

IMPLEMENTATION OF MOVES-BASED PM_{2.5} EMISSIONS APPROACH FOR ONROAD GASOLINE SOURCES USING HOURLY, GRIDDED TEMPERATURES

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ABSTRACT

The impending release of the Motor Vehicle Emissions Simulator (MOVES) has prompted interest in using these emissions in air quality modeling. The MOVES PM_{2.5} emissions are significantly higher for onroad gasoline mobile sources due to temperature dependencies built into MOVES. Thus, these emissions are expected to be different from emissions based on the Mobile Source Emission Factor Model, version 6.2 (MOBILE6). These differences are important for modeling applications and include (1) higher overall values, (2) greater daily and hourly variability, and (3) greater spatial variability, with colder regions experiencing significantly higher emissions. The computationally intense nature of MOVES makes it difficult to run MOVES directly for all temperatures needed using gridded, hourly temperatures. The work reported here defines a methodology for using MOVES-based emissions without running MOVES for all temperatures in all counties.

The approach described differs significantly from a “lookup table” approach (used previously for VOCs) or the use of county-monthly emissions that has worked for MOBILE6-based processing using the National Mobile Inventory Model (NMIM). The approach relies on adjustments of start and running emissions from 72° F for all modeling hours and grid cells predicted by the meteorology data to be below 72° F, down to a maximum adjustment at -20° F. Implementation of this approach demonstrates that it is a relatively efficient manner for including these emissions improvements.

Results from this work show that in some areas, PM_{2.5} emissions from onroad gasoline sources can be many times higher than previously estimated using a MOBILE6-based approach, created with NMIM. We show the impact on temporal and spatial variability of the emissions from using this approach. Further, we show that our approach can provide significantly different emission estimates from both a NMIM/MOBILE6-based approach and a MOVES-based approach that uses state-month temperatures for air quality modeling.

1 INTRODUCTION

The Environmental Protection Agency (EPA) Office of Transportation and Air Quality (OTAQ) and Office of Air Quality Planning and Standards (OAQPS) have recently developed and implemented significant improvements for onroad gasoline mobile emissions using the Motor Vehicle Emissions Simulator (MOVES). This paper describes the impact of those changes on both the emissions data and air quality modeling results on a national, 36-km resolution modeling domain using the Community Multiscale Air Quality (CMAQ) model.

The purpose of this paper is not only to provide the results of using these data, but also to provide our methodology for applying temperature adjustments to emissions of particulate matter less than 2.5 microns ($PM_{2.5}$). In Section 2, we describe the MOVES model updates and the changes intended to improve estimation of onroad mobile source emissions. In Section 3 we provide our modeling approach, including the modeling configuration, MOVES application, MOVES pre- and post-processing, including $PM_{2.5}$ temperature adjustments. The final results section describes both the significant impact on the emissions, particularly in northern cities, and the impact on the modeled air quality.

2 BACKGROUND

2.1 *Underestimation of onroad PM*

Onroad mobile $PM_{2.5}$ emissions are known to be key contributors to air pollutants based on monitoring results, particularly in urban areas. In particular, organic mass is a key concern because of its large contribution to ambient $PM_{2.5}$ relative to other $PM_{2.5}$ components. A good summary and analysis that identifies these issues is provided in Brown et al., (2006). This report concludes that a major source of organic mass is mobile sources. In addition, it concludes that primary local sources, including mobile and industrial sources, are more important to ambient organic mass than transport or secondary sources.

The emission inventory has not traditionally been consistent with these conclusions, and the uncertainty in mobile $PM_{2.5}$ emissions has long been identified as the cause. To address this uncertainty, EPA created a consortium of sponsors in 2003 to support and advise a multi-year test program of onroad motor vehicles to collect data needed to support improved emission inventories for mobile sources. This test program is now commonly referred to as the Kansas City study. Previous work by Stump et al. (2002) and Cadle et al (1999) had suggested that temperature might influence the amount of PM emitted from light-duty vehicles, particularly at lower temperatures. To further investigate and quantify a temperature impact, EPA divided the test program into summer and winter periods, with overlap of 41 vehicles tested in both periods. This work incorporates these new data through use of the MOVES model, as explained further below.

