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Emissions Modeling Final Report: Pre02b_36

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Prepared by:

Andrew P. Holland
Zachariah Adelman

UNC-Chapel Hill, Carolina Environmental Program
Bank of America Plaza, CB# 6116
137 E. Franklin St.
Chapel Hill, NC 27599-6116

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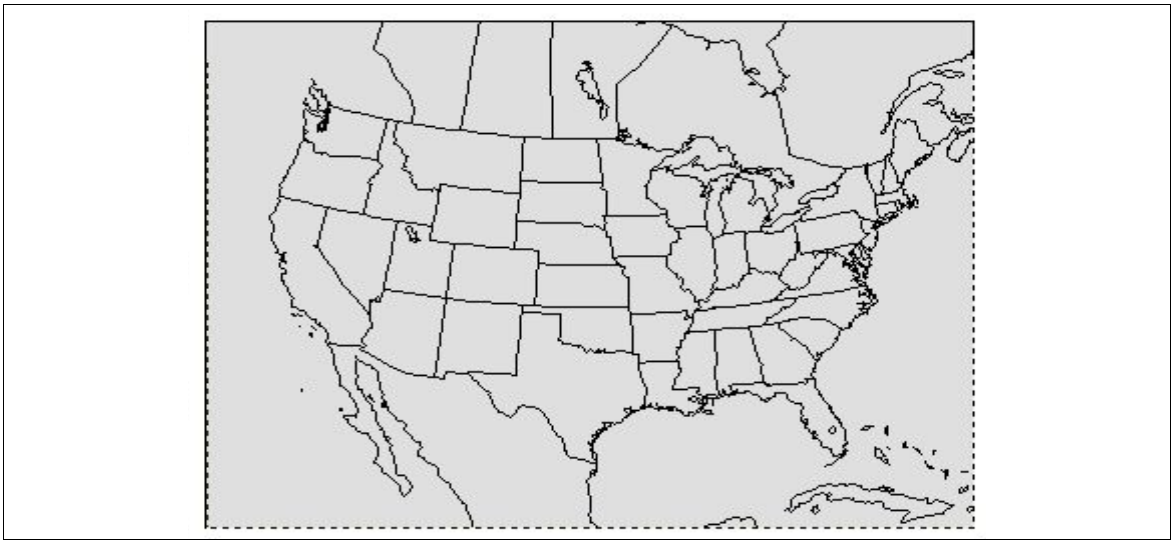
1 Executive Summary

Emissions case Pre02b_36 addresses many of the issues discovered in the inventory and SMOKE configuration discovered during the Pre02a_36 modeling. This report details the work completed by the Western Regional Air Partnership – Regional Modeling Center (WRAP-RMC) to prepare emissions case Pre02b_36. Collection and preprocessing of the inventories, modeling the inventories, addressing problems in the modeling, and quality assurance of emissions case Pre02b_36 are all covered in this report.

2 Introduction

This report summarizes the work completed to prepare the WRAP-RMC emissions simulation Pre02b_36. Performed under Task 3 of the WRAP-RMC 2004 work plan (Tonnesen, 2004), emissions case Pre02b_36 fixed many of the issues discovered during the semi-annual simulation Pre02a_36, as well as adding the offshore inventory. The results from the Pre02b_36 emissions simulation are to be combined with WRAP fire emissions and used by the WRAP-RMC for a preliminary source attribution simulation with the Community Multiscale Air Quality Model (CMAQ). is a graphic of the 2002 regional planning organization (RPO) unified modeling domain used for emissions case Pre02b. The projection and grid definitions are also contained in this figure.

Figure 1: CMAQ 36-km modeling domain



Grid Specification	Value
Columns	148
Rows	112
Layers	19
X-origin	-2,736,000 m
Y-origin	-2,088,000 m
X-center	-97 degrees
Y-center	40 degrees
X-cell	36,000 m
Y-cell	36,000 m
Vertical Top	10,000 m
Vertical Layers (σ)	1.0, 0.995, 0.99, 0.985, 0.98, 0.97, 0.96, 0.95, 0.94, 0.92, 0.9, 0.88, 0.86, 0.82, 0.77, 0.7, 0.6, 0.45, 0.25

3 Emissions Modeling

The purpose of this modeling simulation was to prepare emissions for annual regional haze modeling to prepare for §308 SIP/TIP development. This simulation was based on the "shakeout" simulation, Pre02a_36. The RMC emissions modeling team that worked on this simulation consisted of modelers at CEP with QA being done at CEP and UCR. We completed a twelve month emissions simulation for 2002 on the RMC computing cluster in March and April 2004.

The emissions modeling that we performed for this simulation consisted of the following components:

- Receive emissions inventory (EI) from WRAP EI contractors.
- Ensure all regions and inventories are covered (but not duplicated) by filling in gaps with base year or projected emissions from 1996 and/or 1999 National Emission Inventory (NEI).
- Set up and run SMOKE for a trial period (e.g., one month).
- Perform QA on the trail period results.
- Run SMOKE for the annual simulation.
- Perform QA on the annual period results.
- Deliver emissions to the WRAP RMC for use in air quality model.

We address these components as they were applied to the Pre02b_36 simulation using the following format. In Section 3.1 we describe the SMOKE input data used for this Task, including both inventory files and SMOKE ancillary files, such as cross-reference files, temporal

profiles, speciation profiles, and spatial surrogates. In Section 3.2, we describe the overall processing strategy used in SMOKE for this project and describe the SMOKE run scripts. In Section 3.3, we describe the processing approach and emissions results for stationary area sources, non-road mobile sources, on-road mobile sources, road dust sources, point sources, fire sources and biogenic emission sources. In Section 3.4, we describe the problems and issues from this Task and make recommendations about what can be done in the next round of §308 modeling to improve the data collection, modeling and QA efforts. In Section 3.5, we provide summaries and descriptions that illustrate the application of the QA protocol developed in 2003 to the emissions modeling for this task. This section will conclude in Section 3.6 with a discussion about what the RMC emissions modeling team is expecting to complete during the next phase of the 2002 modeling and how the QA protocol will be improved for the next round of modeling.

3.1 SMOKE input files

The emissions input files used in the Pre02b_36 modeling were the same files used in the Pre02a_36 modeling with fixes for errors caught in the first round of modeling. The details of all the SMOKE input files used in the Pre02b_36 modeling are described below.

3.1.1 Inventory and land use data

Table A-1 in Appendix A lists details about the inventory files used in the Pre02b_36 modeling. The information contained in Table A-1 includes exact emissions inventory file names, the source agency of the files with the delivery date to the RMC, the number of records in the files, the spatial and temporal coverage of the files, and the pollutants contained in the files. The inventory files used in the Pre02b_36 modeling are a combination of files created by WRAP inventory contractors, the NEI99, and the NEI96 grown to 2002 with SMOKE. The files prepared by the WRAP contractors are actual 2002 or 2003 inventories for the WRAP region, while the inventories for the non-WRAP states were collected and prepared by the RMC emissions modeling team to represent 2002 emissions in other parts of the modeling domain. Table 3-1 lists the inventory data sources for the RPO's, Mexico and Canada in the 2002 modeling domain. In the table "WRAP" refers to an inventory generated by a WRAP contractor, "NEI96+" is the NEI96 inventory grown to 2002 by the RMC, "NEI99" is the base NEI99 inventory, "BRAVO" is the 1999 Big Bend Regional Aerosol & Visibility Observations Study emissions data for Mexico, and "Clear Skies" is the 1995 Canadian national inventory used for the US EPA Clear Skies modeling project. Table 3-1 is also color coded to indicate the temporal extent of the inventories with green representing annual inventories, yellow representing seasonal inventories and blue representing inventories derived from daily meteorology information.

Table 3 -3.1: Sources of emissions inventory data for the WRAP modeling domain regions.

Inventory	WRAP	CENRAP	MWRPO	VISTAS	MANEVU	Mexico	Canada
Area	WRAP	WRAP	NEI96+	NEI96+	NEI96+	BRAVO	ClearSkies
Road Dust	WRAP	WRAP	WRAP	WRAP	WRAP	BRAVO	ClearSkies
Non Road	WRAP	NEI96+	NEI96+	NEI96+	NEI96+	BRAVO	ClearSkies
On Road	WRAP	NEI99	NEI99	NEI99	NEI99	BRAVO	ClearSkies
On Road (CA)	WRAP	n/a	n/a	n/a	n/a	n/a	n/a
Point	WRAP	WRAP	NEI96+	NEI96+	NEI96+	NEI96+	NEI96+
Biogenic	VISTAS	VISTAS	VISTAS	VISTAS	VISTAS	VISTAS	VISTAS

Annual inventory | Seasonal inventory | Daily meteorology dependent emissions

3.1.1.1 U.S. inventories

We anticipate that the 2002 WRAP area and point source inventory delivered to the RMC in 2003 will be the final version of that inventory for the §308 modeling. The WRAP inventory contains area and point source data for the WRAP and CENRAP states for 2002. The RMC amended the WRAP inventory with the NEI96 grown to 2002 with EGAS 4.0 growth factors to cover the rest of the United States.

