APPENDICES

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

Appendix A: Revisions to PTIPM Sector SO2 and NOX emissions from V4 to V4.1

Table A-1. Plant level summary of V4.1 differences for SO2 and NOX, ptipm sector

state	count y	plant_id	Plant name	Plant-level annual tons NOX, V4	Plant-level annual tons NOX, V4.1	NOX DIFFERE NCE : Platfor m V4.1 minus V4	Plant-level annual tons SO2, V4	Plant-level annual tons SO2, V4.1	SO2 DIFFERE NCE : Platform V4.1 minus V4	Data Source of data in V4	Comments on updated emissions
CA (06)	San Diego (073)	37122772	SouthBay Power Plant	108.23	45.34	(62.9)	21.4	4.2	(17.2)	NOx and SO2 from 2002 NEI	
CA (06)	San Diego (073)	37122773	Encina Power Plant	301.93	289.40	(12.5)	51.0	47.2	(3.8)	NOx and SO2 from 2002 NEI	
CA Total						**(75.4)**			**(21.1)**		
MA (25)	Hamp den (013)	0420001	StonyBroo Energy er	458.07	176.02	(282.1)				NOx and SO2 from 2002 NEI	
MA (25)	Middl esex (017)	1190128	EXELON MYSTIC LLC	1,154.92	953.94	(201.0)	5007.1	3473.7	(1,533.4)	NOx and SO2 are a mixture of 2002 (carried forward) and 2005 CEM (created by EPA).	CEMs are reporting nearly every day for all units. Updated boiler matching is for data from 2002, which is replaced by 2005.
MA Total						**(483.0)**			**(1,533.4)**		
MS (28)	Choct aw (019)	28019000 11	CHOCTA NERATION LLP,REDHI ENERA				1918.0	2847.7	929.7	2005 State data.	Confirmed 2 boilers in CEM and only one matched previously.
MS											

state	county	plant_id	Plant name	Plant-level annual tons NOX, V4	Plant-level annual tons NOX, V4.1	NOX DIFFERENCE : Platform V4.1 minus V4	Plant-level annual tons SO2, V4	Plant-level annual tons SO2, V4.1	SO2 DIFFERENCE : Platform V4.1 minus V4	Data Source of data in V4	Comments on updated emissions
Total									929.7		
NY (36)	Nassau (059)	1282000553	EFBARRET POWER STATION	1,227.53	1,078.20	(149.3)				2005 State data.	
NY Total						**(149.3)**					
SC (45)	Beaufort (013)	0360-0006	SANTEE COOPER HILTONHE	162.09	12.74	(149.3)				NOx and SO2 from 2002 NEI	
SC (45)	Charleston (019)	0560-0244	COGENSO	1,487.10	707.34	(779.8)				2002 NEI carried forward	
SC (45)	Darlington (031)	0820-0002	PROGRES ENERGY ROBINSO STATION	3,092.95	2,855.88	(237.1)	11066.9	11065.6	(1.3)	NOx and SO2 from 2002 NEI (except other large CEM source that EPA inserterd for 2005)	
SC Total						**(1,166.2)**			**(1.3)**		
WV (54)	Marion (049)	5404900026	AMERICA BITUMIN POWER-GRANTTO PLT	8.36	150.84	142.5				2005 State data.	
WV Total						**142.5**					NOx only (assume state just didn't report NOx)
Total						**(1,731.5)**			**(625.9)**		

Appendix B: Creation of the modeling file ("ORL point file") parameters from the Boiler MACT ICR unit level emissions

The following table shows how the ICR unit level Hg emissions were developed into non-EGU (ptnonipm) sector file (ORL format)that was used in SMOKE. We used the annual emissions from 080310 version of Boiler MACT ICR database (Aug 3), provided by Brian Shrager, SPPD. Revisions to that database prior to development of the ORL file were:

1. Removed units identified by CAMD as EGUs
2 Excluded units without NEI_UNIQUE_ID assignment (sum of 0.177 tons)
3. Shortened plantid to 16 characters
4. Created a "POINTID" (unit ID) such that the first character of the POINTID indicates whether unit(s) are boilers (B) or process heaters (P), the rest of the ID field was a sequential number.

ORL fields were populated as provided by the table below.

FORMAT FOR INVENTORY DATA- POINT SOURCES

Position in ORL file (column)	**ORL variable name**	**Description**	**Approach to Populate from Boiler MACT ICR database**
A	FIPS	Five digit FIPS code for state and county (required)	Taken from Boiler MACT ICR database – these were added based on Facility/county by matching to the NEI
B	PLANT ID	Plant Identification Code (15 characters maximum) (required; this is the same as the State Facility Identifier in the NIF)	Used "FacilityID" from Boiler MACT database. If ID was too long, then shortened the FacilityID where needed and added to Boiler MACT database
C	POINT ID	Point Identification Code (15 characters maximum) (required; this is the same as the Emission Unit ID in the NIF)	the letter "P" or "B" based on whether the unit is a process heater "P" or boiler "B" concatenated with a number, where the number is a numerical increment assigned to each boiler mact record
D	STACKID	Stack Identification Code (15 characters maximum) (recommended; this is the same as the Emissions Release Point ID in the NIF)	BOILERMACTICR
E	SEGMENT	DOE Plant ID (15 characters maximum) (recommended; this is the same as the Process ID in the NIF)	BOILERMACTICR
F	PLANT	Plant Name (40 characters maximum) (recommended)	Use "FacilityID" from Boiler MACT database
G	SCC	Source Classification Code (10 characters maximum) (required)	based on XWALK "default_scc_for_boilerMACT_hg.xlsx" which depends on both unit type (boiler or process heater, as defined in the Boiler MACT database in the column