2.2 *Summary of onroad mobile improvements included in MOVES*

MOVES includes many improvements over the Mobile Source Emission Factor Model, version 6.2 (MOBILE6), among them user interface, flexibility in specifying operating modes, expanded technology and fuel choices, ease in updating, and improved emission factors, fuel effects, $PM_{2.5}$ temperature effects, and deterioration factors. PM emissions were derived from the Kansas City study, using approaches described by Nam et al. (2008). The version of MOVES used for this work was an intermediate version of the recently released Draft MOVES2009. The latter estimates criteria and major hazardous air pollutants for onroad mobile sources. Emissions from heavy-duty diesel vehicles in MOVES2009 were derived from more than 300 in-use vehicles in a number of detailed studies.

However, they were not sufficiently developed in time to use in the work described in this paper. MOVES2009 also includes updated national default information on vehicle fleet and activity. For consistency, however, we used VMT from NMIM for the work described in this paper.

MOVES provides the $PM_{2.5}$ emissions as total $PM_{2.5}$, primary elemental carbon (PEC), and primary sulfate (PSO₄). The temperature adjustments apply only to the primary organic mass (POM) and PEC parts of $PM_{2.5}$. As part of our post-processing approach, we compute the primary organic carbon (POC) needed for CMAQ by making assumptions about the composition of POM from MOVES. Temperature adjustments also impact exhaust naphthalene emissions because these are computed as a fraction of $PM_{2.5}$. The details and formulations of the speciation and temperature adjustments are provided in Section 3, below.

MOBILE6 places start and non-running evaporative emissions on the twelve highway performance monitoring system (HPMS) road types; MOVES adds a thirteenth "road type, called "parking areas," for emissions that do not actually occur on roadways, including starts and non-running evaporative emissions. For the inventories described here, we allocated parking area emissions for light duty gasoline vehicles to grid cells by urban and rural local road VMT; for the heavy duty gasoline vehicles, we allocated parking area emissions to commercial, industrial and institutional land.

3 APPROACH

To show the impact of using MOVES-based emissions, we created emissions and ran the CMAQ air quality model for three cases. For each of these cases, we changed the onroad mobile approach as follows:

- **NMIM case:** Used emissions as described in Section 3.1, with monthly emissions based on month-specific and county-specific 2005 temperatures.
- **MOVES72 case:** Used MOVES-based data for available pollutants. For $PM_{2.5}$ and exhaust naphthalene, used emission factor *without* temperature adjustment, which is the emission factor at 72° F, as described in Section 3.3.
- **MOVES case:** Same as the MOVES72 case except $PM_{2.5}$ and exhaust naphthalene temperature adjustments were applied on an hourly grid-cell basis, as described in Sections 3.2 through 3.4.