The WRAP RMC received a 2003 road dust emissions inventory for paved and unpaved roads in late 2003 for use in the preliminary §308 modeling. The 2003 road dust inventory uses the same methodology to account for the transportable fraction reductions as was used in developing the 1996 and 2018 inventories for the WRAP §309 modeling performed in 2001-2003 (Pollack, 2004). The WRAP inventory contractor supplied the road dust inventory for all states in the CMAQ domain, and it includes $PM_{2.5}$ and PM_{10} emissions only.

The RMC received 2003 on-road and non-road mobile source inventories covering the WRAP states for use in the 2002 §308 modeling from the WRAP mobile inventory contractor in December 2003. Both are seasonal inventories and contain pre-computed emissions with speciated $PM_{2.5}$. The on-road mobile inventory is split between California and the rest of the 12 WRAP states. We are supplementing the WRAP on-road and non-road inventories with annual NEI99 activity data and NEI96 emissions grown to 2002, respectively. For the non-WRAP on-road emissions we are using the MOBILE6/SMOKE integration to calculate CO, NOx, VOC, SO_2, NH_3 and PM emissions from the NEI99 activity data.

The RMC received 1996 offshore emissions data for the Gulf of Mexico and the 2002 offshore emissions data for California in early 2004. The Gulf of Mexico data came from the US EPA Clear Skies project and is available at the following URL: ftp://ftp.epa.gov/modelingcenter/Clear_skies/CSA2003/Emissions. The California data was developed by the RMC using a spreadsheet from the California Air Resources Board (CARB).

3.1.1.2 Foreign inventories

We modeled the area and point source inventories for Mexico and Canada as their base years of 1999 and 1995, respectively. The Big Bend Regional Aerosol & Visibility Observations Study (BRAVO) produced the Mexico inventory used in Task 2E. The ten northern Mexican states contained in this inventory include San Luis Potosi, Baja California Norte, Sonora, Chihuahua, Coahuila de Zaragoza, Nuevo Leon, Tamaulipas, Sinaloa, Durango and Zacatecas. The Mexico inventory is available from the US EPA at the following URL: http://www.epa.gov/ttn/chief/net/mexico.html. The US EPA distributes a SMOKE ready version of the 1995 Canadian national inventory as part of the Clear Skies modeling project. This inventory is available from the US EPA at the following URL: ftp://ftp.epa.gov/modelingcenter/Clear_skies/CSA2003/Emissions. While we have been notified that updated inventories will become available, we are uncertain whether the amended US inventories derived from the NEI96 or the Mexico and Canada inventories will be replaced by updated inventories before the final 2002 modeling begins.

The BRAVO area source inventory contains road dust $PM_{2.5}$ and PM_{10} emissions for the 10 Mexican states covered in the inventory. The Clear Skies area source inventory contains road dust emissions for Canada for the following pollutants: SO_2, NOx, CO, VOC, NH_3, $PM_{2.5}$ and PM_{10}.

For Canada and Mexico we extracted the on-road and non-road mobile SCC's from the Clear Skies and BRAVO area source inventories, respectively, and grouped them with the US mobile source inventories.

3.1.1.3 Land use data

While most of the inventory data came either directly from WRAP inventory contractors or from the EPA through CEP, the WRAP RMC benefited from the unified 36-km RPO domain by using gridded biogenic land use files developed by Alpine Geophysics for the Visibility Improvement State and Tribal Association of the Southeast (VISTAS) modeling. The VISTAS gridded land use data came in the form of binary input files for running BEIS3 in SMOKE. We anticipate using the VISTAS gridded biogenic land use data for the final §308 modeling.

3.1.1.4 Inventory summaries

Table 3 -3.2: mass of inventory pollutants by source category for U.S. states.

	CO	NOX	VOC	NH3	SO2	PM10	PM2_5	PMC
Area	8788585	2133791	8743374	4547733	1328943	7381849	2351239	5030603

Biogenic	7488941	975295	68968097	0	0	0	0	0
On Road	69371953	8078587	5868161	251904	273748	225877	170672	55205
Non Road	25336215	5320217	3166860	12032	942749	471442	423330	48382
Road Dust	0	0	0	0	0	2917582	507809	2409776
Point	5458565	9515094	2462456	282919	16967419	1275162	753570	521592
Offshore	32293	139377	48474	0	107	40	39	2
Total	**129522895**	**26451372**	**89883729**	**5156807**	**19590788**	**13542065**	**5298888**	**8243442**

Table 3 -3.3: Annual mass of inventory pollutants by source category for WRAP states.

	CO	NOX	VOC	NH3	SO2	PM10	PM2_5	PMC
Area	1448071	453881	1741918	961371	153465	2117539	640254	1477275
Biogenic	3395628	306924	27815801	0	0	0	0	0
On Road	12630468	1399267	1097751	45603	32312	53796	42621	11175
Non Road	4059991	1101916	422651	4537	155124	75230	69735	5767
Road Dust	0	0	0	0	0	470112	82714	387403
Point	667508	1005001	232292	26501	907063	187296	107393	79901
Offshore	0	0	0	0	0	0	0	0
Total	**35248009**	**4556000**	**31936720**	**1100233**	**1325785**	**4174084**	**2034945**	**2139403**

Table 3 -3.4: Annual mass of inventory pollutants by source category for Canada.

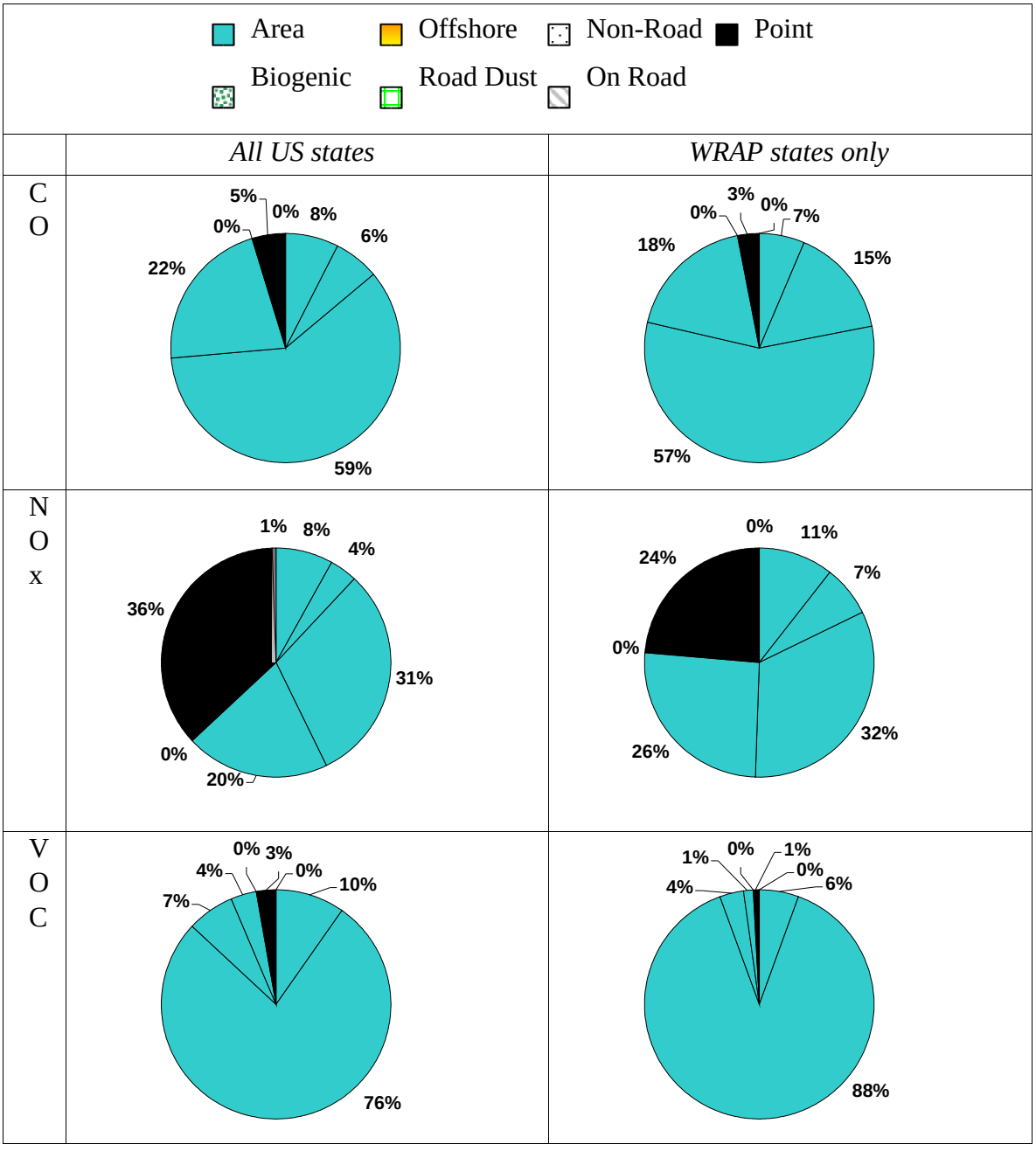
	CO	NOX	VOC	NH3	SO2	PM10	PM2_5	PMC
Area	675273	53908	677827	317131	200754	258783	161367	97417
Biogenic	0	0	0	0	0	0	0	0
On Road	6497880	357657	727668	0	20386	22613	21982	632
Non Road	19730	12518	3100	0	14	2145	2049	0
Road Dust	0	0	0	0	0	600395	124610	475780
Point	2611140	333696	1141813	0	2719516	558179	279062	279128
Offshore	0	0	0	0	0	0	0	0
Total	**9804024**	**757779**	**2550408**	**317131**	**2940671**	**1442116**	**589070**	**852956**