FORMAT FOR INVENTORY DATA- POINT SOURCES

Position in ORL file (column)	**ORL variable name**	**Description**	**Approach to Populate from Boiler MACT ICR database**
			entitled "Classification")and the ICR fuel type – see note 1 below.
H	ERPTYPE	Emissions release point type (2 characters maximum); indicates type of stack (used by SMOKE for ASPEN, ISCST3, AERMOD): 01 = fugitive, 02 = vertical stack, 03 = horizontal stack, 04 = goose neck, 05 = vertical with rain cap, 06 = downward-facing vent	02
I	SRCTYPE	Source type (2 characters maximum); used by SMOKE in determining applicable MACT-based controls and for data summaries (required), 01 = major, 02 = Section 112 area source. 03=nonroad source	01
J	STKHGT	Stack Height (ft) (required)	Use value from Hg NATA inventory unit from same NEI_UNIQUE_ID that has same fuel type. (SO LITTLE HG FROM PROCESS HEATERS – DON't USE THEM TO MATCH THE TYPE OF UNIT). Use the "nata_nei_scc-to-fuel_xwalk.xlsx" -- see Note 2 below. to assign nata and nei inventories a fuel TYPE based on the SCC, and use the "fuelxwalk_for_tagging_revision1.xls" (first two columns of the Primary XWALK tab) (see Note 3 below) to match ICR unit to a unit in the NEI based on NEI fuel. Once there is at least one matching unit, can use to get stack parameters. 2. If no match to Hg inventory, use secondary fuel xwalk. 3. If still no match, then match to CAP inventory unit. 4. if still no match, then use default parameters from the following file:ftp://ftp.epa.gov/EmisInventory/2002finalnei/documentation/point/augmentation_point/2002nei_stackparameterdefault.mdb see item 4 for if there is no SCC match to that file. See note 4 below. 5. if there are multiple units that match the ICR unit, then choose stack parameters from stack with largest total emissions --either across all polls or just pick Hg for nata and CO for NEI.
K	STKDIAM	Stack Diameter (ft) (required)	same as above
L	STKTEMP	Stack Gas Exit Temperature (°F) (required)	same as above
M	STKFLOW	Stack Gas Flow Rate (ft3/sec) (optional; automatically calculated by **Smkinven** from velocity and diameter if not given in file)	leave blank
N	STKVEL	Stack Gas Exit Velocity (ft/sec) (required)	same as above
O	SIC	Standard Industrial Classification Code (recommended)	use value based on NEI_UNIQUE_ID. If multiple values, then choose the mode

FORMAT FOR INVENTORY DATA- POINT SOURCES

Position in ORL file (column)	**ORL variable name**	**Description**	**Approach to Populate from Boiler MACT ICR database**
P	MACT	Maximum Achievable Control Technology Code which identifies a source categories defined by Maximum Achievable Control Technology rules or rules that are done under other programs such as Section 129 standards (6 characters maximum) (optional)	0107
Q	NAICS	North American Industrial Classification System Code (6 characters maximum) (optional)	use value based on NEI_UNIQUE_ID. If multiple values, then choose the mode
R	CTYPE	Coordinate system type (1 character maximum) (required); U = Universal Transverse Mercator ; L = Latitude/longitude	L
S	XLOC	X location (required), If CTYPE = U, Easting value (meters); If CTYPE = L, Longitude (decimal degrees)	same as stack params except if no unit match then use site avge lat/lon
T	YLOC	Y location (required), If CTYPE = U, Northing value (meters), If CTYPE = L, Latitude (decimal degrees)	same as stack params except if no unit match then use site avge lat/lon
U	UTMZ	UTM zone (required if CTYPE = U)	-9
V	POLCODE	Code representing the pollutant contained in the inventory (required, can be up to 10 characters)	7439976
W	ANN_EMIS	Annual Emissions (tons/year) (required)	emissions are in the boiler MACT database
X	AVD_EMIS	Average-day Emissions (tons/average day) (optional)	Put in a value of -9 for this variable
Y	CEFF	Control Efficiency percentage (give value of 0-100) (recommended, if left blank, SMOKE default is 0)	leave blank
Z	REFF	Rule Effectiveness percentage (give value of 0-100) (recommended, if left blank, SMOKE default is 100)	leave blank
AA	CPRI	Primary Control Equipment Code (not used by SMOKE)	leave blank
BB	CSEC	Secondary Control Equipment Code (not used by SMOKE)	leave blank