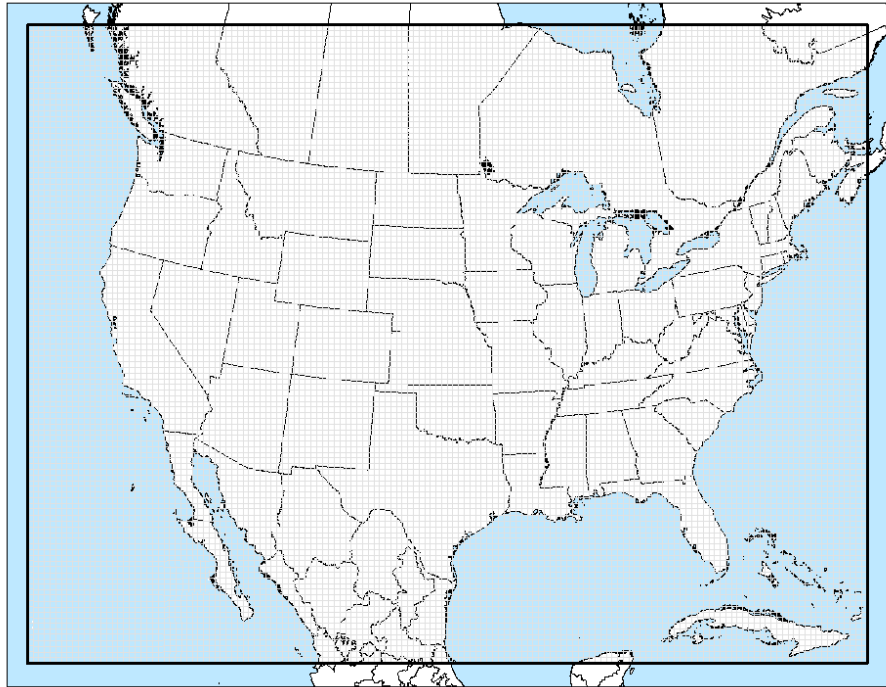
3.1 Model and emissions configuration

We processed emissions for all three cases using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system version 2.4, along with custom post-processing for the MOVES steps. The air quality modeling was done using CMAQ version 4.7, which includes secondary organic aerosol (SOA) chemistry relevant for improved $PM_{2.5}$ model predictions. We derived the gridded meteorological input data for the entire year of 2005 from simulations of the Pennsylvania State University / National Center for Atmospheric Research Mesoscale Model (Grell et al., 1994). This model, commonly referred to as MM5, was evaluated and shown to replicate the actual meteorological patterns of 2005 with sufficient accuracy for use in CMAQ.

We modeled all three cases for an annual episode on the 36-km gridded national U.S. domain shown in Figure 1. This domain uses a Lambert projection with a center at 40° latitude and -97° longitude, meridians at 33° and 45° latitude, a lower left corner at (-2736 km,-2088 km), and 148 cells in the X direction and 112 cells in the Y direction. We used the SOA-enhanced CB05 ozone chemical mechanism, which includes emissions of benzene and sesquiterpenes that play a role in SOA formation in CMAQ's chemical computations. We used SMOKE to prepare the hourly gridded data needed for air

quality modeling using an intermediate version of OAQPS’s “version 4” modeling platform, using a 2005 base year.

Figure 1: National modeling domain using a 36-km resolved grid.



For all three cases, we used emissions data based primarily on the 2005 National Emission Inventory (NEI), except for wildfire and prescribed burning, which used an “average fire” approach developed for modeling purposes. The following list summarizes the modeling sectors and the source of the data used for the modeling.

- **Point sources:** 2005 NEI v1 emissions for electric generating units (EGUs) and nonEGU point sources. For nonEGU emissions, this inventory was simply the 2002 NEI v3, with plant closures applied between 2002 and 2005. For EGUs, the 2005 continuous emissions monitoring (CEM) data were used for the annual values, and the emissions were allocated to days using an approach that calculates monthly emissions using 2004, 2005, and 2006 CEM data and further calculates daily emissions using 2005 CEM data. This approach is described in EPA’s documentation of its 2002 modeling platform (Strum et al., 2008).
- **Stationary nonpoint sources:** 2005 NEI v1 emissions, which contained 2002 NEI v3 emissions values, with corrections that reduced residential wood combustion VOC. This sector also includes portable fuel container emissions for 2002. For fugitive dust sources (e.g., building construction, road construction, paved roads, unpaved roads, agricultural dust), the emissions included reductions based on county-specific transportable fractions to PM₁₀ and PM_{2.5} using information on vegetation and surface features (Pace, 2005). Since most of this inventory uses 2002 values, additional details about it are available in Strum et al. (2008).
- **Wildfires and prescribed burning:** “Average year” fire emissions described in Section 2.3.3 of Strum et al. (2008).
- **Nonroad mobile:** There are three parts to the nonroad mobile inventory:
 - Monthly emissions that sum to the same values as the annual 2005 NEI v2 emissions. Created by NMIM running the NONROAD model, using state-provided NMIM inputs