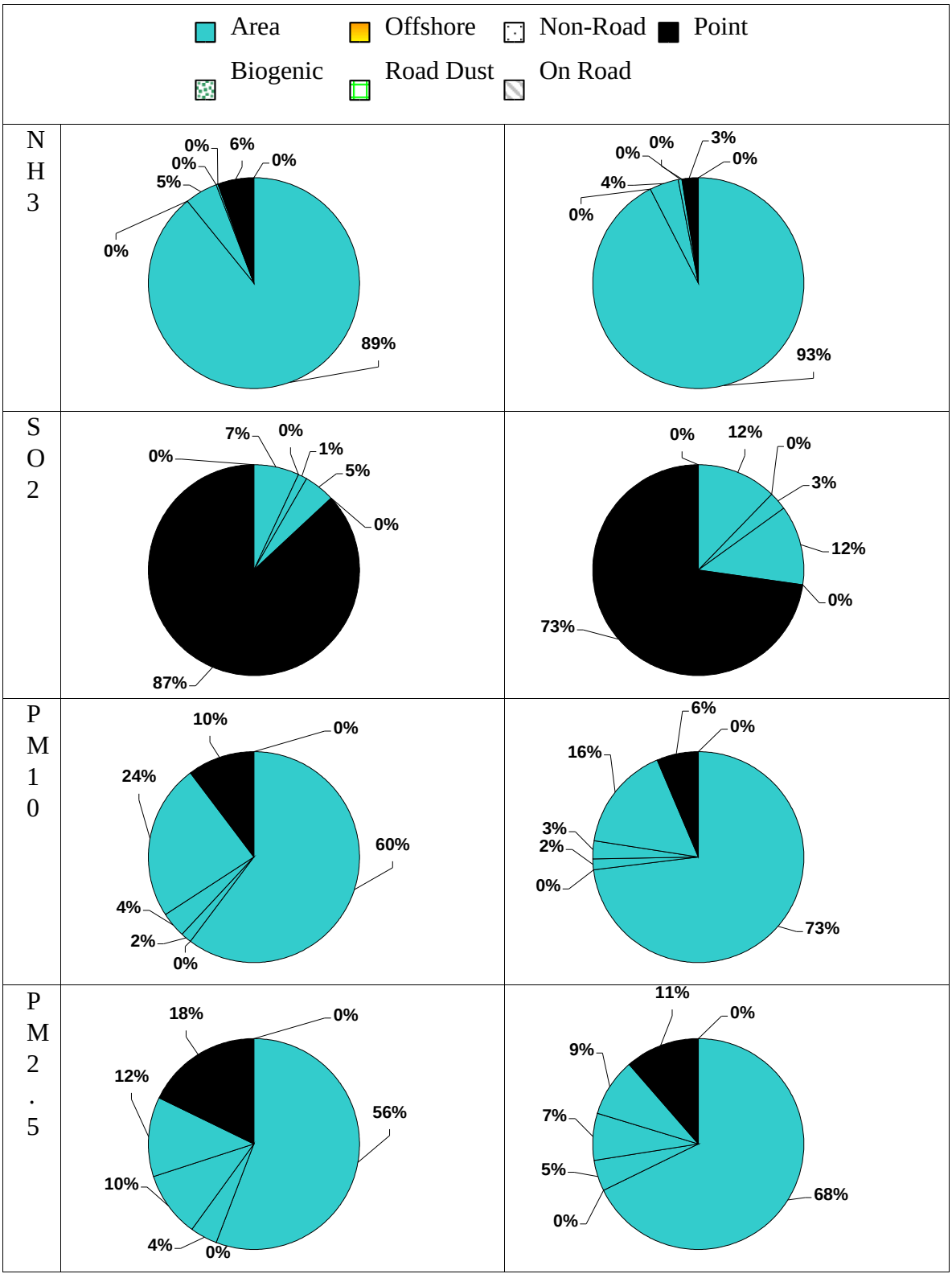
Table 3 -3.5: Annual mass of inventory pollutants by source category for Mexico.

	CO	NOX	VOC	NH3	SO2	PM10	PM2_5	PMC
Area	8629662	499089	2527588	548298	230560	1861774	854541	1007236
Biogenic	0	0	0	0	0	0	0	0
On Road	1846215	425262	186630	20875	1892	10588	9766	822
Non Road	4194002	834190	279884	1292	92442	53602	45346	0

Road Dust	0	0	0	0	0	696246	118294	577950
Point	745278	165384	168511	1046	1531262	0	0	0
Offshore	0	0	0	0	0	0	0	0
Total	**15415157**	**1923925**	**3162613**	**571511**	**1856156**	**2622210**	**1027947**	**1586008**

Figure 2: Break down of 2002 base emissions by source category.




Area
Offshore
Non-Road
Point
Biogenic
Road Dust
On Road
NH3
0%
6%
0%
0%
5%
0%
89%
0%
0%
3%
0%
4%
0%
93%
SO2
7%
0%
0%
1%
5%
0%
87%
0%
12%
0%
3%
12%
0%
73%
PM10
10%
0%
24%
60%
4%
2%
0%
6%
0%
16%
3%
2%
0%
73%
PM2.5
18%
0%
12%
56%
10%
4%
0%
11%
0%
9%
7%
5%
0%
68%

3.1.2 SMOKE ancillary inputs

Tables A-2 and A-3 in Appendix A list details abou the ASCII and binary SMOKE ancillary input files used in the Pre02b_36 modeling, respectively. The RMC created the 2002 meteorology files with MM5 and preprocessed the data with MCIP to prepare them for SMOKE. All of the ancillary emissions input files except the temporal profile/cross-reference files and the spatial surrogates/cross-reference files originated from the SMOKE version 2 distribution. We used the temporal profile and cross reference files that the RMC used for the WRAP §309 modeling (Houyoux, 2003). The RMC used spatial surrogates created by the US EPA (http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html) for the US and Canada and supplemented this with VISTAS surrogates for Mexico, instead of the VISTAS surrogates used in case Pre02a_36. The reasons behind using the EPA surrogates are twofold. First, the EPA surrogates use more land use categories and thus provide for higher resolution spatial allocation information. Second, the EPA provides surrogates for three different spatial resolutions, 36-km, 12-km and 4-km. By starting with the 36-km unified surrogates, we can use the finer resolution data in subsequent modeling simulations that will be on 12-km and 4-km grids within the WRAP region. Table 3-3 shows the data sources for the spatial surrogates.

3.2 Processing with SMOKE

This section describes SMOKE and the techniques used to build the model ready inventory.

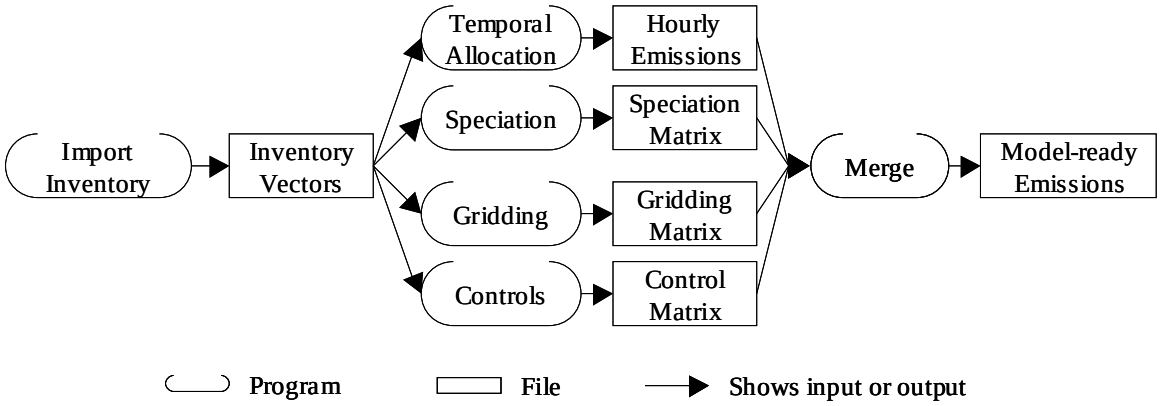
3.2.1 SMOKE background

The purpose of SMOKE (or any emissions processor) is to convert the resolution of the emission inventory data to the resolution needed by an air quality model. Emission inventories are typically available with an annual total emissions value for each emissions source, or perhaps with an average-day emissions value. The air quality models, however, typically require emissions data on an hourly basis, for each model grid cell (and perhaps model layer), and for each model species. Consequently, emissions processing involves (at a minimum) transformation of emission inventory data by temporal allocation, chemical speciation, spatial allocation, and perhaps layer assignment, to achieve the input requirements of the air quality model. For the WRAP modeling effort, all of these steps are needed. In addition, the WRAP processing requires special MOBILE6 processing and growth and control of emissions. Finally, the biogenic emission processing using BEIS2 includes additional processing steps.