FORMAT FOR INVENTORY DATA- POINT SOURCES

Position in ORL file (column)	**ORL variable name**	**Description**	**Approach to Populate from Boiler MACT ICR database**
CC	NEI_UNIQUE_ID	Unique ID that ties together HAP and CAP emissions within a common facility ID, and ties together emissions obtained from multiple data sources (e.g., TRI, State, ESD) which may have different StateFacilityIdentifiers but really belong to a single FACILITY (optional)	use value from boiler mact database
DD	ORIS_FACILITY_CODE	Provides ORIS code at the plant level (optional)	leave blank
EE	ORIS_BOILER_ID	ORIS boiler ID (optional)	leave blank
FF	IPM_YN	Y or N single character flag indicating whether the point source belongs in the IPM sector (optional)	if in HG inventory, NEI UNIQUE ID is in both, then B, if it is in IPM then Y if nonIPM then blank. If source is in CAP inventory but NOT Hg inventory then use the same criteria but base it on the CAP values
GG	DATA_SOURCE	flag indicating the source of the data (e.g., state-submitted, toxics release inventory, Clean Air Markets Division, etc.) (optional)	the Data source code indicates the emissions estimation method: BMICR_ET means test was done, BMICR_BSAVmeans used Emission Factor (see Baseline memo in Boiler MACT docket) Since only allowed 10 characters, use BSAV is used if the Hg source field is BaselineAverage
HH	STACK_DEFAULT_FLAG	flag indicating how NEI defaulted stack params (optional)	if the stack came from Hg or CAP inventory use same value as unit you used. If you used default by SCC then the value is 11111
II	LOCATION_DEFAULT_FLAG	flag indicating how NEI defaulted locations (optional)	if the stack came from Hg or CAP inventory use same value as unit you used. If you used siteave then "DEF_SITEAVG"
JJ	YEAR	Allows us to see what year was used to represent 2002 emissions (optional)	2008
KK	TRIBAL_CODE	Indicates the particular tribe that submitted the data (optional)	TRIBAL_CODE
LL	HORIZONTAL_AREA_FUGITIVE	related to AXLEN, AYLEN which are optional params for ISCST3/AERMOD (optional) (units are square feet)	leave blank
MM	RELEASE_HEIGHT_	related to optional params for ISCST3/AERMOD (ARELHT?) (optional) (units are feet)	leave blank

Remainder of the fields are left blank

NOTES

1. Below are the default_scc_for_boilerMACT_hg.xlsx:

ICR Fuel Category for Unit	Default SCC	Rationale
Gas 1 (NG Only)	10200601	arbitrarily chosen industrial boiler natl gas
Coal	10200201	arbitrarily chosen industrial boiler coal
Light Liquid	10200501	arbitrarily chosen industrial boiler distillate oil
Gas 1 (Other)	10200701	used refinery gas SCC since Brian Shrager (project lead) said that was Gas 1 (other)
Wet Biomass	10200901	arbitrarily chosen industrial boiler wood: bark
Heavy Liquid	10200401	arbitrarily chosen industrial boiler: residual oil
Dry Biomass	10200908	chose dry wood since there is no SCC with lumber or sanderdust or hog fuel or other dry biomass examples
Gas 2	10200799	chose scc for process gas - unspecified
Bagasse	10201101	chose scc for bagasse - industrial boilers all sizes

2. Fuels are provided in the SCC description; therefore we do not provide the “"nata_nei_scc-to-fuel_xwalk.xlsx"” . We do provide, below, a list of SCCs for which fuels were extracted to use for the characterizing inventory sources

Source Classification Code

10200101 10200104 10200107 10200117 10200201 10200202 10200203 10200204 10200205 10200206 10200210 10200212 10200213 10200217 10200218 10200219 10200221 10200222 10200223 10200224 10200225 10200226 10200229 10200300 10200301 10200302 10200303 10200304 10200306 10200307 10200401 10200402 10200403 10200404 10200405 10200501 10200502 10200503 10200504 10200505 10200601 10200602 10200603 10200604 10200701 10200704 10200707 10200710 10200711 10200799 10200802 10200804 10200901 10200902 10200903 10200904 10200905 10200906 10200907 10200908 10200910 10200911 10200912 10201001 10201002 10201003 10201101 10201201 10201202 10201301 10201302 10201303 10201601 10201701 10300101 10300102 10300103 10300203 10300205 10300206 10300207 10300208 10300209 10300211 10300214 10300216 10300217 10300218 10300221 10300222 10300223 10300224 10300225 10300226 10300300 10300305 10300306 10300307 10300309 10300401 10300402 10300403 10300404 10300501 10300502 10300503 10300504 10300601 10300602 10300603 10300701 10300799 10300811 10300901 10300902 10300903 10300908 10300910 10300911 10300912 10301001 10301002 10301003 10301201 10301202 10301301 10301302 10301303 10500102 10500105 10500106 10500110 10500113 10500114 10500202 10500205 10500206 10500209 10500210 10500213 10500214

