Table 2-9 lists the new area source SCCs that were created to describe the new WRAP oil and gas emissions inventory. We converted the WRAP's average day "IDA"-formatted inventory to the SMOKE annual "ORL" (one record per line) format and retained only non-zero emissions, leaving us with the following pollutants (also seen in Table 2-8): CO, NO_x, SO₂, and VOC. The first two SCC Tier descriptions "Industrial Processes, Oil and Gas Production" are not repeated in this table.

Table 2-9. New SCCs from the Phase II WRAP Oil and Gas Inventory

SCC	Description
2310000220	All Processes, Drill Rigs
2310000330	All Processes, Artificial Lift
2310000440	All Processes, Saltwater disposal engines
2310010100	Crude Petroleum, Heaters
2310010200	Crude Petroleum, Tanks - Flashing & Standing/Working/Breathing
2310010300	Crude Petroleum, Pneumatic Devices
2310010700	Crude Petroleum, Fugitives
2310010800	Crude Petroleum, Truck Loading
2310020600	Natural Gas, Compressor Engines
2310020700	Natural Gas, Fugitives
2310020800	Natural Gas, Truck Loading
2310021100	Natural Gas, Heaters
2310021300	Natural Gas, Pneumatic Devices
2310021400	Natural Gas, Dehydrators

SCC	Description
2310021500	Natural Gas, Completion - Flaring & Venting
2310021600	Natural Gas, Venting
2310023000	Natural Gas, CBM - Dewatering pump engines
2310030210	Natural Gas Liquids, Tanks - Flashing & Standing/Working/Breathing, Uncontrolled
2310030220	Natural Gas Liquids, Tanks - Flashing & Standing/Working/Breathing, Controlled

Updates RWC emissions

The updates for RWC emissions were done between the 2002 v3 and 2005 v2; no additional updates were made for the platform. Currently the documentation of RWC changes is not available on the website so we document these changes here. First, emissions were replaced for Oregon and New York, because these areas submitted changes to their 2002 v3 emissions that they indicated were improvements. Second, analysis of PM_{2.5} and VOC for RWC indicated that, with the exception of California, states and local agencies that submitted emissions, used the AP-42-based VOC emissions factor (229 lb VOC per ton wood) for fireplaces, which we have subsequently determined overestimated VOC by over an order of magnitude. Therefore, we replaced the AP-42-based VOC factor of 229 lbs VOC/ton wood burned with a factor from a Mid-Atlantic Regional Air Management Association (MARAMA) study (Marama, 2006) of 18.9 lbs VOC/ton wood burned, using a series of conditional analyses detailed in Appendix A. The conditional part of the changes was required because many states included fireplaces together with woodstoves or did not include VOC with all RWC-related SCCs.

The net effect of the RWC updates and the VOC recalculation on annual national emission totals between the 2002 and 2005 platform is shown in Table 2-10.

Table 2-10. RWC Emissions Changes for CAPs between 2002 and 2005 platforms.
Emissions values provided in short tons/year.

Pollutant	2002	2005	% Change
VOC	1,476,756	40,754	-97.2%
NO _x	40,707	38,369	-5.7%
CO	3,061,043	2,857,985	-6.6%
SO ₂	5,705	5,307	-7.0%
NH ₃	8,700	7,238	-16.8%
PM _{2.5}	405,777	382,192	-5.8%
PM ₁₀	416,488	384,295	-7.7%

The 2005 platform also contains corrected HCl emissions for Stationary Source Fuel Combustion Coal fired Industrial and Commercial/Institutional boilers (SCCs 2102002000 and 2103002000). The EPA Office of Research and Development (ORD) identified overestimated HCl in the 2002 platform nonpt sector and provided revised HCl emissions in Georgia, Utah, and Virginia that lowered these emissions by approximately 100,000 tons/year.

2.3 Fires (*ptfire* and *avefire*)

Wildfire and prescribed burning emissions are contained in the *ptfire* and *avefire* sectors. The nonptfire sector in the 2002 platform is not needed for the 2005 platform because the 2005 platform *ptfire* sector contains these emissions. The *ptfire* sector has emissions provided at geographic coordinates (point locations) and has daily emissions values, whereas the *avefire* sectors are county-summed inventories and have annual total emissions values. For the 2005 evaluation case, we modeled 2005 year-specific fires using the emissions from the *ptfire* sector. For the 2005 base case, the *ptfire* sector was replaced by the *avefire* sector.

For the 2005 Platform, the following SCCs from the 2005 NEI are considered “fires” (note that the actual SCC description includes “Miscellaneous Area Sources” as the first tier level description).

Table 2-11. 2005 NEI SCCs representing emissions in the *ptfire* and *avefire* modeling sectors

SCC	SCC Description *
2810001000	Other Combustion;Forest Wildfires;Total
2810015000	Other Combustion;Prescribed Burning for Forest Management;Total
2810005000	Managed Burning, Slash (Logging Debris);Total

* all SCC descriptions begin with “Miscellaneous Area Sources;”

Both the *ptfire* and *avefire* sectors for the 2005 Platform exclude agricultural burning and other open burning sources, which are included in the nonpt sector. We chose to keep agricultural burning and other open burning sources in the nonpt sector because these categories were not factored into the development of the average fire sector (as described in 2.3.3). Additionally, their year-to-year impacts are not as variable as wildfires and non-agricultural prescribed/managed burns.

2.3.1 Day-specific point source fires (*ptfire*)

The *ptfire* sector includes wildfire and prescribed⁶ burning emissions occurring in 2005, which were used for the 2005 model evaluation case. Note that Agricultural Burning is not included in the *ptfire* sector as it is included in the nonpt sector. We did not include emissions from this sector in the 2005 base case or any of the future year cases. This sector includes emissions for all 2005 wildfires and many prescribed burns with daily estimates of each fire’s emissions. It includes a satellite derived latitude/longitude of the fire’s origin and other parameters associated with the emissions such as acres burned and fuel load, which allow estimation of plume rise.

The SCCs in the *ptfire* sector are listed in Table 2-12.

⁶ For purposes of this document prescribed burning also includes managed burning, i.e., “Other Combustion; Managed Burning, Slash (Logging Debris)”

Table 2-12. SCCs in the ptfire sector

SCC	SCC Description *
2810001000	Other Combustion;Forest Wildfires;Total
2810005000	Other Combustion;Managed Burning, Slash (Logging Debris);Total

* all SCC descriptions begin with “Miscellaneous Area Sources;”

The use of point source and day-specific data for fires was a new feature to EPA’s modeling for the 2002 platform and is described in the 2002 platform documentation.

The point source day-specific emission estimates for 2005 fires rely on Sonoma Technology, Inc.’s Satellite Mapping Automated Reanalysis Tool for Fire Incident Reconciliation (SMARTFIRE) system (Sullivan, et al., 2008). This system involves the use the National Oceanic and Atmospheric Administration’s (NOAA’s) Hazard Mapping System (HMS) fire location information as input combined with CONSUMEv3.0 (Joint Fire Science Program, 2009) and the Fuel Characteristic Classification System (FCCS) fuel-loading database to estimate fire emissions from wildfires and prescribed burns on a daily basis. The method involves the reconciliation of ICS-209 reports (Incident Status Summary Reports) with satellite-based fire detections to determine spatial and temporal information about the fires. The ICS-209 reports for each large wildfire are created daily to enable fire incident commanders to track the status and resources assigned to each large fire (100 acre timber fire or 300 acre rangeland fire). The SMARTFIRE system of reconciliation with ICS-209 reports is described in an Air and Waste Management Association report (Raffuse, et al., 2007).

Figure 2-1 shows a functional diagram of the SMARTFIRE process.