- for Maine, Maryland, Michigan, Utah, and Wisconsin. Pre-calculated emissions provided by states for California.
- Aircraft, locomotive, and marine emissions from the 2002 NEI v3 for criteria pollutants and hazardous air pollutants.
- C3 commercial marine vessel emissions, including at-sea emissions out to 200 nautical miles (Corbett et al., 2006). These are also included in the 2005 NEI v2.
- **Onroad mobile:** The 2005 NEI v2 emissions were used for all three cases, in varying degrees depending on whether MOVES data were also used. We created these using NMIM running the MOBILE6 model (US EPA, 2008a). These NMIM runs included state-provided VMT NMIM inputs for Delaware, Georgia, Idaho, Nevada, Pennsylvania, Tennessee, Texas, and West Virginia. They also included state-provided non-VMT NMIM inputs for Arizona, Colorado, Delaware, District of Columbia, Georgia, Idaho, Maine, Maryland, Michigan, Nevada, North Carolina, Pennsylvania, South Carolina, Tennessee, Texas, Utah, Virginia, and West Virginia. Pre-calculated emissions were used as provided by California. Depending on the case, some of these emissions were replaced with MOVES-based emissions, as described in Section 3.2.
- **Biogenic emissions:** We created these emissions using 2005 meteorology and the BEIS3.14 model, including the sesquiterpenes needed for the CMAQ v4.7 used for the modeling.
- **Non-US inventories:** 2000 Canadian inventory and 1999 Mexican inventory described in Section 2.6 of Strum et al. (2008).

3.2 Overview of MOVES-based approach

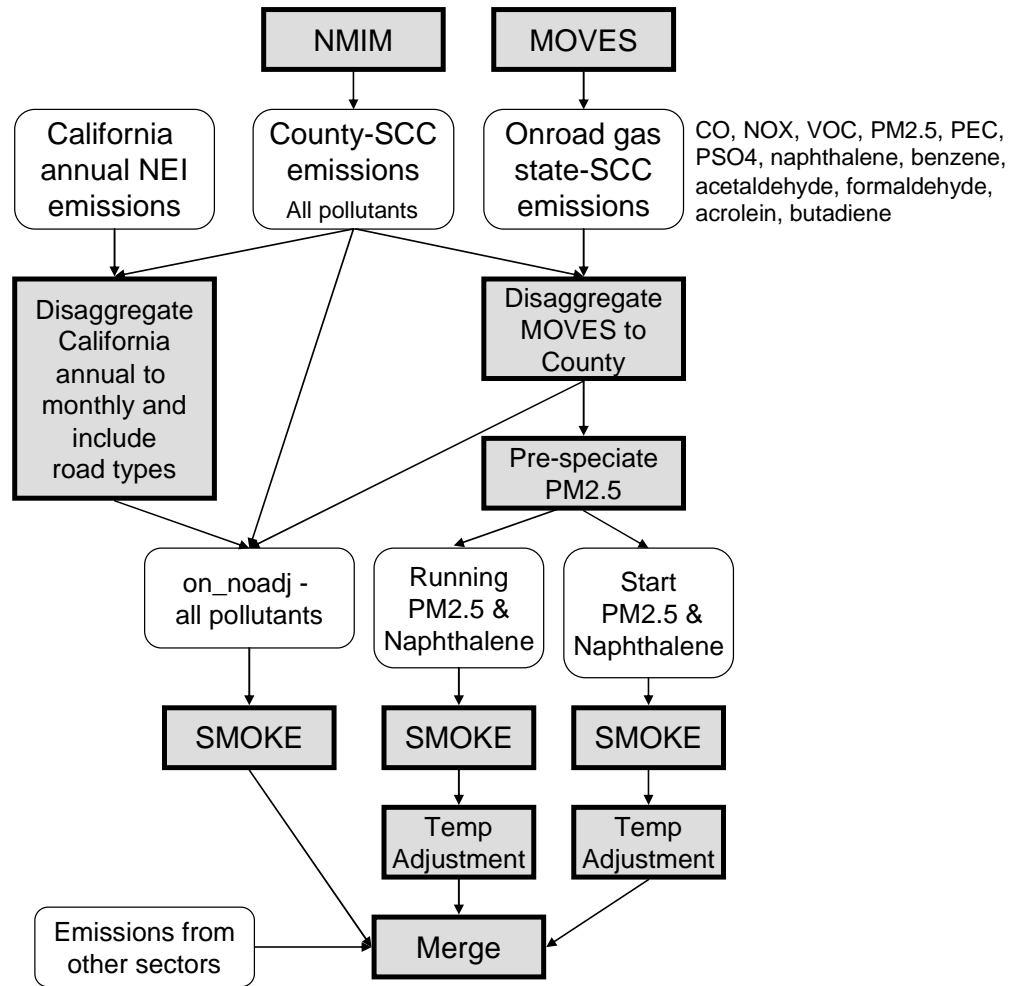
As described above, two of the three modeling cases described by this paper used MOVES-based emissions for onroad gasoline sources. For those cases, MOVES-based emissions were used for all states except California and for pollutants CO, NO_x, VOC, species of exhaust PM_{2.5}, naphthalene, benzene, acetaldehyde, formaldehyde, acrolein, and butadiene. The species of exhaust PM_{2.5} provided by MOVES are PEC and PSO₄. For the MOVES case, the POC, PEC, coarse PM (PMC) and exhaust naphthalene emissions received a temperature adjustment. For the MOVES72 case, we did not apply that adjustment. Section 3.4 provides more details of the speciation and temperature adjustment approaches.