2102001000 2102002000 2102004000 2102005000 2102006000 2102006001 2102006002 2102007000 2102008000 2102009000 2102010000 2102011000 2102012000 2103001000 2103002000 2103004000 2103005000 2103006000 2103007000 2103007005 2103007010 2103008000 2103010000 2103011000 2103011005 2103011010 2199001000 2199002000 2199003000 2199004000 2199004001 2199004002 2199005000 2199006000 2199006001 2199006002 2199007000 2199008000 2199009000 2199010000 2199011000

30190001 30190002 30190003 30190004 30290001 30290002 30290003 30290005 30390001 30390002 30390003 30390004 30490001 30490002 30490003 30490004 30590001 30590002 30590003 30590005 30600101 30600102 30600103 30600104 30600105 30600106 30600107 30600108 30600111 30600199 30790001 30790002 30790003 30890001 30890002 30890003 30890004 30990001 30990002 30990003 31000401 31000402 31000403 31000404 31000405 31000406 31000411 31000412 31000413 31000414 31000415 31390001 31390002 31390003 39900501 39900601 39900701 39900711 39900721 39900801 39901001 39901601 39901701 39990001 39990002 39990003 39990004 10100101 10100102 10100201 10100202 10100203 10100204 10100205 10100211 10100212 10100215

10100217 10100218 10100221 10100222 10100223 10100224 10100225 10100226 10100235 10100237 10100238 10100300 10100301 10100302 10100303 10100304 10100306 10100316 10100317 10100318 10100401 10100404 10100405 10100406 10100501 10100504 10100505 10100601 10100602 10100604 10100701 10100702 10100703 10100704 10100707 10100711 10100712 10100801 10100818 10100901 10100902 10100903 10100908 10100910 10100911 10100912 10101001 10101002 10101003 10101101 10101201 10101202 10101204 10101205 10101206 10101207 10101208 10101301 10101302 10101304 10101305 10101306 10101307 10101308 10101601 10101801 10101901 10102001 10102018

3. fuelxwalk_for_tagging_revision1.

SCC fuel category	ICR Fuel Category for Unit
Bagasse	Bagasse
coal	Coal
Coal-based Synfuel	Heavy Liquid
crude oil	Heavy Liquid
Digester Gas	Gas 2
Distillate Oil	Light Liquid
Distillate Oil (Diesel)	Light Liquid
gas	Gas 2
Gasified Coal	Gas 1 (Other)
Gasoline	Light Liquid
Hydrogen	Gas 1 (Other)
Kerosene	Light Liquid
Kerosene/Naphtha (Jet Fuel)	Light Liquid
Landfill Gas	Gas 2
Liquid Waste	Heavy Liquid
Liquified Petroleum Gas (LPG)	Gas 1 (Other)
LPG	Gas 1 (Other)
Methanol	Heavy Liquid
Natural Gas	Gas 1 (NG Only)
oil	Light Liquid
Other Oil	Light Liquid
Petroleum Coke	Coal
Process Gas	Gas 2
propane/butane	Gas 1 (Other)
Refinery Gas	Gas 1 (Other)
Residual Oil	Heavy Liquid
Solid Waste	Wet Biomass
unknown	Gas 1 (NG Only)
Waste Coal	Coal
Waste oil	Heavy Liquid
Wood	Dry Biomass
Wood/Bark Waste	Wet Biomass

4. Stack parameters for sources without an NEI UNIQUE ID / fuel type match in existing inventories: As some of the SCCs we needed default stack parameters for were not present in 2002nei_stackparameterdefault.mdb (retrieved from ftp.epa.gov). In these cases, we used default stack parameters for a different SCC instead, an SCC that has the same ICR fuel type (according to nonunique_icr

fuel and nei fuel mapping.xls) as the original SCC. Here are the substitutions:

10200908: use default stackparms for SCC=10100902
10200101: use default stackparms for SCC=10200201
10101308: use default stackparms for SCC=10200901
39900701: use default stackparms for SCC=31000415
39900711: use default stackparms for SCC=31000406

Appendix C: Pollutants in the onroad emission sectors generated from NMIM or MOVES2010