Once the fire reconciliation process is completed, the emissions are calculated using the U.S. Forest Service’s CONSUMEv3.0 fuel consumption model and the FCCS fuel-loading database in the Bluesky Framework (Ottmar, et. al., 2007),

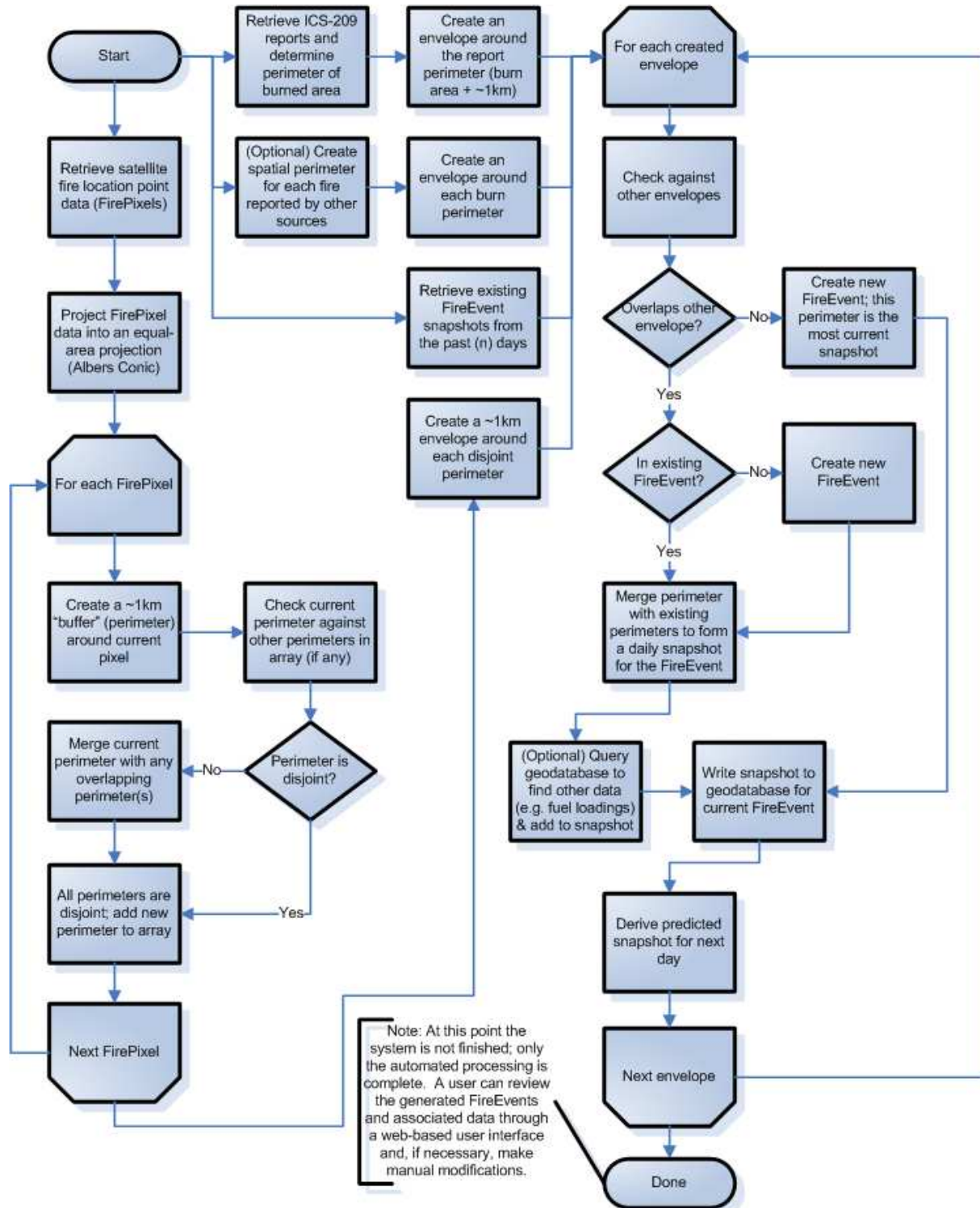
This method of estimating emissions in the ptfire sector is significantly different than that described in the 2002 platform documentation. First, the fire locations are satellite-based instead of ground-based. This means that many more fires are detected in space and time. Fires that could be matched in space and time with an ICS-209 report were designated as wildfires; all other fires were designated as prescribed burning. This point leads to the second difference from 2002: the distinction between wildfire and prescribed burn is not as precise as with ground-based methods. Third, the fire size was based on the number of satellite pixels and a nominal fire size of 100 acres/pixel was assumed for a significant number of fire detections when the first detections were not matched to ICS 209 reports. This means that the fire size information is not as precise as ground based methods. Finally, because the HMS satellite product from NOAA is based on daily detections, the emission inventory represents a time-integrated emission estimate. For example, a large smoldering fire will show up on satellite for many days and would count as acres burned on a daily basis whereas a ground-based method would count the area burned only once even it burns over many days.

Additional references for this method are provided in (McKenzie, et al., 2007), (Ottmar, et al., 2003), (Ottmar, et al., 2006), and (Anderson et al., 2004).

Figure 2-1. SMARTFIRE System

SMARTFIRE System

Functional Diagram



The SMOKE-ready “ORL” files created from the raw daily fires contain both CAPs and HAPs. The HAPs were generated using the same emission factors as were used in the 2002 Platform and described in Section 2.3 of the CAP and HAP 2002-Based Platform, Version 3 (<http://ftp.epa.gov/EmisInventory/2002v3CAPHAP/documentation>)

2.3.1.1 Speciation of “isomers of xylenes” in ptfire

Although xylenes are not HAPs that are used in the 2005 CAP-BAFM platform, they are used in the RFS2 version. We modified “Xylenes (Mixed Isomers)” emissions present in the raw daily fires files, represented only by pollutant code 1330207 by apportioning the emissions to m-xylene (108383), o-xylene (95476) and p-xylene (106423). We did this because pollutant code 1330207 (representing “Xylenes (Mixed Isomers)”) is mapped (during the speciation process that occurs in SMOKE) to m, o, and p, xylene and ethylbenzene. The mapping (developed by the chemical mechanism developers) treats pollutant code 1330207 as a solvent as opposed to a combustion byproduct. We apportioned the code 1330207 emissions using the following percentages: 61.41% m-xylene, 16.58% p-xylene and 22.01% o-xylene. These were derived from measurements of the flaming and smoldering xylene emission rate (Lee, et. al, 2005) and the assumption that 75% of the emissions are flaming and 25% smoldering⁷.

2.3.1.2 Creation of “NONHAPVOC” in ptfire

We used the BAFM HAP emissions from the inventory rather than from VOC speciation in this sector (though it is listed as a limitation below). To accomplish this, we computed the NONHAPVOC as an input to SMOKE, because SMOKE is limited to computing NONHAPVOC for annual emissions data but not the daily data we used for fires. Daily NONHAPVOC for each fire was computed for each source by subtracting the fire’s daily BAFM mass from the daily VOC mass. We also then dropped the pollutant “VOC” from the data files since it was no longer needed and if we had kept it, then we would be double counting emissions.

2.3.1.3 Limitations of the ptfire data in the 2005 platform

There were several limitations of the ptfire data approach that we identified after the data were prepared and modeled. Only the first issue listed affects a species that was modeled, and that issue only affects the model evaluation case; it had no impact on the base case used in RRF calculations because ptfire was not used in the base case. The limitations are listed below.

(1) Benzene (Pollutant code and CAS =71432): Emissions were inadvertently dropped during format conversion. Raw data annual total = 58,346 tons/yr and ORL file annual total = 263.47 tons/yr.