We did not use MOVES-based emissions in California because our modeling approach uses California emissions provided by that state, and no information was available on how to apply the MOVES-based temperature adjustments to that state. Additionally, the MOVES motorcycle and diesel emissions estimates were not available at the start of this effort and therefore were not used.

Because of the long processing times to run MOVES, we realized at the start of the project that we could not run MOVES for each county using gridded temperature data for an entire year. Even using county-specific monthly average temperatures would have taken longer than our project's time would allow. Because of the significantly higher PM emissions at lower temperatures, we also wanted to use gridded, hourly temperatures rather than averaging temperatures in space or time. We determined that it is a good assumption for this work to adjust emissions based only on whether those emissions were for the start or running exhaust modes, because the adjustments do not depend on county, vehicle type, month, or hour. This assumption allowed us to process the unadjusted (or 72° F) PM_{2.5} and exhaust naphthalene start emissions separately from other running emissions, and then apply temperature adjustments using gridded, hourly temperatures to the gridded, speciated, hourly emissions.

Figure 2 summarizes our overall approach. The MOVES emissions (far right) were created for gasoline vehicle exhaust at the state-SCC level for the pollutants available from MOVES. The PM_{2.5} MOVES data were also separated by running and start exhaust modes, needed for downstream processing.

Figure 2: Overall approach for incorporating MOVES data into emissions processing to support CMAQ.



The NMIM (center) was also run for all onroad pollutants, processes, vehicles, and counties as part of the 2005 NEI v2 (see <http://www.epa.gov/ttn/chief/net/2005inventory.html>), and these emissions were used for three purposes. First, the onroad NMIM emissions supplied county-SCC-month emissions for pollutants not available from MOVES, including the brake and tire wear PM_{2.5} emissions because MOVES provided only exhaust PM_{2.5}. These emissions went to the “on_noadj” sector shown in the middle left of the figure. Second, the onroad NMIM emissions were used to allocate the MOVES emissions from the state-process-pollutant level to the county-process-pollutant level, shown by the box labeled “Disaggregate MOVES to County”. Finally, we used the NMIM data to disaggregate the annual California emissions to obtain monthly California data and add the road type detail of the SCC (needed for spatial allocation), shown in the middle left of the figure. Prior to processing in SMOKE, we created three processing sectors: (1) “on_noadj” includes all onroad emissions other than the MOVES start and running PM_{2.5}, (2) “on_moves_startpm” includes the starting PM_{2.5} emissions, and (3) “on_moves_runpm” includes the running PM_{2.5} emissions.