SECTOR /Mobile emissions approach	Pollutants	Pollutants used in Case
on_noadj / NMIM	EVP_10041 (ETHYLBENZ), EXH_100414(ETHYLBENZ), EXH_100425(STYRENE), EVP_108883(TOLUENE), EXH_108883(TOLUENE), EVP_110543(HEXANE), EXH_110543(HEXANE), EXH_120127(ANTHRACEN), EXH_123386(PROPIONAL), EXH_129000(PYRENE), EVP_108383 (MXYL as 0.68 of EVP_1330207(XYLS)), EVP_95476 (OXYL as 0.32 of EVP_1330207(XYLS)), EXH__108383 (MXYL as 0.74 of EXH_1330207 (XYLS)), EXH_95476 (OXYL as 0.26 of EXH_1330207(XYLS)), EXH_16065831(CHROMTRI), EXH_1634044(MTBE), EXH_18540299(CHROMHEX), EXH_191242(BENZOGHIP), EXH_193395(INDENO123), DESC EXH_200(HG), EXH_201(HGIIGAS), EXH_202(PHGI), EXH_205992(BENZOBFLU), EXH_206440(FLUORANTH), EXH_207089(BENZOKFLU), EXH_208968(ACENAPHTY), EXH_218019(CHRYSENE), EXH_50328(BENZOAPYR), EXH_53703(DIBENZAHA), EVP_540841(TRMEPN224), EXH_54084(TRMEPN224), EXH__56553(BENZAANTH), EXH_7439965(MANGANESE),EXH__7440020(NICKEL), EXH_83329(ACENAPENE), EXH_85018(PHENANTHR), EXH_86737(FLUORENE), EXH_93(ARSENIC)	EXH_200(HG), EXH_201(HGIIGAS), EXH_202(PHGI)
on_noadj sector/ MOVES .	BRK_PM10, BRK_PM2_5 ,TIR_PM10, TIR_PM2_5 ,EVP_VOC ,EVP_71432 (benzene), EVP_91203 (naphthalene), EXH_106990 (butadiene), EXH_107028 (acrolein), EXH_50000 (formaldehyde), EXH_71432, EXH_75070 (acetaldehyde), EXH_CO, EXH_NH3, EXH_NOX, EXH__SO2, EXH_VOC, EXH_91203 (Naphthalene), PEC POC PNO3 PSO4 PMFINE and PMC (exhaust mode) for onroad diesel sources	All <u>except</u>: EVP_91203 (naphthalene), EXH_106990 (butadiene), EXH_107028(acrolein)EXH_91203 (Naphthalene)
on_moves_start PM and on_moves_runpm sectors/ MOVES	PEC_72 POC_72 PNO3 PSO4 OTHER PMFINE_72 PMC_72	All <u>except</u>: NAPHTH_72 (all exhaust)

Appendix D: Approach to develop CMAQ PM2.5 species from Partially-speciated MOVES2010 EXHAUST PM2.5 for the 2005 Platform, version 4.1

Introduction

This document presents the interim approach developed by OTAQ and OAQPS to speciate the partially speciated PM2.5 exhaust emissions from MOVES2010. The advantage of using this approach over the approach used for speciating total PM2.5 is that it allows the speciated emissions from MOVES; i.e., elemental carbon and particulate sulfate to be retained and only the remainder of the PM2.5 to rely on speciation profiles.

The table below shows the MOVES2010 exhaust PM2.5-related species and how they relate to the five CMAQ 4.7 model species: PEC, POC, PSO4, PNO3, and PMFINE

MOVES2010 Pollutant Name	shortName	Variable name for Equations	Relation to CMAQ model species
Primary Exhaust PM2.5 - Total	PM2.5 Total Exh	PM25_TOTAL	
Primary PM2.5 - Organic Carbon	PM2.5 Organic C	PM25OM	Sum[2] of **POC**, **PNO3** and **PMFINE**
Primary PM2.5 - Elemental Carbon	PM2.5 Elem C	PM25EC	**PEC**
Primary PM2.5 - Sulfate Particulate	PM2.5 Sulfate	PM25SO4	**PSO4**

We need to further disaggregate the MOVES species "PM25OM" into the CMAQ model species.

MOVES species are related as follows: PM25_TOTAL = PM25EC + PM25OM + PSO4

The five CMAQ species also sum to total PM2.5:

PM2.5 = POC+PEC+PNO3+PSO4+PMFINE

The next section discusses the procedure we used when using the draft version of MOVES prior to the MOVES2010 release. The issues with this approach and rationale for the changes to MOVES2010 outputs are presented.

Following this explanation, we describe the approach, data and assumptions used.

[2] For draft MOVES, for gasoline sources (in all cases using draft MOVES for the platform including 2005ai , 2005ak, 2005ap), this MOVES pollutant also included PSO4, since it was the difference of total PM2.5 and PEC. With MOVES2010, this species is now the difference between total PM2.5 and the sum of PEC and PSO4.

The last section provides the equations used when when MOVES is run at 72 F, such as the case when pre-computed MOVES emissions are input into SMOKE, and are adjusted based on gridded hourly temperatures prior to be input into CMAQ.

Background: Previous Approach Using Draft MOVES

When we received output from the draft version of MOVES for gasoline vehicles (summer 2008), it did not include Primary Exhaust PM2.5 - Total. MOVES output provided emissions for the following:

1) Primary PM2.5 - Elemental Carbon (PEC)
2) Primary PM2.5 .- Sulfate Particulate (PSO4)
3) The difference between total PM2.5 and PEC, which ***was*** labeled “PM25OC”

The total PM2.5 and PEC (from which the MOVES PM25OC was derived) were based on the Kansas City Study; the MOVES PSO4 was based on the fuel sulfur content. In our previous approach, we first subtracted PSO4 from PM25OC prior to further speciating it into the necessary CMAQ inputs.