(2) Benzo[g,h,i]Perylene (Pollutant code and CAS= 191242): A portion of the emissions were inadvertently dropped during format conversion. Raw data annual total = 263 tons and ORL file annual total = 266.58 tons.

⁷ When reviewing the calculations, it turns out an equal flaming and smoldering fraction was used by mistake, a 75/25 split would have resulted in the following percentages: 59.07, 19.25 and 21.68 for m, p, and o-xylene, respectively.

(3) Benzo[k]Fluoranthene (Pollutant code and CAS= 207089): Emissions were missing from the ORL file. Raw data annual total = 134.84 tons and ORL file annual total = 0 tons.

(4) Benzofluoranthenes (Pollutant code and CAS 56832736) double counts emissions of CAS= 203338 (Benzo(a)Fluoranthene) and CAS= 207089 Benzo[k]Fluoranthene). Therefore this pollutant should not have been in the file.

As noted earlier, items 2 through 4 above impact HAPs that are not used in the modeling, but that are included with incorrect emissions values in the data we posted at the 2005v4 website (see the end of Section 1). The first error, however, impacts the modeling results because benzene emissions were integrated with the VOC and used as part of the speciation approach described in Section 3.1.2.1.

Finally, our use of the HAP emissions to “integrate” the HAP VOCs with the VOC (described in Section 2.3.1.2) was an approach that we have since dropped in favor of using VOC speciation without BAFM integration. Due to the introduction (in this platform) of a new speciation profile (5560) that is based on a compilation and critical evaluation of a large variety of species emitted from biomass fires (Andrae, 2001), we have not established whether or not HAP emissions from the NEI are more or less accurate. Therefore in subsequent modeling, we will choose to use the “no-integrate”, “no-hap-use” case which means VOC from these sources is speciated to provide all model species including BAFM.

2.3.2 Average fires (avefire)

The average fire sector includes emissions from wildfires, prescribed burning, and managed burning. We used this sector for the 2005 base case, and all future year cases. As noted above, avefire emissions are annual, county-level emissions.

The purpose of the avefire sector is to represent emissions for a typical or average 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 changing the fires would otherwise cause. 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.

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. Emissions provided in short tons/year

SCC	SCC Description *	2002 VOC	2005 VOC	CO	$PM_{2.5}$
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

Pollutant Description	CAS	PM_{2.5} factor
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
Methylanthracene	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)

For CMAQ, we computed the biogenic emissions based on 2005 meteorology data using the BEIS3.14 model from 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)

The biggest differences in the U.S. mobile emissions between the 2002 and 2005 platforms are (1) the apportioning of the emissions into additional platform sectors to allow for processing differences among the sectors; (2) the use of new emissions methods and data sets, particularly the use of a draft version of the Motor Vehicle Emissions Simulator (MOVES) model including temperature affects on gasoline PM_{2.5} exhaust emissions; and (3) the update of most of the data to 2005. A summary of these differences is presented below; details are provided in the subsections that follow.

For the 2005 platform, as indicated in Table 2-2, we have separated the previous 2002 sectors “onroad” and “alm”. The result is the 2005 onroad emissions are now broken out into three sectors: (1) “on_moves_startpm”; (2) “on_moves_runpm”; and (3) “on_noadj”. The aircraft, locomotive, and commercial marine emissions are now divided into two nonroad sectors: “alm_no_c3” and “seca_c3”, and as previously mentioned, the aircraft emissions are now in the nonEGU point inventory.

While the previous EPA platforms have used NMIM for the onroad and nonroad sectors⁸, some of the onroad emissions in the 2005 platform were based on a draft version⁹ of the MOVES model run for the year 2005. We used this draft MOVES model to make sure to include the PM_{2.5} emissions from onroad gasoline vehicles, which include temperature effects and are much larger than previous versions of onroad PM_{2.5}. The onroad gasoline emissions, except for motorcycles, were based on MOVES for the pollutants listed in Table 2-15. Unlike our use of NMIM, we used the MOVES data to create emissions by state and month and then allocated these to counties based on 2005 NMIM-based county-level data. The reason for the state resolution was due to (a) run time issues that made a county run done for the nation infeasible in the timeframe required and (b) uncompleted 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 2005 NEI v2.

Table 2-15. Pollutants covered by the draft MOVES model in the 2005 Platform¹

Used in the 2005 CAP-BAFM Platform	Available from draft MOVES, but not used in 2005 CAP-BAFM Platform
PM _{2.5} ; exhaust, partially speciated ²	Naphthalene ³
VOC; except refueling	1,3 butadiene ⁴
CO	Acrolein ⁴
NO _x	
Benzene; except refueling	
Formaldehyde	
Acetaldehyde	

¹ Draft MOVES data were used only for onroad gasoline vehicles with the exception of motorcycles. Draft MOVES

⁸ Other than California which were provided by CARB and were based on the mobile models used by California, EMFAC and OFFROAD, for onroad and nonroad emissions, respectively.

⁹ As of December 2009, this draft version was replaced by the publicly released MOVES2010 version at www.epa.gov/otaq/models/moves/

data were not used for any California onroad emissions

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”). Brake wear and tire wear PM_{2.5} emissions were not available from draft MOVES.

³ Used for the RFS2 version of the platform

⁴ Used for the RFS2 and LD GHG versions of the platform

The 2005 v2 NEI does not contain the draft 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.¹⁰ The NMIM data was used for all of the remaining onroad mobile sources 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.

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 2005 NEI v2 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 are now modeled separately as point sources in the new “seca_c3” sector for the 2005 platform.

The nonroad sector is the only 2002 mobile sector with U.S. emissions that was left intact and is still based on NMIM; however, for the 2005 platform, NMIM was run for 2005.

California onroad and nonroad emissions, which use neither MOVES nor NMIM, are based on an updated submittal to the NEI for 2005.

With the exception seca_c3 point source-formatted sector, the mobile sectors are at county and SCC resolution. 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.

All mobile sectors that have benzene, acetaldehyde, formaldehyde or methanol present in the inventory data, use these HAPs via “integration” for input into the air quality model, as described in Section 3.1.2.1. A few categories of nonroad sources (CNG and LPG-fueled equipment) do not have BAFM and therefore utilize the “no-integrate”, “no-hap-use” case which means VOC from these sources is speciated to provide BAFM.

¹⁰ 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.