Next, we processed the three sectors separately through SMOKE’s temporal allocation, spatial allocation, and chemical speciation steps as separate emissions sectors. Finally, we applied the start emissions temperature adjustments to the on_moves_startpm sector and the running emissions temperature adjustments to on_moves_runpm sector. The temperature adjustments step also included special considerations for handling the pre-speciated PM emissions provided by MOVES, which is described further in Section 3.4.

Using the extra temperature adjustments steps requires more processing time as compared to running with NMIM only, and that additional time depends on the number of grid cells. For our 36-km domain, we ran the temperature adjustments simultaneously for the exhaust and running emissions, and ran sequentially for all days in the year. These steps took about 12 hours for each mode. We could have further reduced the time taken by processing quarter-year periods in parallel. For the NMIM case, the SMOKE processing steps took 5.5 hours running quarter-year periods in parallel. For the MOVES case, the SMOKE processing steps took 5.25 hours also running quarter-year periods in parallel. Thus, the total increase in processing time for the MOVES case as compared to the NMIM case is 11.75 hours or a 214% increase for the onroad sector. These timing data include not only creating the temperature adjusted gridded, model-ready data, but also county-SCC inventories with adjusted emissions that we used for summary purposes. Processing times could be further reduced by not calculating the county-SCC emissions values or running this step outside of the critical processing path needed for CMAQ-ready emissions. In contrast, we estimate that performing county-specific MOVES runs using detailed temperature data would have taken months of processing time. While these performance times are dependent on our particular processors and system configuration, they provide an indication of the relative efficiency of the approach.

3.3 Application of MOVES

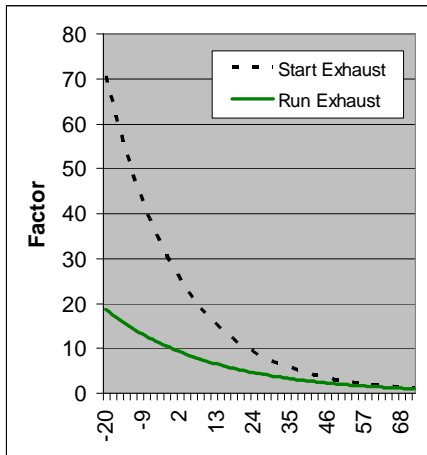
We ran MOVES to produce output for all MOVES SCCs for only gasoline vehicles, which excludes motorcycles. These vehicles comprise four SCC vehicle types: light duty gasoline vehicles, light duty gasoline trucks 1 and 2, light duty gasoline trucks 3 and 4, heavy duty gasoline vehicles 2b through 8b and buses. Because there are twelve HPMS roadway types plus a thirteenth “parking area” roadway type added to MOVES for emissions not on roads, there were a total of 52 MOVES SCCs. The additional SCCs due to the new “parking area” roadway type (and not familiar from NMIM) are listed in Table 1.

Table 1: Onroad gasoline SCCs from MOVES

SCC	Description*
2201001350	Gasoline;Light Duty Gasoline Vehicles (LDGV);Parking Area: Rural
2201001370	Gasoline;Light Duty Gasoline Vehicles (LDGV);Parking Area: Urban
2201020350	Gasoline;Light Duty Gasoline Trucks 1 & 2 (M6) = LDGT1 (M5);Parking Area: Rural
2201020370	Gasoline;Light Duty Gasoline Trucks 1 & 2 (M6) = LDGT1 (M5);Parking Area: Urban
2201040350	Gasoline;Light Duty Gasoline Trucks 3 & 4 (M6) = LDGT2 (M5);Parking Area: Rural
2201040370	Gasoline;Light Duty Gasoline Trucks 3 & 4 (M6) = LDGT2 (M5);Parking Area: Urban
2201070350	Gasoline;Heavy Duty Gasoline Vehicles 2B thru 8B & Buses (HDGV);Parking Area: Rural
2201070370	Gasoline;Heavy Duty Gasoline Vehicles 2B thru 8B & Buses (HDGV);Parking Area: Urban

* Description preface “Mobile Sources; Highway Vehicles -” applies to all descriptions, but was left out for formatting purposes.