When we tried to implement the same approach for draft MOVES for diesel vehicles, the PM2.5 Sulfate exceeded the PM25OC. Therefore we chose not to subtract PM2.5 Sulfate. Note that the diesel results did not come from the Kansas City study and the actual relationship between PM2.5 Total Exhaust, PM2.5 Organic Carbon, and PEC is not necessarily the same as in the Kansas City study.

It should also be noted, that for the gasoline approach, the sulfates included in the gasoline-based “PM25OC” would have been specific to Kansas City and very small. It is possible that in other parts of the country or that for different years, the sulfate is much larger and would be inconsistent with the “PM25OC” of the Kansas City study. As a result, it was decided at the OTAQ/OAQPS Inventory Coordination Team meeting on February 25, 2010, that in the interim we will no longer remove PSO4 mass from MOVES “PM25OC” **for neither gasoline nor diesel vehicles.**

In addition to the above changes, there were also changes to the values used for the speciation approach. Attachment 1 provides the details.

Ultimately, the plan is for MOVES to provide all of the species that CMAQ requires. In the meantime, adjustments will continue be made in a post processing step of the MOVES outputs that we describe in this document.

Approach for MOVES 2010

MOVES 2010 output provides total $PM_{2.5}$ and three components of $PM_{2.5}$: two pre-speciated components of PM2.5 which are: 1) *PEC*, and 2) *PSO4*, and a non-speciated component termed "*PM25OM*", which is defined as the difference between total $PM_{2.5}$ and PEC.

It is important to note that *PM25OM* is not solely made up of organic matter, but is defined as the following:

$$\text{MOVES total } PM_{2.5} = PEC + PM25OM + PSO4 \qquad (1)$$

We can compute the CMAQ PM2.5 species from (1) the MOVES2010 output pollutants: PEC, PSO4 and PM25OM, and (2) the speciation profile for total PM2.5 exhaust. The equations used are presented below.

MOVES total $PM_{2.5}$ is the sum of the two pre-speciated components of PM2.5 and a remainder term, *R*.

$$\text{MOVES total } PM_{2.5} = PEC + PSO4 + R \qquad (2)$$

The remainder term is provided as a MOVES output

$$R = PM25OM \qquad (3)$$

The *R* term includes POM, which consists of POC and the hydrogen and oxygen atoms attached to the carbon as part of the organic matter, PNO3, soil oxides and metals (also known as "crustal" and called METAL here), ammonium, and water, and thus can be also written as:

$$R = POM + PNO3 + METAL + NH4 + H_20 \qquad (4)$$

To correctly calculate the five $PM_{2.5}$ species needed for CMAQ, we first needed to break out the POC, PNO3, and PMFINE from *R*. We can use the proportional relationship of known species to unknown species from the speciation profile. Note that there are different speciation profiles for gasoline vehicles, light duty diesel vehicles and heavy duty diesel vehicles. They are provided along with the corresponding data used for these calculations in Table 1. The primary nitrate is computed based on the ratio of nitrate to elemental carbon, i.e., F_{NO3} / F_{EC} and metals component from the ratio of metals to elemental carbon, F_{METAL} / F_{EC} using equations (5) and (6), respectively.

$$PNO3 = PEC \times F_{NO3} / F_{EC} \qquad (5)$$

$$METAL = PEC \times F_{METAL} / F_{EC} \qquad (6)$$

where,

F_{EC} = Fraction of elemental carbon in the speciation profile
F_{NO3} = Fraction of nitrate in the speciation profile
F_{METAL} = Fraction of metals in the speciation profile

Table 1 shows the values for the above fractions and the profiles from which they are to be derived.

Table 1: Values and basis for fractions used to compute PNO3 and METAL

Vehicle Type	**SCC list**	**Speciation Profile Code and Name**[1]	**Profile Percentages**
LDDV	All SCCs that begin with: 2230001 2230002 2230003 2230004 2230005 2230006	92042 LDDV Exhaust – Simplified 91017 LDDV Exhaust - Composite See Note 2	F_{EC} = 57.48051203% F_{NO3}= 0.23% F_{METAL}=0.6513%
HDDV	All SCCs that begin with: 223007	92035 HDDV Exhaust – Simplified 3914 Diesel Exhaust See Note 3	F_{EC} = 77.1241% F_{NO3}= 0.1141% F_{METAL} = 0.2757%
LDGV and HDGV	All SCCs that begin with 2201	92050 Onroad Gasoline Exhaust – Simplified 91022 Onroad Gasoline Exhaust - Composite	F_{EC} = 20.80113619% F_{NO3} = 0.1015% F_{METAL} = 2.2256%

NOTES
1. The values of F_{EC} and F_{NO3} are the same in the simplified and non-simplified profiles. The value for F_{METAL} was computed from the non-simplified profile as the sum of percentages of all ions of the metals and metal elements in the profile.
2. Previously (Attachment 1), for LDDV in the draft MOVES approach, we used the value of F_{NO3} and F_{METAL} from the HDDV profile. We changed so that all fractions for each species come from the LDDV
3. The value of F_{METAL} for HDDV previously used (Attachment 1) was corrected since it had inadvertently excluded the chloride ion percentage in the HDDV speciation profile.