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

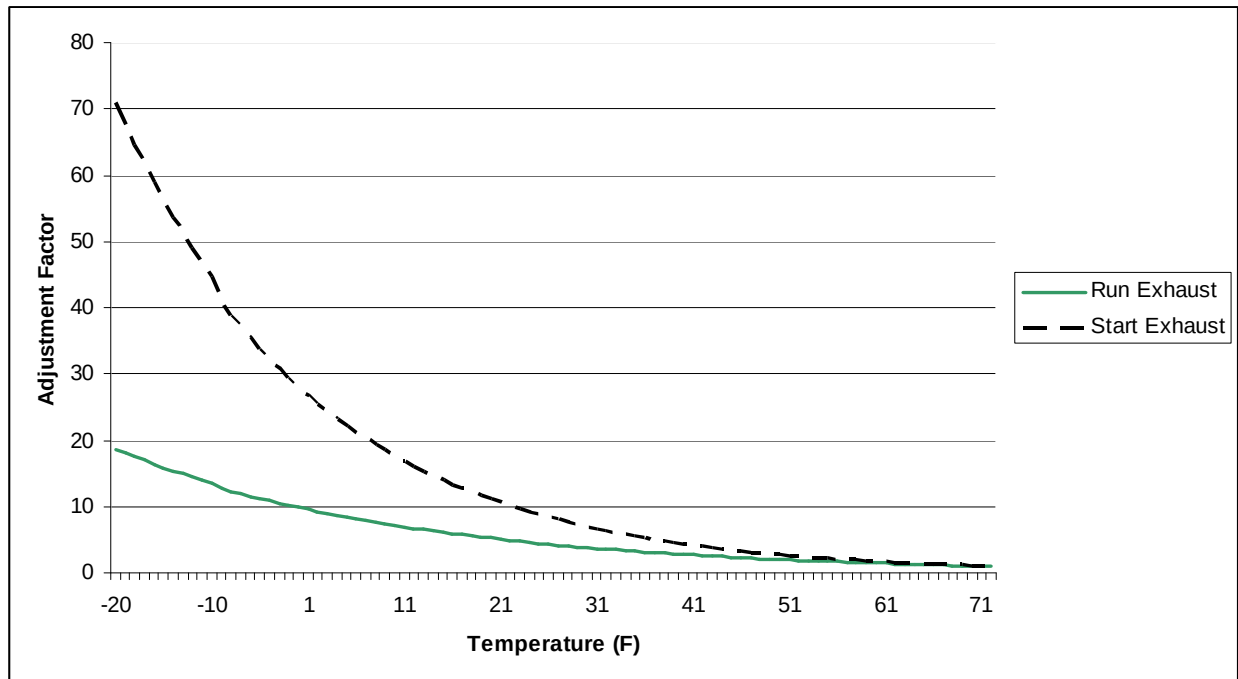
This sector contains draft MOVES emissions for PM and naphthalene¹¹ for non-California onroad gasoline cold-start exhaust except for motorcycles. These emissions (and the on_moves_runpm sector discussed in the next section) are processed separately from the remainder of the onroad mobile emissions because they are subject to hourly temperature adjustments, and these temperature adjustments are different for cold-start and running exhaust modes.

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 for RFS2) adjustments were different for starting and running exhaust and applied to SMOKE gridded, hourly intermediate files using the gridded hourly temperature data also input to the CMAQ model. One result of this approach is that inventory summaries based from 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 2-2 shows how PM (and naphthalene) emissions increase with colder temperatures and how start exhaust emissions increase more than running exhaust emissions.

¹¹ Naphthalene is not used in the 2005 CAP-BAFM platform, but it is contained in the MOVES-based inputs and was used in the version of the 2005 platform used for RFS2 (EPA, 2010)

Figure 2-2. MOVES exhaust temperature adjustment functions.



A number of features of the MOVES output required additional processing to develop county-level monthly ORL files for SMOKE. As stated earlier, the spatial resolution of the MOVES data was at the state level and data were allocated to county level prior to input into SMOKE. In addition, the exhaust $PM_{2.5}$ 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 done only on the species affected by temperature. Finally, because the start 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 below.

- i. We allocated state-level emissions to counties using state-county emission ratios by SCC, pollutant, and emissions mode (e.g., evaporative, exhaust) for each month. The ratios were computed using NMIM 2005 data (same data included in the 2005 NEI v2).
- ii. We assigned these start 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 data. For example, we split 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 B.
- 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. 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 specie “PM25EC”. 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 B.

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 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 2-2).

2.5.3 Onroad no-adjustments mobile sources (on_noadj)

This sector consists of the remaining onroad mobile emissions 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, non-motorcycle, non-PM: These are the monthly non-PM, non-naphthalene MOVES-based emissions from two MOVES inventories:
 - a. Exhaust: VOC, NO_x, CO, 1,3-butadiene (106990), acetaldehyde (75070), acrolein (107028), benzene (71432), and formaldehyde (50000); and
 - b. Evaporative: Non-refueling VOC, benzene, and naphthalene (91203)

For these pollutants listed, these non-California MOVES emissions encompass the same sources as the on_moves_startpm and on_moves_runpm sectors -LDGV, LDGT1, LDGT2, and HDGV- but 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 these emissions did not require species calculations because the raw MOVES emissions translated directly to SMOKE inventory species.

2. California onroad inventory: California year 2005 v2 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 NMIM runs for California. We retained only those HAPs that are also estimated by NMIM for nonroad 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 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 for all onroad diesel, all motorcycles, all refueling, and onroad LDGV, LDGT1, LDGT2, and HDGV emissions for pollutants not covered by the draft MOVES used for this platform (e.g., SO₂, NH₃, and most HAPs). 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.

The remainder of this section discusses the pre-processing required to create monthly ORL files for the remainder of the on_noadj sector (#3 above).

EPA/OTAC created the NMIM 2005v2 onroad mobile CAP/HAP emissions for all states and sources using the MOBILE6 model version M6023ChcOxFixNMIM. We then removed the CO₂ emissions and emissions of dioxins and furans, as well as emissions that were replaced by MOVES and California-submitted data. We also removed onroad refueling emissions since the NEI treats onroad refueling as a stationary source that is included in the nonpt sector (gasoline

distribution, Stage II, SCC=2501060100), and in limited appearance in the point sector in a handful of states (gasoline distribution Stage II; vapor loss or unclassified, SCC=40600401, 40600402, 40600403, and 40600499 in California, Colorado, Kentucky, and North Carolina).

Emissions were converted from monthly totals to monthly average-day based the on number of days in each month. Furthermore, this sector includes exhaust, evaporative, brake wear and tire wear emissions from onroad sources, which allowed us to use speciation profiles that are specific to each of these processes.

Similar to nonroad pre-processing, we reassigned NMIM evaporative xylene (compound XYL or CAS=EVP__1330207) into MXYL (CAS=EVP__108383) and OXYL (CAS=EVP__95476,) using a 68% and 32% ratio to evaporative 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.

The 2005 VMT database was based on 2002 VMT grown to 2005 based on Federal Highway Administration (FWHA) data unless replaced by state-provided VMT. A summary of the 2005 vehicle miles traveled (VMT) inputs (along with future year 2020 VMT used in the projections and will be discussed in a future version of this documentation) is available at: ftp://ftp.epa.gov/EmisInventory/2005_nei/mobile/2005_mobile_nei_version_2_report.pdf

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. 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. Future year nonroad emissions (to be added to Section 4 of this document) used the NR05d-Bond-final version of NONROAD which incorporates the Bond rule revisions. 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 for nonroad sources are not dropped from processing for this sector.

Similar to the on_noadj pre-processing, we also reassigned NMIM evaporative xylene. Since for nonroad sources we kept the refueling emissions in the nonroad sector (unlike onroad, these are not in any other part of the inventory) we also reassigned refueling 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 the on 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. 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). 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. In previous modeling platforms, this sector also contained aircraft emissions, but here we have removed aircraft emissions from the sector because point-source airports were provided in the 2005 NEI v2 point source inventory, and we chose to include them with other point sources in the ptnonipm sector. (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.

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	Mobile Sources; Aircraft: All Aircraft Types and Operations: Total

SCC	Action	SCC Description
	platform	
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 alm sector is available at:
<http://www.epa.gov/ttn/chief/net/2002inventory.html#documentation>

For modeling purposes, the following additional changes were made to the 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 ports 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 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 a 2005 inventory from the 2002 data. These growth factors are provided in

Table 2-17 and are mapped and documented in the following report:

<http://www.epa.gov/oms/regs/nonroad/marine/ci/420r09007-chap2.pdf>

These growth factors are the same for all pollutants except NO_x which includes a Tier 1 Standard.