SMOKE formulates emissions modeling in terms of sparse matrix operations. Figure 3 shows an example of how the matrix approach organizes the emissions processing steps for anthropogenic emissions, with the final step in creating the model-ready emissions being the merge step. This example does not include all processing steps, which can be different for each source category in SMOKE, but does include the major processing steps listed in the previous paragraph, except the layer assignment. Specifically, the inventory emissions are arranged as a vector of emissions, with associated vectors that include characteristics about the sources such as its state and county or SCC. SMOKE also creates matrices that will apply the gridding, speciation, and temporal factors to the vector of emissions. In many cases, these matrices are independent from one another, and can therefore be generated in parallel. The processing approach ends with the merge

step, which combines the inventory emissions vector (now an hourly inventory file) with the control, speciation, and gridding matrices to create model-ready emissions.

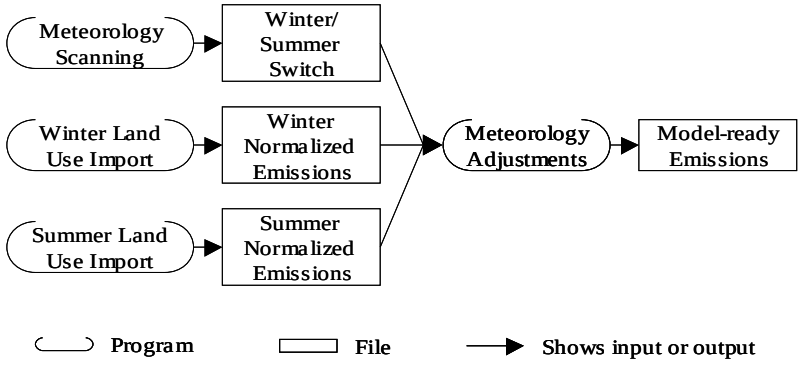
Figure 3: Flow diagram of major SMOKE processing steps needed by all source categories



For the temporal processing step, one can elect to process using representative Mondays, weekdays, Saturdays, and Sundays for each month; we reference this type of processing here as MWSS processing. This approach significantly reduces the number of times the temporal processing step must be run. In the sections below, we have identified the cases in which we have used this processing approach.

In addition, Figure 4 provides a schematic diagram of SMOKE/BEIS2 processing steps used in this project.

Figure 4: Flow diagram of SMOKE/BEIS2 processing steps



3.2.2 SMOKE scripts

The scripts are the interface that emissions modelers use to run SMOKE, and are therefore the items of practical importance for anyone wanting to simply reproduce the work performed as part of this contract. For this project, we created many SMOKE scripts to run the required emissions modeling cases, which we describe in this subsection. In the §309 modeling we modified the SMOKE scripting to use an operational modeling approach that used the number of times that each SMOKE program gets run in the course of a simulation to configure the scripts (Houyoux, 2002). For the §308 modeling we decided to stay with the default SMOKE script set up, which is based on source categories, to configure the scripts. We did make several modifications to the default SMOKE scripts to modularize them, add error checking loops, and break up the report and logs directories by source category. Now we have one script for each source category that we are modeling that calls all of the SMOKE programs required for simulating that source. Table 3-6 lists all of the SMOKE scripts used for the Pre02b_36 modeling and the SMOKE programs called by each script. In addition to the source-specific scripts listed in Table 3-6, we also listed the SMOKE utility scripts that actually call executables, manage the log files, and manage the configuration of the SMOKE simulations.

Table 3 -3.6: Summary of SMOKE scripts.

Source Category	**Script Name**	**SMOKE Programs/Function**
Area	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts /run/smk_ar_Pre02b.csh	*Smkinven, Grdmat, Spcmat, Temporal, Smkmerge, Smkreport*
Non-road mobile	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts /run/smk_nr_Pre02b.csh	*Smkinven, Grdmat, Spcmat, Temporal, Smkmerge, Smkreport*
Road Dust	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts /run/smk_rd_Pre02b.csh	*Smkinven, Grdmat, Spcmat, Temporal, Smkmerge, Smkreport*
On-road mobile (non-VMT)	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts /run/smk_mb_Pre02b.csh	*Smkinven, Grdmat, Spcmat, Temporal, Smkmerge, Smkreport*
On-road mobile (VMT-based)	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts /run/smk_mb_Pre02b.csh_vmt	*Smkinven, Mbsetup, Premobl, Emisfac, Grdmat, Spcmat, Temporal, Smkmerge, Smkreport*
Point	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts /run/smk_pt_Pre02b.csh	*Smkinven, Grdmat, Spcmat, Laypoint, Temporal, Smkmerge, Smkreport*

Source Category	Script Name	SMOKE Programs/Function
Offshore	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts/run/smk_ofs_Pre02b.csh	*Smkinven, Grdmat, Spcmat, Laypoint, Temporal, Smkmerge, Smkreport*
Biogenic	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts/run/smk_bg_Pre02b_beis3.12.csh	*Normbeis, Tmpbeis, Smkmerge*
Merge	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts/run/smk_mrgall_Pre02b.csh	*Mrggrid, Smkreport*
n/a	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts/run/make_invdir.csh	*creates inventory output directories by source category*
n/a	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts/run/movelog.csh	*moves existing log file to a back up file*
n/a	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts/run/smk_run.csh	*calls the SMOKE executables for everything but projection, controls, and QA*
n/a	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts/run/qa_run.csh	*calls the SMOKE executables for running the QA programs*
n/a	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts/run/smoke_calls.csh	*calls smk_run.csh, qa_run.csh and performs configuration management; used to clean up the source-specific run scripts*

3.2.3 SMOKE directory structures

The SMOKE directories can be divided into three broad categories, the first one being the program directories. These directories contain the model source code, assigns files, scripts and executables needed to run SMOKE. The second category includes the input directories. These directories contain the raw emissions inventories, the meteorological data and the ancillary input files. The third category, output directories, contains all of the output from the model. The directories are described in the Table 3-7.

Table 3 -3.7: Summary of SMOKE directories

Category	Directory location	Directory contents
Program	/home/aqm3/edss2/Pre02b/subsys/smokev2/src	*SMOKE source code*
	/home/aqm3/edss2/Pre02b/subsys/smokev2/assigns	*SMOKE assigns files*
	/home/aqm3/edss2/Pre02b/subsys/smokev2/scripts	*SMOKE make and run scripts*
	/home/aqm3/edss2/Pre02b/subsys/smokev2/Linux2_x86ifc	*SMOKE executables*
Input	/home/aqm3/edss2/Pre02b/data/inventory	*Raw emissions inventory files*
	/home/aqm3/edss2/Pre02b/data/met	*MCIP output meteorology files*
	/home/aqm3/edss2/Pre02b/data/ge_dat	*SMOKE ancillary input files*
Output	/home/aqm3/edss2/Pre02b/data/run_Pre02b/static	*Non-time dependent SMOKE intermediate outputs*
	/home/aqm3/edss2/Pre02b/data/run_Pre02b/scenario	*Time dependent SMOKE intermediate outputs*
	/home/aqm3/edss2/Pre02b/data/run_Pre02b/outputs	*Model-ready SMOKE outputs*
	/home/aqm3/edss2/Pre02b/data/reports	*SMOKE QA reports*

3.2.4 SMOKE Configuration

The RMC emissions modeling team configured SMOKE to generate emissions for all months of 2002 on the 36 km unified RPO modeling domain. A full listing of the SMOKE configuration options for this simulation is listed in Appendix C. For the anthropogenic emissions sources that use hourly meteorology (on road mobile and agricultural fires) we configured SMOKE to represent the daily emissions explicitly. For the non-meteorology dependent emissions, we used a representative Saturday, Sunday, Monday, and weekday for each month as surrogate days for the entire month's emissions (we refer to this as the MWSS processing approach). For these non-meteorology dependent emissions sources we explicitly represented the holidays as Sundays. Table 3-8 lists the days that we modeled as representative days in the months that we simulated for the Pre02b_36 modeling. Table 3-9 lists the holidays in 2002 that will be modeled.