Ammonium is based on stoichiometric calculations; the formula is shown in equation (7).

$$NH4 = (PNO3/MW_{NO3} + 2 \times PSO4/MW_{SO4}) \times MW_{NH4} \quad (7)$$

MW_{SO4} = Molecular weight of sulfate (**96.0576**)
MW_{NO3} = Molecular weight of nitrate (**62.0049**)
MW_{NH4} = Molecular weight of ammonium (**18.0383**)

The final component of PMFINE is the non-carbon mass of organic carbon. To calculate the non-carbon mass, we first needed to compute organic carbon from the remainder term, *R*.

A key assumption is that POM is a factor of 1.2 greater than the mass of primary organic carbon, which is also used in the CMAQ postprocessing software at EPA.

$$POM = 1.2 \times POC \qquad (8)$$

Using this assumption and assuming that the $H_2 0$ is negligible, the equation needed for the calculation of POC is shown in equation (9) below.

$$POC = 5/6 \times (R - METAL - NH4 - PNO3) \qquad (9)$$

From equation (8), the non-carbon portion of the organic carbon matter is 20%, of the POC. By definition, PMFINE is the sum of the non-carbon portion of the mass, METAL and NH4.

$$PMFINE = METAL + NH4 + 0.2 \times POC \qquad (10)$$

For gasoline mobile sources, the PMC is 8.6% of the $PM_{2.5}$ mass

Gasoline vehicles only: PMC = 0.086 × (PMFINE + PEC + POC + PSO4 + PNO3)

For diesel mobile sources, the PMC is 3.09% of the $PM_{2.5}$ mass

Diesel vehicles only: PMC = 0.0309 × (PMFINE + PEC + POC + PSO4 + PNO3)

Implementation for when MOVES-based emissions at 72 Fahrenheit are Input into SMOKE[3]

The equations below utilize the following MOVES 2010 outputs:

PM25OM
PM25EC
PM25SO4

However, EXH_PM25 can be used for QA

All red-fonted variables are fed into SMOKE
All blue-fonted varilables are from MOVES output
Table 1 provides the values of the constants (italics): *FNO3, FEC, FMETAL and* $R_{PM10\text{-}to\text{-}PM25}$*-1*

The equations are

- **(1)** PEC_72 = PM25EC
- **(2)** PSO4 = PM25SO4
- ***(3)*** PNO3 = PEC_72 × *FNO3 / FEC*
- ***(4)*** METAL = PEC_72× *FMETAL / FEC*
- **(5)** NH4 = (PNO3/**62.0049** + 2×PSO4/**96.0576**) × **18.0383**
- **(6)** POC_72 = 5/6 × (PM25OM – METAL – NH4 – PNO3)
- **(7)** OTHER = METAL+NH4

A program is used to compute temperature adjustments are made to the SMOKE intermediate files to produce POC and PEC. That program also computes the remainder of the species that are needed prior to the final SMOKE merge using the adjusted POC and PEC and other intermediate species. These species are shown in green font.

- **(8)** **POC** = Look-up-table_Function (Temperature, POC_72)
- **(9)** **PEC** = Look-up-table_Function (Temperature, PEC_72)
  See below for lookup table functions
  Note that OTHER, PNO3 and PSO4 are not temperature-adjusted and come directly from the SMOKE intermediate files
- **(10)** **PMFINE** = OTHER + 0.2 × POC
- **(11)** **PMC** = ($R_{PM10\text{-}to\text{-}PM25}$*-1)* × (PMFINE + PEC + POC + PSO4 + PNO3)

[3] This procedure is only needed for gasoline particulate exhaust emissions. For diesel emissions, we use the same equations but without the "_72" appended.