Table 2-17. Regional growth factors used to project 2002 C3 emissions to 2005

Region	NO_x	All_other pollutants
Alaska	1.054	1.102
East Coast	1.091	1.141
Gulf Coast	1.042	1.090
Hawaii	1.107	1.158
North Pacific (Washington)	1.054	1.102
South Pacific (Oregon and California)	1.107	1.158
Great Lakes	1.047	1.052

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 this conference paper:

<http://www.epa.gov/ttn/chief/conference/ei17/session6/mason.pdf>

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.

Table 2-18 shows how these C3 emissions generally increase from the 2002 v3 platform (from the old methods used in the NEI) and this 2005 v4 platform. Note that the 2002 NEI-based C3 emissions are confined to the immediate coast and ports, whereas the 2005 C3 emissions cover most of the northern hemisphere Atlantic and Pacific oceans, including the Great Lakes/St. Lawrence seaway and Gulf of Mexico. The conference paper also shows gridded emissions maps comparing the 2002 NEI and 2002 ECA datasets. 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).

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

Pollutant	2002 platform	2005 platform	% Change
CO	28,195	53,746	91%
NH ₃	131	0	-100%
NO _x	244,988	642,089	162%
PM ₁₀	13,687	53,581	291%
PM _{2.5}	12,620	49,294	291%
SO ₂	150,532	417,307	177%
VOC	7,377	22,367	203%

We applied factors to compute HAP emissions (based on emissions ratios) to either VOC or PM_{2.5} to obtain HAP emissions values. Table 2-19 below shows these factors and whether they were applied to VOC, PM_{2.5}, or PM₁₀. 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.

Table 2-19. HAP emission ratios for generation of HAP emissions from criteria emissions for C3 commercial marine vessels

Pollutant	Apply to	Pollutant Code	Factor
Acetaldehyde	VOC	75070	0.0002286
Benzene	VOC	71432	9.795E-06
Formaldehyde	VOC	50000	0.0015672
Benz[a]Anthracene	PM _{2.5}	56553	5.674E-07
Benzo[a]Pyrene	PM _{2.5}	50328	1.844E-07
Benzo[b]Fluoranthene	PM _{2.5}	205992	1.56E-07
Benzo[k]Fluoranthene	PM _{2.5}	207089	1.56E-07
Chrysene	PM _{2.5}	218019	9.929E-08
Indeno[1,2,3-c,d]Pyrene	PM _{2.5}	193395	1.418E-08
Acenaphthene	PM _{2.5}	83329	3.404E-07
Acenaphthylene	PM _{2.5}	208968	5.248E-07
Anthracene	PM _{2.5}	120127	5.248E-07
Benzo[g,h,i]Perylene	PM _{2.5}	191242	1.277E-07
Fluoranthene	PM _{2.5}	206440	3.12E-07
Fluorene	PM _{2.5}	86737	6.95E-07
Naphthalene	PM _{2.5}	91203	1.987E-05
Phenanthrene	PM _{2.5}	85018	7.943E-07
Pyrene	PM _{2.5}	129000	5.532E-07
Beryllium	PM ₁₀	7440417	5.459E-07
Cadmium	PM ₁₀	7440439	7.642E-06
Chromium VI	PM ₁₀	18540299	2.948E-06
Chromium III	PM ₁₀	16065831	1.343E-05
Lead	PM ₁₀	7439921	3.002E-05
Manganese	PM ₁₀	7439965	5.732E-05
Nickel	PM ₁₀	7440020	0.0016377
Selenium	PM ₁₀	7782492	1.337E-05

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 CMAQ domain, which is the largest domain used for this effort.

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

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. There are two new sectors in the 2005 platform, othpt_hg and othar_hg. These sectors contain year 2000 Canadian speciated mercury emissions for point and area inventories. 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 (discussed in a future version of this documentation). 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 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 2005 NEI v2 point source inventory. The offshore sources were provided by the Mineral Management Services (MMS).

Table 2-20 summarizes the data in the "oth" sectors and indicates where these emissions have been updated from the 2002 platform.

Table 2-20. Summary of the othpt, othpt_hg, othar, othar_hg, and othon sectors in the 2005 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: 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.

Sector	Components	Changes from 2002 Platform
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 “HGNRVA” 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 temporalize 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 were the same as were used in the 2002 Platform.

2.7.1 Mercury

As discussed in the CAP and HAP 2002-based Platform 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
- mercury emissions from land
- mercury emissions from volcanoes

Annual fluxes of recycled elemental mercury for 2001 were created using the deposition results from a CMAQ4.5.1 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. This fraction is subject to future adjustment as the processes controlling the recycling of mercury are better understood.

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 2005 Platform, but using 2005-specific factors:

$$\begin{aligned} \text{Ocean: } & \frac{SOLRAD_{hr} * (SFCTMP_{hr} - 273)}{\sum_{allhrs} [SOLRAD * (SFCTMP - 273)]} \quad \text{or exactly zero for } SFCTMP < 273 \text{ K} \\ \text{Land: } & \frac{SOLRAD_{hr} * (SFCTMP_{hr} - 253)}{\sum_{allhrs} [SOLRAD * (SFCTMP - 253)]} \quad \text{or exactly zero for } SFCTMP < 253 \text{ K} \end{aligned}$$

where SOLRAD is the solar radiation in W/m^2 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 model requires 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 CMAQ, 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 CMAQ. 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 pollutants for all sectors except for biogenics, natural, recycled and volcanic mercury and ocean chlorine are those inventoried for the NEI. 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 (and scripts, at a later date) for the 2005 Platform emissions are available at the 2005v4 website (see the end of Section 1).

We used SMOKE to pre-process the raw emissions to create the emissions inputs for CMAQ. Although we used SMOKE version 2.5, the SMOKE version 2.6 source code and executables

can be used to reproduce our emissions modeling, and these are available from the Community Multiscale Analysis System (CMAS) Center at <http://www.cmascenter.org>. The scripts used for running the 2002 platform in SMOKE are available on the CHIEF website provided at the end of Section 1. The 2005 scripts will be provided at a later date.

One of the largest processing differences compared to the 2002v3 platform is the use of the CMAQ in-line emissions capability, which we used to create source-based emissions files rather than the 3-dimensional files for sectors that have plume rise. SMOKE was also 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.

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). 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 2005 Platform, we did not have SMOKE compute vertical plume rise; this was done in CMAQ using stack data in 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 temporalized source-based CMAQ inputs for seca_c3 were used for the vertical allocation. The in-line approach was not done for the 2002 Platform, as this was a new feature in CMAQ and SMOKE that was not available at that time.