Table 3 -3.8: Representative model days for Pre02b_36 simulation.

Saturday	Sunday	Monday	Weekday
January 5	January 6	January 7	January 4
February 2	February 3	February 4	February 5
March 2	March 3	March 4	March 5
April 6	April 7	April 8	April 2
May 4	May 5	May 6	May 7
June 8	June 9	June 3	June 4

July 6	July 7	July 8	July 3
August 3	August 4	August 5	August 6
September 7	September 8	September 9	September 10
October 5	October 6	October 7	October 8
November 2	November 3	November 4	November 5
December 7	December 8	December 9	December 10

Table 3 -3.9: 2002 modeled holidays.

Holiday	**Date**
New Years	January 1, 2002 January 2, 2002
Good Friday	March 29, 2002 March 30, 2002
Memorial Day	May 27, 2002 May 28, 2002
Independence Day	July 4, 2002 July 5, 2002
Labor Day	September 2, 2002 September 3, 2002
Thanksgiving Holiday	November 28-30, 2002
Christmas Holiday	December 24-26, 2002

We used the designations in Table 3-10 to determine which months fell into each season when temporally allocating the seasonal emissions inventories.

Table 3 -3.10: Assignments of months to seasons for use of seasonal inventory files in SMOKE.

Month	**Season**
January	Winter
February	Winter
March	Spring
April	Spring
May	Spring
June	Summer
July	Summer
August	Summer
September	Fall
October	Fall
November	Fall

December	Winter

3.3 SMOKE processing for WRAP source categories

SMOKE has four different processing approaches: processing for area, on-road mobile, point, and biogenic source. The WRAP source categories map to these processing approaches as shown in Table 3-11.

Table 3 -3.11: WRAP source categories mapped to processing approaches in SMOKE.

WRAP Source category	SMOKE processing approach
Stationary area	Area
Nonroad mobile	Area
Road dust	Area
On-road mobile	On-road mobile
Point	Point
Offshore	Point
Biogenics	Biogenics

Each SMOKE processing approach is for a specific SMOKE source category, which has its own source characteristics. These correspond to the identifiers used in creating the emission inventory (e.g. state/county FIPS code and SCC). The source categories also have source attributes, which are the other useful data in the emission inventories that SMOKE uses for processing them (e.g., point-source flue gas exit height and temperature). Source characteristics *define* the sources as area, mobile, or point sources for SMOKE processing and also distinguish one source in the inventory from another. Source attributes are additional data about the source that do not contribute to the source's uniqueness in SMOKE.

In SMOKE, each source category is defined by source characteristics, as follows:

- **Area sources** are defined by (1) country, state, and county codes, (2) SCC codes, or optionally (3) grid cell only.
- **On-road mobile sources** are defined by (1) country, state, and county codes, (2) SCC codes, and optionally (3) link codes.
- **Point sources** are defined by (1) country, state, and county codes, (2) plant codes, and (3) characteristics 1 through 5, one of which should be the SCC code.
- **Biogenic sources** are defined differently depending on the type of processing that you are using. They can be defined either by (1) country, state, and county codes and (2) land use code, or by (1) grid cell and (2) land use code.

In the following subsections, we describe the processing that we performed for each of the WRAP source categories.

3.3.1 Area emissions processing

Area-source processing includes emissions for the stationary area inventory (including Mexican and Canadian area, nonroad mobile, and road dust), the U.S. road dust inventory, and the U.S. nonroad mobile inventory. For the Pre02b_36 emissions modeling we grouped the area inventories by source category and applied the MWDSS temporal allocation approach to distribute the emissions in each month. We used the following grouping for the area inventory processing,

Group 1: Stationary Area

- **WRAP 2002 area inventory**: WRAP and CENRAP states, annual inventory
- **NEI96_02 area inventory**: MWRPO, VISTAS, and MANE-VU states, annual inventory, NEI96 grown to 2002 with EGAS4.0 growth factors
- **BRAVO Mexico 1999 area inventory**: 10 Northern Mexican states, annual inventory
- **Clear Skies Canada 1995 area inventory**: All Canadian provinces, annual inventory

Group 2: Non-road Mobile

- **WRAP 2003 non-road inventory**: WRAP states, seasonal inventory
- **NEI96_02 non-road inventory**: CENRAP, MWRPO, VISTAS, and MANE-VU states, annual inventory, NEI96 grown to 2002 with EGAS4.0 growth factors
- **BRAVO Mexico 1999 non-road inventory**: 10 Northern Mexican states, annual inventory extracted from BRAVO area source inventory
- **Clear Skies Canada 1995 non-road inventory**: All Canadian provinces, annual inventory extracted from Canada area source inventory

Group 3: Road Dust

- **WRAP 2002 paved road dust inventory**: Entire US, seasonal inventory
- **WRAP 2002 unpaved road dust inventory**: Entire US, seasonal inventory
- **BRAVO Mexico 1999 paved road dust inventory**: 10 Northern Mexican states, annual inventory extracted from BRAVO area source inventory
- **BRAVO Mexico 1999 unpaved road dust inventory**: 10 Northern Mexican states, annual inventory extracted from BRAVO area source inventory
- **Clear Skies Canada 1995 paved road dust inventory**: All Canadian provinces, annual inventory extracted from Canada area source inventory
- **Clear Skies Canada 1995 unpaved road dust inventory**: All Canadian provinces, annual inventory extracted from Canada area source inventory

For a flow diagram on how the inventories are processed through SMOKE refer to the WRAP Jumpstart Final Report (Houyoux, 2002).

3.3.2 On-road mobile-source emissions processing

The SMOKE processing for WRAP included two approaches for processing on-road mobile sources. The first approach was to compute mobile emissions values prior to providing them to SMOKE; we call this the precomputed-emissions approach. The second approach was to provide SMOKE with VMT data, meteorology data, and MOBILE6 inputs, and let SMOKE compute the mobile emissions based on these data. We call this the VMT approach. These approaches are not mutually exclusive for a single SMOKE run; therefore, we performed single SMOKE runs in which both approaches were used.

As described in Section 3.1.1, the on-road mobile inventory contains a combination of inventories:

- Precomputed, seasonal MOBILE6-based emissions of all pollutants for the 13 WRAP states that included prespeciated $PM_{2.5}$ data.
- Annual VMT for computing CO, NO_x, VOC, and PM using MOBILE6 for the rest of the United States.
- Precomputed, annual 1999 BRAVO emissions of all pollutants for Mexico
- Precomputed, annual 1995 Clear Sky emissions of all pollutants for Canada

Consequently, we used both the precomputed-emissions and VMT approaches for this effort. In SMOKE, the precomputed emissions approach is quite similar to processing for area sources. All SMOKE on-road mobile runs were performed as a single group using the following inventory set-up,

- **WRAP 2003 on road mobile inventory**: 2003 WRAP states (without California) precomputed, prespeciated $PM_{2.5}$ seasonal emissions
- **CA 2003 on road mobile inventory**: 2003 California precomputed, prespeciated $PM_{2.5}$ seasonal emissions
- **NEI99 on-road VMT**: 1999 CENRAP, MWRPO, VISTAS, and MANE-VU states, annual NEI activities for input to MOBILE6
- **BRAVO Mexico 1999 on road mobile inventory**: 10 Northern Mexican states, annual inventory extracted from BRAVO area source inventory
- **Clear Skies Canada 1995 on road mobile inventory**: All Canadian provinces, annual inventory

3.3.3 Point-source emissions processing

Point-source processing for the WRAP Pre02b_36 modeling includes emissions for the point-source inventory and offshore inventory. The point-source inventory included both Mexican and Canadian point sources. In SMOKE, one of the major factors distinguishing stationary-point source inventory processing from the other source categories is the calculation by SMOKE of plume rise and subsequent allocation of the emissions vertically. In addition, point-source

processing can include day-specific and hour-specific emission inventories and hour-specific precomputed plume rise.

We grouped the point source emissions by stationary point and offshore sources using the following set up,

Group 1: Stationary Point

- **WRAP 2002 point inventory**: WRAP and CENRAP states, annual inventory
- **NEI96_02 point inventory**: MWRPO, VISTAS, and MANE-VU states, annual inventory, NEI96 grown to 2002 with EGAS4.0 growth factors
- **BRAVO Mexico 1999 point inventory**: 10 Northern Mexican states, annual inventory
- **Clear Skies Canada 1995 point inventory**: All Canadian provinces, annual inventory; version 1 of this inventory of which there have been two subsequent versions.