Table D-1. Correction Factors to Adjust 72 F PM OC and EC Emissions for colder temperatures (supplied by Harvey Michaels, OTAQ, 9/5/2008)			
Year	Temperature (degrees F)	Correction Factor for Running Exhaust	Correction Factor for Start Exhaust
2005	-20	18.6454	70.7816
2005	-19	18.0618	67.5797
2005	-18	17.4965	64.5218
2005	-17	16.9488	61.6025
2005	-16	16.4183	58.8153
2005	-15	15.9045	56.1542
2005	-14	15.4067	53.6136
2005	-13	14.9244	51.1878
2005	-12	14.4573	48.8719
2005	-11	14.0048	46.6607
2005	-10	13.5665	44.5495
2005	-9	13.1418	42.5339
2005	-8	12.7305	40.6095
2005	-7	12.332	38.7722
2005	-6	11.9461	37.018
2005	-5	11.5721	35.3431
2005	-4	11.2099	33.744
2005	-3	10.8591	32.2173
2005	-2	10.5192	30.7596
2005	-1	10.1899	29.3679
2005	0	9.87099	28.0392
2005	1	9.56203	26.7706
2005	2	9.26275	25.5594
2005	3	8.97281	24.4029
2005	4	8.69197	23.2988
2005	5	8.41992	22.2447
2005	6	8.15638	21.2382
2005	7	7.90109	20.2773
2005	8	7.65378	19.3599
2005	9	7.41422	18.484
2005	10	7.18216	17.6477
2005	11	6.95736	16.8492
2005	12	6.73959	16.0868
2005	13	6.52865	15.359
2005	14	6.3243	14.6641
2005	15	6.12635	14.0006
2005	16	5.9346	13.3672
2005	17	5.74885	12.7624
2005	18	5.56891	12.1849
2005	19	5.39461	11.6337
2005	20	5.22576	11.1073
2005	21	5.06219	10.6048
2005	22	4.90375	10.125
2005	23	4.75026	9.66683
2005	24	4.60158	9.22946
2005	25	4.45755	8.81189
2005	26	4.31803	8.41321
2005	27	4.18288	8.03256
2005	28	4.05196	7.6691
2005	29	3.92513	7.32215
2005	30	3.80228	6.99088
2005	31	3.68327	6.67456
2005	32	3.56798	6.37257
2005	33	3.4563	6.08424
2005	34	3.34812	5.80897

Table D-1. Correction Factors to Adjust 72 F PM OC and EC Emissions for colder temperatures (supplied by Harvey Michaels, OTAQ, 9/5/2008)			
2005	35	3.24333	5.54614
2005	36	3.14181	5.29521
2005	37	3.04347	5.05563
2005	38	2.94821	4.82689
2005	39	2.85593	4.6085
2005	40	2.76655	4.39999
2005	41	2.67995	4.20091
2005	42	2.59607	4.01085
2005	43	2.51481	3.82938
2005	44	2.4361	3.65612
2005	45	2.35985	3.4907
2005	46	2.28599	3.33277
2005	47	2.21444	3.18198
2005	48	2.14513	3.03801
2005	49	2.07799	2.90055
2005	50	2.01295	2.76932
2005	51	1.94994	2.64403
2005	52	1.88891	2.5244
2005	53	1.82979	2.41018
2005	54	1.77252	2.30114
2005	55	1.71704	2.19702
2005	56	1.66329	2.09762
2005	57	1.61123	2.00271
2005	58	1.5608	1.9121
2005	59	1.51195	1.82559
2005	60	1.46463	1.74299
2005	61	1.41878	1.66413
2005	62	1.37438	1.58883
2005	63	1.33136	1.51695
2005	64	1.28969	1.44832
2005	65	1.24932	1.38279
2005	66	1.21022	1.32022
2005	67	1.17234	1.26049
2005	68	1.13564	1.20346
2005	69	1.1001	1.14901
2005	70	1.06567	1.09703
2005	71	1.03231	1.04739
2005	72	1	1

ATTACHMENT 1

Fractions of Utilized in Draft MOVES approach and rationale for the changes for MOVES 2010

PNO3 = PEC × *FNO3 / FEC*

METAL = PEC × *FMETAL / FEC*

Vehicle/ SCC s	**FNO3 value and basis**	**FEC value and basis**	**FMETAL value and basis**
LDDV: 2230001000 through 2230060334	Previously used 0.1141% Based on **HDDV** speciation profile (92035-simplified, 3914-composite containing all species).	57.4805% Based on LDDV speciation profile (92042 simplified, 91017, composite)	Previously used 0.2663% based on Value provided by Catherine Yanca and Joe Somers (OTAQ) to OAQPS in email provided 11/6/2009. It

Vehicle/ SCC s	**FNO3 value and basis**	**FEC value and basis**	**FMETAL value and basis**
	Updated to use LDDV (92042 simplified, 91017, composite) the value is 0.23%		was based on the HDDV profile (3914) Updated to use the LDDV profile for all LDDV fractions. Value changed to 0.6513% , computed using LDDV profile 91017
HDDV: 2230071110 through 2230075330	0.1141% Based on HDDV speciation profile (92035-simplified, 3914-composite containing all species).	77.1241% Based on HDDV speciation profile (92035-simplified, 3914-composite containing all species).	Previously used 0.2663% based on Value provided by Catherine Yanca and Joe Somers (OTAQ) to OAQPS in email provided 11/6/2009 "Equations for diesel MOVES speciation use in CMAQ 110609.doc" Recomputed as 0.2757% using 3914. The difference is that the chloride ion percent was inadvertently left out of the 0.2663% value
LDGV and HDGV 2201001 through 220107	0.1015% based on 92050 simplified, 91022-composite	20.80113619% based on 92050 simplified, 91022-composite	2.2256% based on 91022-composite