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	

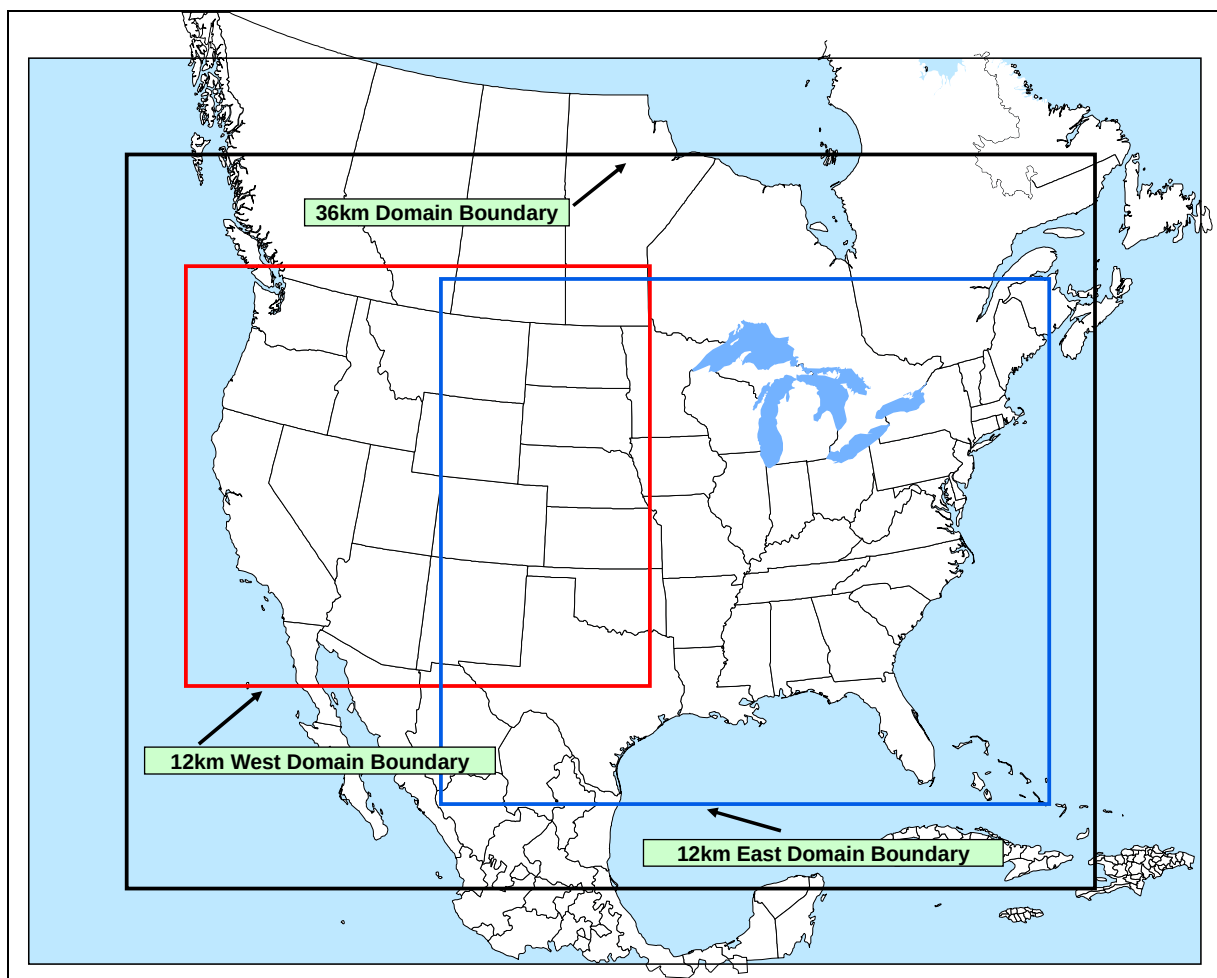
Platform sector	Spatial	Speciation	Inventory resolution	Plume rise
othar	surrogates	Yes	annual	
seca_c3	point	Yes	annual	in-line
alm_no_c3	surrogates & area-to-point	Yes	annual	
on_noadj	surrogates	Yes	monthly	
on_noadj	surrogates	Yes	monthly	
on_moves_startpm	surrogates	Yes	monthly	
on_moves_runpm	surrogates	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 BEIS	hourly	
ptfire	point	Yes	daily	in-line
nonptfire	surrogates	Yes	annual	
avefire	surrogates	Yes	annual	

One of the issues we found was that when using in-line processing, the PELVCONFIG file cannot allow grouping, otherwise the “inline” versus “offline” (i.e., processing whereby SMOKE creates 3-dimensional files) will not give identical results. Since we used a PELVCONFIG file with grouping, anyone wanting to exactly replicate our results should use the “inline” approach.

3.1.1 Spatial configuration

For the 2005 Platform, we ran SMOKE and CMAQ for modeling domains with 36-km and 12-km spatial resolution. These are the same domains as were used for the 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_148X12	'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 Carbon Bond 05 (CB05) mechanism (Yarwood, 2005) with secondary organic aerosol (SOA) and HONO enhancements as described in http://www.cmascenter.org/help/model_docs/cmaq/4.7/RELEASE_NOTES.txt. From the perspective of emissions preparation, it is the same mechanism 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; 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

Inventory Pollutant	Model Species	Model species description
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

The approach for speciating PM_{2.5} emissions is the same as that described for the 2002 platform except that two of the onroad sectors, and Canadian emissions contained pre-speciated PM emissions which were not further speciated in SMOKE . The approach for speciating VOC emissions from non-biogenic sources is different in two major ways: 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 on the fly given the fraction of each specific profile to use for the 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 2005 Platform.

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 2005 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.

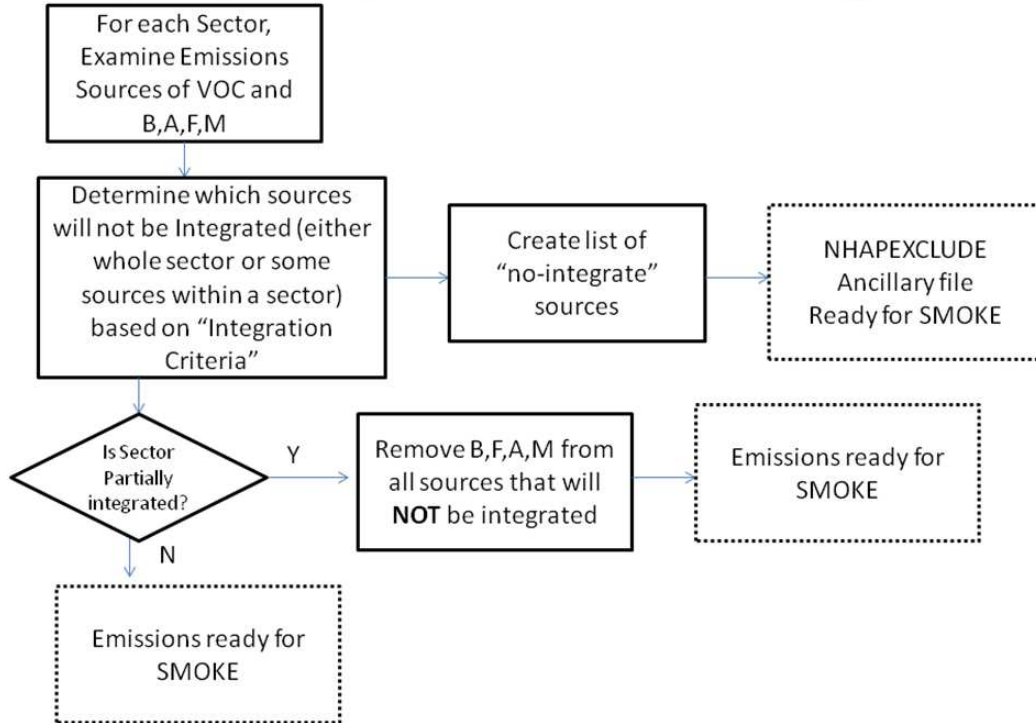
We chose these HAPs because, with the exception of BENZENE, they are the only explicit VOC HAPs in the base version of CMAQ 4.7 (CAPs only with chlorine chemistry) model. By “explicit VOC HAPs,” we mean model species that participate in the modeled chemistry using the CB05 chemical mechanism. We denote 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 integration¹²). 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 CMAQ VOC species not including the integrated HAPs. This process is illustrated in Figure 3-2. Note that we did not need to remove B,A,F,M 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 B,A,F,M in that sector.