Group 2: Offshore Sources

- **Clear Skies 1996 US offshore inventory:** Gulf of Mexico annual inventory
- **California Air Resources Board 2002 offshore inventory:** West US annual inventory

3.3.4 Biogenic emissions processing

Biogenic inventories depend heavily on the meteorological conditions of each day and hour. Temperature and solar radiation data are components of the biogenic inventory calculation. For this modeling effort, we used the Biogenic Emission Inventory System, version 3.12 (BEIS3) within SMOKE and the prognostic meteorological data provided by MCIP for input to the CMAQ. For the meteorology variables used to calculate the biogenic emissions, we used ambient temperatures (TA) and radiation reaching the ground (RGRND). Since the inventory is really a modeling exercise, the inventory is computed by the SMOKE system during emissions processing, and not as a separate inventory preparation process. The main preparation activity is creating the gridded land use data, which in this case was done by the VISTAS inventory contractor and supplied to the WRAP. Alpine Geophysics, LLC prepared the 36 km gridded landuse data that the RMC used for the Pre02b_36 modeling. Contact Greg Stella at Alpine Geophysics for additional information (gms@alpinegeophysics.com).

3.4 Problems encountered and remaining processing issues

Lessons learned during the WRAP Jumpstart project resulted in an overhaul to the RMC emissions modeling protocol. Many of the issues that we faced during the Jumpstart period, such as a multitude of data sources, errors in the data, delays in the data delivery and limited resources for QA still presented themselves, but we took these issues into account when developing the modeling protocol for the §308 modeling. In this section, we describe the QA issues that we encountered in the Pre02b_36 modeling and how they were resolved. In detailing these problems we distinguish between inventory problems, ancillary input file problems, and problems encountered with the SMOKE configuration. We also address unresolved issues with

the emissions modeling. Processing errors that we caught through the procedures in the draft QA protocol are summarized in Appendix D.

3.4.1 Emissions inventory issues

Most of the emissions inventory issues were resolved in the Pre02a_36 modeling run. However; we did find and resolve some more issues. We discovered that we were double counting NH_3 and SO_2 emissions for the non-WRAP states. This was due to the fact that MOBILE6 produces these pollutants and we were including the NEI99 emissions for the mobile source processing. We simply removed the NEI99 file from the processing to fix this problem. Another issue arose from the addition of the offshore inventory. Several of the longitudes for sources off the California coast were incorrect and were placing the emissions over land. This problem was corrected by fixing the longitudes in the inventory file. Using the NEI96 files grown to 2002 caused an issue with the gridding surrogates. The NEI96 files used the old FIPS code for Dade County, Florida, while the surrogates file used the new Miami-Dade FIPS code. We replaced the old FIPS code with the new one in all of the NEI96 files.

3.4.2 SMOKE ancillary input issues

Most of the ancillary input issues were from the use of a new gridding surrogates file from the EPA. The first problem was a simple formatting issue. SMOKE requires a six digit FIPS code and the file only had five digit codes. Also, the Canadian surrogates were using an incorrect county code. We found that many SCC's were missing from gridding surrogates file. This problem was fixed when were received a new surrogates file from the EPA in mid-April. However; this new surrogates file's Mexican surrogates appeared to be bogus. To address this problem we used the VISTAS Mexican surrogates from Alpine Geophysics. The final ancillary issue pertains to the Canadian temporal profiles. The US profiles vary by season, that is, January, February and December use the same factor. However; in the Canadian profiles, January, February and March use the same factor, see Table 3-12. We believe that this may be a formatting issue.

Table 3 -3.12: Temporal profiles for a major nonroad source.

Country	Profile number	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Canada	623	60	60	60	80	80	80	100	110	100	90	90	90
US	22	52	52	84	84	84	115	115	115	83	83	83	52

3.4.3 Computing issues

Many of the model-ready files contained values of infinity in them. After we reran the merge step the values would be corrected. We can only assume that this has to do with computer memory.

3.4.4 Unresolved emissions problems

A few issues with the SMOKE emissions remained unresolved at the completion of the Pre02b_36 simulation. A listing of these issues follows.

- Friday emissions slightly higher than the rest of the week for sources using MWSS temporal processing – in the MWSS approach the emissions for Tuesday-Friday should be exactly the same in a given month. For some reason the emissions on Fridays are slightly (~1%) higher than the rest of the week.
- The Clear Skies version 1 point source inventory for Canada contains only the eastern provinces.
- The Canadian mobile source inventory does not contain SO_2.

3.5 Emissions quality assurance

The Pre02b_36 simulation used the QA protocol that was developed by CEP and was tested in the Pre02a_36 simulation. Complete details on the modeling protocol are contained in Adelman, 2004. The different types of analysis used in the QA process are listed in the QA protocol. The QA products for tracking and documenting the QA process are contained in the Appendices of this report.

The WRAP RMC maintains a website with documentation and QA graphics for the Pre02b_36 simulation. The base page for the §308 emissions modeling documentation is here: http://pah.cert.ucr.edu/aqm/308/emissions.shtml. Documents with the same information contained in the Appendices of this report are linked to off of this page. The set of emissions QA regression spreadsheets are located here: http://pah.cert.ucr.edu/rmc/2002/QA_pre02b36.reports/sheets and the web page containing links to the various QA graphics is here: http://pah.cert.ucr.edu/aqm/308/qa_pre02b36.shtml.

4 References

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Pollack, A. et al. "Final Report: Development of WRAP Mobile Source Emission Inventories," presented to the Western Governors' Association, February 9, 2004,

List of Appendices

Appendix A - COMPLETE LISTING OF EMISSIONS INPUT and OUTPUT FILES

The tables listed in Appendix A detail the emissions inventories and ancillary SMOKE inputs used in the Pre02b_36 modeling. Table A-1 lists the names and brief descriptions of the inventory input files used for the Pre02b_36 simulation. Table A-2 lists the names and brief descriptions of the SMOKE ancillary input files used for this simulation. Table A-3 lists the names and locations of the binary meteorology and SMOKE output files on the RMC computers.

Table A -5.1. WRAP Pre02b_36 emissions inventory sources

SMOKE Simulation ID: Pre02b_36				
Date, source	**File name**	**# of records**	**Description**	**Species/contents**
12/4/03, Pechan	arinv.WRAP2002_v1_ida.txt	114,867	2002 Area source inventory; WRAP, Tier1 and Tier2 states	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
12/10/03, CEP	arinv.nei96_02.ida.txt	122,832	1996 NEI Area source inventory grown to 2002 using EGAS factors; EastUS states	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
EPA/Clear Skies	arinv.ClearSkies_Canada95_v3_ida.txt	19,782	1995 Area source inventory; Canadian sources only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
BRAVO	arinv.BRAVO_Mexico99_ida.txt	10,792	1999 BRAVO Area source inventory; Mexican sources only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
12/4/03, Environ	nrinv.Environ_WRAP_${season}03_ida.txt	13,987	2003 Seasonal nonroad source inventory; WRAP states only	VOC,NOx,CO,NH3,SO2,SO4_2.5,PMC_PRE,EC2.5,OC2.5,OTHER2.5
12/10/03, CEP	nrinv.nei96_02.ida.txt	52,526	1996 NEI Nonroad source inventory grown to 2002 using EGAS factors; Tier1, Tier2 and EastUS states	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
BRAVO	nrinv.BRAVO_Mexico99_ida.txt	446	1999 BRAVO Nonroad source inventory; Mexican sources only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
EPA/Clear Skies	nrinv.ClearSkies_Canada95_v3_ida.txt	7,376	1995 Nonroad source inventory; Canadian sources only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
RMC	rdinv.pvd_US_${season}02_ida.txt	3,080	2002 Seasonal paved road dust source inventory; WRAP, Tier1, Tier2 and EastUS states	PM10,PM2.5
12/9/03, CEP	rdinv.pvd.BRAVO_Mexico99_ida.txt	441	1999 BRAVO paved road dust source inventory; Mexican sources only	PM10,PM2.5
EPA/Clear Skies	rdinv.pvd.ClearSkies_Canada95_v3_ida.txt	284	Extracted from Clear Skies inventory	PM10,PM2.5
RMC	rdinv.unp_US_${season}02_ida.txt	3,108	2002 Seasonal unpaved road dust source inventory; WRAP, Tier1, Tier2 and EastUS states	PM10,PM2.5

SMOKE Simulation ID: Pre02b_36				
12/9/03, CEP	rdinv.unp.BRAVO_Mexico99_ida.txt	441	1999 BRAVO unpaved road dust source inventory; Mexican sources only	PM10,PM2.5
EPA/Clear Skies	rdinv.unp.ClearSkies_Canada95_v3_ida.txt	287	Extracted from Clear Skies inventory	PM10,PM2.5
12/4/03, Pechan	ptinv.WRAP2002_v1_ida.txt	210,078	2002 Point source inventory; WRAP, Tier1 and Tier2 states	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
12/10/03, CEP	ptinv.NEI96_02_EastUS_ida.txt	293,376	1996 NEI Point source inventory grown to 2002 using EGAS factors; EastUS states	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
EPA/Clear Skies	ptinv.ClearSkies_Canada96_v3_ida.txt	1,321	1996 Point source inventory; Canadian sources only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
BRAVO	ptinv.BRAVO_Mexico99_ida.txt	109	1999 BRAVO Point source inventory; Mexican sources only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
EPA/Clear Skies	ptinv.ClearSkies_USoffshore96_v1_ida.txt	4,899	Clear Skies offshore point inventory	CO,NOx,VOC
CARB/UCR	ptinv.CARB_WestUSoffshore2002_v1_ida.txt	141	UCR developed this inventory from a spreadsheet supplied by CARB	CO,NOx,SO2,VOC,PM10,PM2.5
7/31/02, AirSciences	pthour_agbase_073102.mod.$month.ida	varies by month	2018 Hourly Agricultural Fire inventory; WRAP states only	N/A
7/31/02, AirSciences	ptday_agbase_073102.mod.$month.ida	varies by month	2018 Daily Agricultural Fire inventory; WRAP states only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
7/31/02, AirSciences	ptinv_wrap.agbase.073102.$month.ida	varies by month	2002 Latitude and Longitude for the Agricultural Fire inventory; WRAP states only	N/A
AirSciences,4/04	pthour_wf_2002v1.mod.$month.ida	varies by month	Hourly Wildfire inventory; WRAP states only	N/A
AirSciences,4/04	ptday_wf_2002v1.mod.$month.ida	varies by month	Daily Wildfire inventory; WRAP states only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3

SMOKE Simulation ID: Pre02b_36				
AirSciences,4/04	ptinv_wrap.wf.2002v1.$month.ida	varies by month	Latitude and Longitude for the Wildfire inventory; WRAP states only	N/A
AirSciences,4/04	pthour_rxbase_2002v1.mod.$month.ida	varies by month	Hourly Prescribed Fire inventory; WRAP states only	N/A
AirSciences,4/04	ptday_rxbase_2002v1.mod.$month.ida	varies by month	Daily Prescribed Fire inventory; WRAP states only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
AirSciences,4/04	ptinv_wrap.rxbase.2002v1.$month.ida	varies by month	Latitude and Longitude for the Prescribed Fire inventory; WRAP states only	N/A
Environ	mbinv.Environ_CA_${season}03_v1_ida.txt	464	2003 Seasonal Mobile source inventory; California sources only	VOC,NOx,CO,NH3,SO2,SO4_2.5,PMC_PRE,EC2.5,OC2.5,OTHER2.5
Environ	mbinv.Environ_WRAP_${season}03_v1_ida.txt	45,600	2003 Seasonal Mobile source inventory; WRAP states	VOC,NOx,CO,NH3,SO2,SO4_2.5,PMC_PRE,EC2.5,OC2.5,OTHER2.5
BRAVO	mbinv.BRAVO_Mexico99_ida.txt	2,640	1999 BRAVO Mobile source inventory; Mexican sources only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
EPA/Clear Skies	mbinv.ClearSkies_Canada95_v3_ida.txt	2,269	1995 Mobile source inventory; Canadian sources only	VOC,NOx,CO,SO2,PM10,PM2.5,NH3
CEP	mbinv.nei99v1.nowrap.ida_emis.txt	175,692	1999 NEI Mobile sources inventory emissions data; Tier1, Tier2 and EastUS states	SO2,NH3
CEP	mbinv.nei99.nowrap.ida_vmt.txt	250,045	1999 NEI Mobile sources inventory activity data; Tier1, Tier2 and EastUS states	SPEED,VMT
VISTAS	b3_a.VISTAS36_148X112.beld3.ncf	N/A	Biogenics gridded landuse, File A	N/A
VISTAS	b3_b.VISTAS36_148X112.beld3.ncf	N/A	Biogenics gridded landuse, File B	N/A
VISTAS	b3_t.VISTAS36_148X112.beld3.ncf	N/A	Biogenics gridded landuse, totals file	N/A

Table A -5.2. WRAP Pre02b_36 modeling SMOKE ancillary input files

SMOKE Simulation ID:Pre02b_36			
File name	**SMOKE logical name**	**Creation date, source**	**Description**
pstk.m3.txt	PSTK	12/5/03, CEP	Replacement stack parameters file
costcy.txt	COSTCY	12/5/03, CEP	Country, state, county names and time zones
holidays.txt	HOLIDAYS	12/5/03, CEP	Holidays date list
scc_desc.txt	SCCDESC	12/5/03, CEP	SCC descriptions file
oris_info.txt	ORISDESC	12/5/03, CEP	ORIS ID descriptions file
gscnv.txt	GSCNV	12/5/03, CEP	Pollutant to pollutant conversion file
GRIDDESC	GRIDDESC	12/11/03, CEP	Grid descriptions file
amptref.m3.032003.us+can.WRAP.txt	[A|M|P]TREF		Temporal cross-reference file
amptpro.m3.121702.us+can.txt	[A|M|P]TPRO		Temporal profiles file
gsref.cmaq.cb4p25.txt	GSREF	12/12/03, CEP	Speciation cross-reference file
gspro.cmaq.cb4p25.txt	GSPRO	12/12/03, CEP	Spreciation profiles file
b3fac.beis3_efac_v0.98.txt	B3FAC		BEIS3 emissions factors
meproc.txt	MEPROC	CEP	Mobile emissions processes
mvref.txt	MVREF	CEP	Mobile source county settings file
mcref.txt	MCREF	CEP	Mobile source county cross-reference file
mcodes.nti99_VISTAS.txt	MCODES	CEP	Mobile vehicle type and road codes
bioseason.2002.RPO_US36.ncf	BIOSEASON	CEP	Season switch file
srg_desc_EPA1999.txt	SRGDESC	EPA	Surrogate description file
amgref_us_can_mex_091503.txt	[A|M]GREF	EPA	Gridding surrogates cross-reference file
amgpro.36km_102903.us_can_mex.txt	[A|M]GPRO	EPA	Gridding surrogates profiles file

Table A -5.3. WRAP Pre02b_36 modeling binary meteorology

SMOKE Simulation ID:Pre02b_36			
File name	**SMOKE logical name**	**Creation date, source**	**Description**
pstk.m3.txt	PSTK	12/5/03, CEP	Replacement stack parameters file
costcy.txt	COSTCY	12/5/03, CEP	Country, state, county names and time zones
holidays.txt	HOLIDAYS	12/5/03, CEP	Holidays date list
scc_desc.txt	SCCDESC	12/5/03, CEP	SCC descriptions file
oris_info.txt	ORISDESC	12/5/03, CEP	ORIS ID descriptions file
gscnv.txt	GSCNV	12/5/03, CEP	Pollutant to pollutant conversion file
GRIDDESC	GRIDDESC	12/11/03, CEP	Grid descriptions file
amptref.m3.032003.us+can.WRAP.txt	[A|M|P]TREF		Temporal cross-reference file
amptpro.m3.121702.us+can.txt	[A|M|P]TPRO		Temporal profiles file
gsref.cmaq.cb4p25.txt	GSREF	12/12/03, CEP	Speciation cross-reference file
gspro.cmaq.cb4p25.txt	GSPRO	12/12/03, CEP	Spreciation profiles file
b3fac.beis3_efac_v0.98.txt	B3FAC		BEIS3 emissions factors
meproc.txt	MEPROC	CEP	Mobile emissions processes
mvref.txt	MVREF	CEP	Mobile source county settings file
mcref.txt	MCREF	CEP	Mobile source county cross-reference file
mcodes.nti99_VISTAS.txt	MCODES	CEP	Mobile vehicle type and road codes
bioseason.2002.RPO_US36.ncf	BIOSEASON	CEP	Season switch file
srg_desc_EPA1999.txt	SRGDESC	EPA	Surrogate description file
amgref_us_can_mex_091503.txt	[A|M]GREF	EPA	Gridding surrogates cross-reference file
amgpro.36km_102903.us_can_mex.txt	[A|M]GPRO	EPA	Gridding surrogates profiles file

Appendix B - EMISSION INVENTORY BAR CHARTS

The charts in Appendix B summarize the contributions of each state in the 2002 modeling domain to the inventory pollutants in each of the major source categories, not including fires or biogenic emissions.

Appendix C - SMOKE CONFIGURATION OPTIONS

The table in Appendix C lists the SMOKE configuration options for each of the source categories processed for the Pre02b_36 simulation.