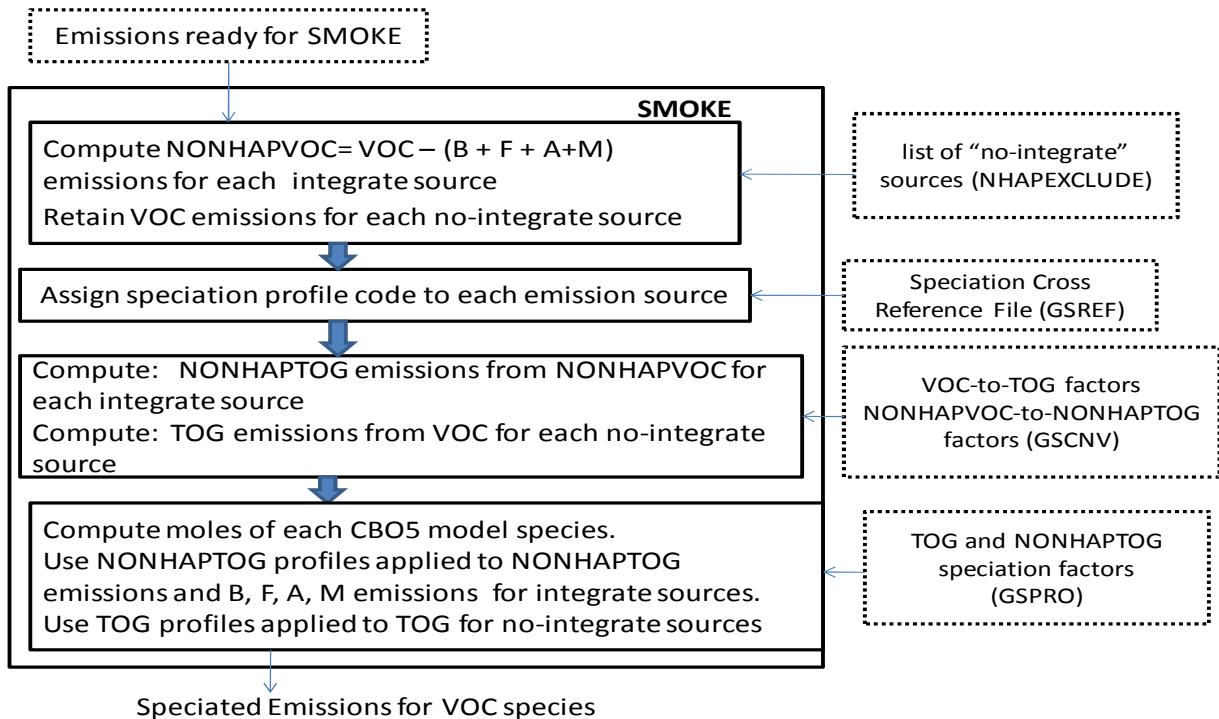
¹² In SMOKE version 2.6 the options to specify sources for integration are expanded so that a user can specify the particular sources to include or exclude from integration, and there are settings to include or exclude all sources within a sector.

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
ptfire	Full integration (However, NONHAPVOC computed outside of SMOKE since SMOKE cannot do this calculation for the day-specific fire formatted files)
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 B, A, F or M emissions were from the 1996 NEI were not integrated (data source code contains a “96”),
2. Any source for which the sum of B, A, F, or M 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 B,A,F and M specified in the first column. For a few source categories, we designated all sources as “no-integrate”.

4. For source categories not covered in Table 3-5 (i.e., that don't comprise the top 80% of VOC emissions), then as long as the source has emissions of one of the B, F, A or M 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
B	2461850000	Solvent Utilization;Miscellaneous Non-industrial: Commercial;Pesticide Application: Agricultural	profile has no benzene. Benzene came from solvent utilization data (Fredonia) for "other markets" for the year 1998. Consider changing this to no-integrate in the future since benzene no longer allowed in pesticides.
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.

minimum HAP(s) needed	SCC Tier 3	SCC Tier 3 Description	Comments
M	2460200000	Solvent Utilization;Miscellaneous Non-industrial: Consumer and Commercial;All Household Products	profile is 3146 contains only nonzero methanol.
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, Freedonia 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 (Fredonia) 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 2002 platform.

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.

Table 3-6. Temporal Settings Used for the Platform Sectors in SMOKE

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	aveday	aveday	
biog	hourly		n/a	n/a	
ptfire	daily		all	all	
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 2005 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 2005 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.

3.2.1 Spatial allocation ancillary files

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 2002 Platform. For Canada, for which we used a 2006 inventory, we used a new set of Canadian surrogates provided by Environment Canada along with their emissions data. 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) websites (see the end of Section 1).

- **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 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
- **ancillary_2005v4_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 66 spatial surrogates available for spatially allocating U.S. county-level emissions to the CMAQ 36-km and 12-km grid cells; they are the same as for the 2002 Platform. As described in Section 3.3.1.2, 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 2002 and 2005 Platforms

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
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	700	Airport Areas
300	Low Intensity Residential	710	Airport Points
310	Total Agriculture	720	Military Airports
312	Orchards/Vineyards	800	Marine Ports
320	Forest Land	807	Navigable Waterway Miles
330	Strip Mines/Quarries	810	Navigable Waterway Activity
340	Land	850	Golf Courses
350	Water	860	Mines
400	Rural Land Area	870	Wastewater Treatment Facilities
500	Commercial Land	880	Drycleaners
505	Industrial Land	890	Commercial Timber

Code	Surrogate Description	Code	Surrogate Description
510	Commercial plus Industrial		

We did not use all of the available surrogates to spatially allocate sources in the 2002 Platform; that is, some surrogates in Table 3-7 were not assigned to any SCCs. Appendix B provides the U.S. emissions assigned by the available surrogates for the CONUS domain region.

The creation of surrogates and shapefiles for the U.S. via the Surrogate Tool was discussed in the 2002 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.

The new onroad off-network (parking area) emissions from the MOVES model, new to the 2005 platform, were allocated as shown in Table 3-8.

Table 3-8. Surrogate assignments to new mobile categories in the 2005 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 thru 8B & Buses (HDGV)- parking areas rural 2201070370 Heavy Duty Gasoline Vehicles 2B thru 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 2002 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.

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 2005 Platform with the exception of the nonpoint Canadian mercury emissions. The updated set completely replaced the 2002 Platform surrogates for allocating the 2006 province-level Canadian emissions. The 2002 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

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_distibution	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	CA_921_NOFILL.txt	cement industries	CA_972_FILL.txt

Surrogate description	Filename of 2005 Platform Surrogate	Surrogate description	Filename of 2005 Platform Surrogate
AGRFORFISH and MANUFACT			
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 DWELLING	CA_925_NOFILL.txt	Electric utilities	CA_976_FILL.txt
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) were the same as were used in the 2002 Platform.

3.2.2 Chemical speciation ancillary files

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 CMAQ model species. SMOKE environmental variable names, used in the file names, are shown using capital letters in parentheses:

- **ancillary_2005v4_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).

3.2.2.1 INVTABLE 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 2005 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. Thus, any BAFM 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 **Error! Reference source not found.**sector-specific NHAPEXCLUDE files that provide the specific sources that are excluded from integration (see Table 3-5). Due to a limitation with SMOKE2.4, we needed to provide an NHAPEXCLUDE file even for sectors for which we integrate all sources in the sector. In this case, we included a source in the file that was not contained in the inventory (this SMOKE limitation has since been resolved).

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 B, A, F and M 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. The 2002-based platform utilized an earlier version, SPECIATE4.0. Note that this update did not impact the PM_{2.5} profiles we used with the 2005-based platform; they were the same as those used for the 2002-based platform.

As with SPECIATE4.0, SPECIATE 4.2 development was a collaboration involving EPA's ORD and EPA's Office of Air Quality Planning and Standards (OAQPS) at Research Triangle Park, NC, 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

One minor issue we found with the PM_{2.5} speciation which was similarly an issue with the 2002-based platform is that we used a bituminous coal combustion profile (92095) that is applicable to numerous inventory sources, but we used it for only a single nonpoint SCC (2101002000). For the other SCCs pertaining to bituminous coal combustion we used the sub-bituminous coal combustion profile (92084). Table 3-10 shows the differences are shown below, though these are quite small and represent only a minor change to the SMOKE results:

Table 3-10. 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

Another issue is that profile 92095 appears to have been inadvertently left out of SPECIATE4.2 (and 4.0); we obtained it from EPA ORD staff using it in their modeling applications.

Key changes to the TOG profiles from the 2002 Platform are as follows:

- Updated the profile for aircraft from 1098 (Aircraft Landing/Takeoff (LTO) – Commercial) which is from SPECIATE3.2 and has a profile date of 1989, to 5565 (Aircraft Exhaust), which has a profile date of 8/2008 and is based on testing conducted in 2005).

- Updated the profile for forest fires from 0307 (Miscellaneous Burning - Forest Fires) which was from SPECIATE3.2 and has a profile date of 1989) to 5560 (Biomass Burning - Extratropical Forest, dated 2/2008 and was based on testing conducted in 2001)
- Changed the assignment of residential wood combustion (including woodstove and fireplace emissions) and other profiles that formerly used 4641 (Fireplace wood combustion-oak wood) to 4642 (Fireplace wood combustion-pine wood) because of all three woods tested in the study (oak, pine and eucalyptus), the most complete testing was done for the pine wood (for example, benzene was only measured for pine)
- Updated the profiles for mobile onroad and nonroad sources to use more up-to-date test data. The updated profiles are:
 - o 8750: Gasoline Exhaust – Reformulated gasoline
 - o 8751: Gasoline Exhaust – E10 ethanol gasoline
 - o 8752¹³: Gasoline Exhaust – E85 ethanol gasoline
 - o 8753: Gasoline Vehicle - Evaporative emission - Reformulated gasoline
 - o 8754: Gasoline Vehicle - Evaporative emission - E10 ethanol gasoline
 - o 8755⁹: Gasoline Vehicle - Evaporative emission - E85 ethanol gasoline
 - o 8756^{9,14}: Composite Profile for Tier 2 vehicles E0, exhaust
 - o 8757^{9,10}: Composite Profile for Tier 2 vehicles E10, exhaust
- Utilized combination profiles comprised of the above updated exhaust and evaporative profiles to match the average ethanol content of fuels used by different counties and for different months of the year. Combinations were created based on the fuel properties data in the NMIM county database.

Table 3-11 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, 8737 is the same as was used in the 2002 Platform, and is used for other nonroad refueling and other fuel-related stationary source emission categories.

Table 3-11. 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

¹³ Profile not used in 2005, but used in future years built off of the 2005 base year.

¹⁴ Profile not included in SPECIATE4.2 (Nov. 2008), per OTAQ documentation, profiles were created October 2008, by OTAQ with EPA Act Phase 1 data, 22 out of 22 valid test cycles. Three vehicles tested: Honda Civic, Toyota Sienna, Chevy Silverado. Composite emission factors calculated using straight weighting for an LA92 drive cycle (1.19 miles, 8.63 miles, 1.19 miles for Bags 1,2 and 3, respectively).

Inventory type and mode	VOC speciation approach for fuels	VOC Profile Codes	2005 sectors
Mobile nonroad Refueling Stationary (no mode assigned to VOC): Portable Fuel Containers, bulk plant -to-pump, refinery-to-bulk terminal	E0	8737 (Composite Profile – Non-oxygenated Gasoline Headspace Vapor)	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 a subsequent version of this document. In summary, we utilized additional profiles in the combinations. The profiles we added were E85 and Tier 2 profiles for E0 and E10. One error (affecting the 2012, 2022 and 2030 future years) is that we used the same onroad and nonroad profiles in the future years. The nonroad profiles in future years should not include any Tier2 vehicles (since Tier 2 impacts only onroad) and should not include any E85.

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 CMAQ 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 CMAQ were generally based on the temporal allocation data used for the 2002 Platform. 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 CMAQ model species. SMOKE environmental variable names, used in the file names, are shown in capital letters in parentheses:

- **ancillary_2005v4_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 2005 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 SCCs¹⁵ 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

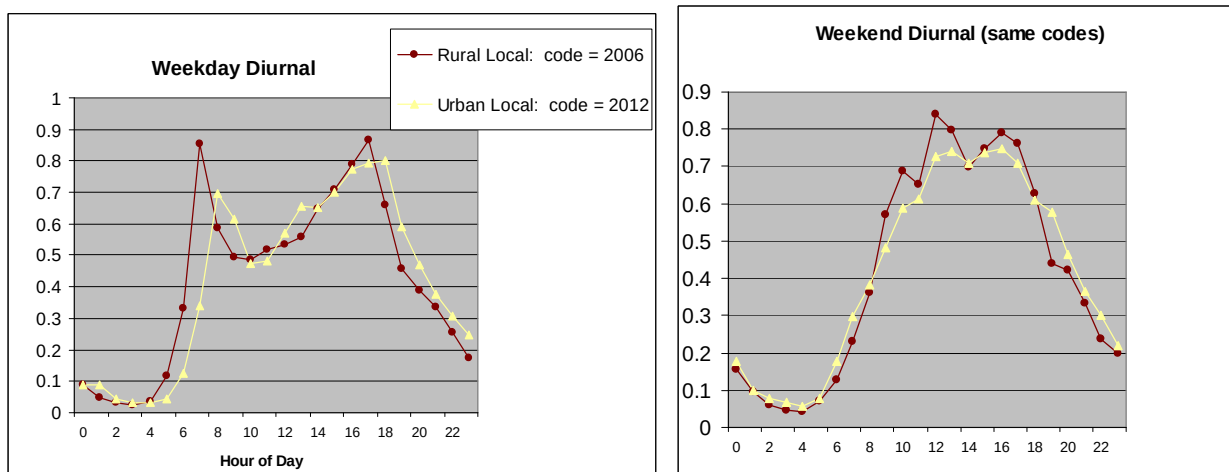
The new SCCs and descriptions, along with the assignments chosen are shown in Table 3-12. Figure 3-3 shows the diurnal profiles referred to in the table.

¹⁵ See Table 2-9: 2310000220, 2310000330, 2310000440, 2310010100, 2310010200, 2310010300, 2310010700, 2310010800, 2310020600, 2310020700, 2310020800, 2310021100, 2310021300, 2310021400, 2310021500, 2310021600, 2310023000, 2310030210, 2310030220

Table 3-12. Temporal Profiles Assigned to New Onroad SCC from the Draft MOVES model:
Parking Areas

SCC & Description	Temporal Profile: Monthly Variation	Temporal Profile: Day of Week Variation	Temporal Profile: Diurnal variation
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	Not applicable – will be receiving 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. Code = 2006 (see Figure 3-3. Diurnal Profiles are based only on road type (use local for “start”) and whether the road is urban versus ruralFigure 3-3, reddish curve)
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	Not applicable – will be receiving 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. Code = 2012 (see Figure 3-3, yellow curve)
2201070350 Heavy Duty Gasoline Vehicles 2B thru 8B & Buses (HDGV)- parking areas rural	Not applicable – will be receiving 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)
2201070370 Heavy Duty Gasoline Vehicles 2B thru 8B & Buses (HDGV)- parking areas urban	Not applicable – will be receiving 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)

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



4 Development of Future Year Emission Inventories

This section will be completed at a later date. Please also see rule-specific documentation, such as the Transport Rule’s Emission Inventory Technical Support Document.

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