Table C -5.1. Simulation Pre02b_36 SMOKE configuration settings

SMOKE Simulation ID:Pre02b_36											
Environment variable	**Description**	**Setting to use**	**Comments/exceptions**	**Checked?***						
				A	F	RD	NR	M	P	B
Time-independent programs										
RUN_SMKINVEN	Run inventory import program			Y	Y	Y	Y	Y	Y	
RUN_SPCMAT	Run speciation matrix program			Y	Y	Y	Y	Y	Y	
RUN_GRDMAT	Run gridding matrix program			Y	Y	Y	Y	Y	Y	
RUN_CNTLMAT	Run control matrix program		Area and point only	N	N	N	N	N	N	
RUN_ELEVPOINT	Run elevated/PinG sources selection		Point only		N				N	
RUN_MBSETUP	Run on-road mobile setup for MOBILE6		On-road only					Y		
RUN_NORMBEIS3	Runs normalized emissions program		Biogenic only							N
Time-dependent programs										
RUN_PREMOBL	Run temperature preprocessing		On-road only					Y		
RUN_EMISFAC	Run MOBILE6 emission factor generation		On-road only					Y		
RUN_LAYPOINT	Run layer fractions program		Point only		Y				Y	
RUN_TEMPORAL	Run temporal allocation program			Y	Y	Y	Y	Y	Y	
RUN_TMPBEIS3	Runs temporal adjustments and speciation		Biogenic only							Y
RUN_SMKMERGE	Run merging program			Y	Y	Y	Y	Y	Y	Y
Quality assurance										
RUN_SMKREPORT	Run for quality assurance reports		Will run this several times to get different QA reports	Y	Y	Y	Y	Y	Y	N
QA_TYPE	Produces particular reports	all	Will also probably use custom as well	all	all	all	all	all	all	n/a
Program-specific controls										
For Smkinven										
FILL_ANN_WSEAS	Fill annual emissions based on seasonal values	Setting	Y for offshore	N	N	N	Y	Y	N	
HOURLY_TO_DAILY	Y reads daily total only from hourly file		Point only		N				N	
HOURLY_TO_PROFILE	Y converts hourly data to source-specific profiles		Point only		N				N	
IMPORT_AVEINV_YN	Y for importing annual-average inventories		Point only		N				Y	
SMK_ARTOPT_YN	Y uses area-to-point conversion	Setting		N	N	N		N		

SMOKE Simulation ID:Pre02b_36											
IMPORT_GRDIOAPI_YN	Y for imported pregridded emissions in I/O API format			N	N	N	N	N	N		
IMPORT_VMTMIX_YN	Y imports VMT mix – EMS-95 inputs		Mobile only					Y			
SMK_VMTMIX_FIXFMT	Y uses fixed-format VMT Mix file		Mobile only					Y			
RAW_DUP_CHECK	Y for errors on duplicate records			N	N	N	N	N	N		
SMK_NHAPEXCLUDE_YN	Y uses NonHAP exclusions file				N		N	N			
SMKINVEN_FORMULA	Formula for calculating an additional pollutant	PMC=PM10-PM2_5	Not used for mobile VMT	Y	Y	Y	Y	N	Y		
SMK_BASYR_OVERRIDE	Override value for base year of all inventories	0		0	0	0	0	0	0		
WKDAY_NORMALIZE	Y normalizes weekly profiles for weekdays	Setting	This assumes that area- and point-source input formats will be provided as average-weekday emissions and VMT will be provided as average-day VMT. This should be confirmed.	N	N	N	N	N	N		
WEST_HSPHERE	Y converts all stack coordinates to western hemisphere		Point only		Y				Y		
For Elevpoint											
SMK_ELEV_METHOD	**0=Laypoint sets elev srcs; 1=use PELVCONFIG**				n/a				n/a		
UNIFORM_STIME	**-1 or HHMMSS for uniform start hour for daily emissions days**				n/a				n/a		
For Grdmat											
SMK_DEFAULT_SRGID	Default surrogate code			100	100	100	100	100			
For Spcmat											
POLLUTANT_CONVERSION	Y uses ROG-to-TOG file			Y	Y	Y	Y	N	Y		
For Cntlmat											
REACTIVITY_POL	Set to VOC or ROG			n/a	n/a	n/a	n/a	n/a	n/a		
For Temporal											
RENORM_TPROF	Y renormalizes temporal profiles			Y	Y	Y	Y	Y	Y		
UNIFORM_TPROF_YN	Y makes all temporal profiles uniform			N	N	N	N	N	N		
ZONE4WM	Y uses time zones for start of day/month			Y	Y	Y	Y	Y	Y		
For Tmpbeis3											
BG_CLOUD_TYPE	Method used to calculate PAR		Biogenic only								1
BIOG_SPRO	Speciation profile code to use for biogenics		Biogenic only								BV309
BIOMET_SAME	Y uses temperature and rad/cld data in same file		Biogenic only								N
BIOSW_YN	Y for using seasons file in Tmpbeis3		Biogenic only								N

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OUTZONE	Output time zone		Biogenic only							0
RAD_VAR	Name of radiation/cloud variable		Biogenic only							RGRND
TMPR_VAR	Name of temperature variable		Biogenic only							TA
PRES_VAR	Name of surface pressure variable		Biogenic only							PRES
For Laypoint										
REP_LAYER_MAX	Layer number for reporting high plume rise		Point only		19				19	
SMK_SPECELEV_YN	Y uses Elevpoint output file to set elevated **sources**		Point only		N				N	
HOUR_PLUMEDATA_YN	PHOUR file contains hourly plume data				Y				N	
For Smkmerge										
MRG_TEMPORAL_YN	Y merges with hourly emissions			Y	Y	Y	Y	Y	Y	Y
MRG_SPCMAT_YN	Y merges with speciation matrix			Y	Y	Y	Y	Y	Y	
MRG_LAYERS_YN	Y merges with layer fractions		Point only		Y				Y	
MRG_GRDOUT_YN	Y outputs gridded file			Y	Y	Y	Y	Y	Y	
MRG_REPSTA_YN	Y outputs for state totals		Reports will be generated by Smkreport	N	N	N	N	N	N	Y
MRG_REPCNY_YN	Y outputs for county totals			N	N	N	N	N	N	N
SMK_ASCIIELEV_YN	Y outputs ASCII elevated file				N				N	
MRG_GRDOUT_UNIT	Units of gridded output file	moles/s		moles/s	moles/s	moles/s	moles/s	moles/s	moles/s	moles/s
MRG_TOTOUT_UNIT	Units of report file	moles/day		moles/day	moles/day	moles/day	moles/day	moles/day	moles/day	moles/day
MRG_REPORT_TIME	Hour in OUTZONE for reporting emissions	230000	So daily totals will be from 0-23 EDT	230000	230000	230000	230000	230000	230000	230000
MRG_MARKETPEN_YN	Apply reactivity controls market penetration		Apply reactivity controls market penetration	N	N	N	N	N	N	
AREA_SURROGATE_NUM	Number for land-area surrogate		Biogenic only							3
Multiple-program controls										
DAY_SPECIFIC_YN	Y imports day-specific inventory				Y	N	N	N	N	
EXPLICIT_PLUME_YN	Y for special wildfire processing or UAM/REMSAD				?				N	
HOUR_SPECIFIC_YN	Y imports hour-specific inventory				Y		N	N	N	
REPORT_DEFAULTS	Y reports default profile application			N	N	N	N	N	N	
SMK_AVGDAY_YN	Y uses average day emissions instead of annual	Setting		N	N	Y	N	N	N	
SMK_PING_METHOD	0=no PinG source, 1=use PELVCONFIG file		No PinG sources to be run		0				0	

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SMK_EMLAYS	Number of emissions layers				19				19	
SMK_MAXWARNING	Maximum number of warnings in log file			100	100	100	100	100	100	100
SMK_MAXERROR	Maximum number of errors in log file			100	100	100	100	100	100	100
OUTZONE	Output time zone of emissions		GMT	0	0	0	0	0	0	0
SMK_DEFAULT_TZONE	Time zone to fix if missing COSTCY file			5	5	5	5	5	5	5
VELOC_RECALC	Y recalculates velocity from diameter and flow		Point only		N				N	
USE_SPEED_PROFILES	Y uses speed profiles instead of inventory speeds		Mobile only					N		
Script settings										
SRCABBR	Abbreviation for naming log files	Setting		ar	agf/wf/rxf	rd	nr	mb/mbv	pt	bg
QA_TYPE	None, all, part1-part4, or custom			all	all	all	all	all	all	all
PROMPTFLAG	Never set to Y for batch processing			N	N	N	N	N	N	N
AUTO_DELETE	Y deletes SMOKE I/O API output files			Y	Y	Y	Y	Y	Y	Y
AUTO_DELETE_LOG	Y automatically deletes logs without asking			Y	Y	Y	Y	Y	Y	Y
DEBUGMODE	Y changes script to use debugger			N	N	N	N	N	N	N
DEBUG_EXE	Sets debugger to use when DEBUGMODE = Y			n/a	n/a	n/a	n/a	n/a	n/a	n/a
NONROAD	Y resets area files to nonroad files						Y			
Episode settings										
G_STDATE	Julian start date			varies	varies	varies	varies	varies	varies	varies
G_STTIME	Start time (HHMMSS)			000000	000000	000000	000000	000000	000000	000000
G_TSTEP	Time step (HHMMSS)			10000	10000	10000	10000	10000	10000	10000
G_RUNLEN	Run length (HHMMSS)		Daily files are from 0-23Z, and they need an extra hour!	250000	250000	250000	250000	250000	250000	250000