Figure 3: 2005 temperature adjustment curves for start and running exhaust gasoline vehicles.



Because at this time, county-month level runs take too long, we ran MOVES at the state-SCC-month resolution and was post-processed using NMIM data to achieve county-SCC-month resolution, as described with more detail in Section 3.4. We performed the MOVES $PM_{2.5}$ runs for gasoline vehicles by state and month the same way as for other pollutants, except that temperatures were fixed at 72° F. We then developed temperature adjustment factors for $PM_{2.5}$ by repeating MOVES runs at one degree increments from -20° F to 72° F for one vehicle type, one county, one month, and one hour. The temperature adjustment factors are the ratio of emissions at each temperature to the emissions at 72° F. These ratios were calculated separately for start and running emissions. As shown in Figure 3, the adjustment factors for start emissions range from 1.0 at 72° F to about 70 times at -20° F, while the factors for running emissions range from 1.0 at 72° F to about 20 times at -20° F.

In our MOVES runs, these ratios do not depend on county, vehicle type, month, or hour, because we did not have county-specific information that impact the temperature affects. If we had needed adjustment factors after 2010, the ratios for the start exhaust emissions would have depended on year because cold start controls from the Mobile Source Air Toxics (MSAT2) Rule begin in 2011. Since these controls affect only new vehicles, their effect increases over time after 2010 as the fleet turns over. The curves are also affected by vehicle age distributions, but that was not a factor in this effort because we assumed a single age distribution everywhere.

We created and used Perl scripts to build each MOVES input set (“runspec”) for temperatures between -20 and 72° F, which was easier than manually creating these inputs. Once the runs for all temperatures were complete, we used another Perl script to combine all temperature runs into a single output database table that records PM emissions by temperature.

3.4 Processing steps for MOVES-based emissions

The temperature impacts on $PM_{2.5}$ from MOVES apply only to some of the species of $PM_{2.5}$ and to PMC and naphthalene. We developed extra processing steps for the purpose of correctly applying MOVES temperature impacts to the $PM_{2.5}$ species, and computing all of the $PM_{2.5}$ species needed by CMAQ. In addition to POC, PEC, and PSO_4 the CMAQ-required species include primary nitrate (PNO₃) and “other” $PM_{2.5}$ (PMFINE). The following steps summarize our approach for both applying the temperature impacts and handling the extra considerations for speciation:

1. Pre-processing

- Disaggregate state/process MOVES emissions to county/process using NMIM
- Compute speciated $PM_{2.5}$ emissions, with those species to be adjusted for temperature effects computed at 72° F
- Compute extra emissions values needed for temperature adjustment calculations during post-processing (the “OTHER” species)
- Compute PMC from $PM_{2.5}$

2. SMOKE processing for MOVES PM sectors without temperature adjustments
 - Process emissions for representative days: month-specific Monday, weekday, Saturday, and Sunday plus holidays and the day after holidays
 - Create two sets of gridded, speciated (unadjusted), hourly data files: one each for sectors on_moves_runpm and on_moves_startpm
3. Post-processing
 - Apply temperature adjustments to POC, PEC, and naphthalene
 - Compute temperature-adjusted part of PMFINE
 - Compute temperature-adjusted PMC

In the remainder of this section, we focus on the pre-processing and post-processing steps, since there was nothing unique about the SMOKE processing step.

3.4.1 Preprocessing

To implement a temperature adjustment to exhaust PM_{2.5}, exhaust PMC, and exhaust naphthalene based on MOVES, we first used the MOVES run described in Section 3.3 to compute PM_{2.5} and naphthalene emissions at 72° F and at the state-process level. We developed a pre-processing SAS[®] program with two functions: (1) disaggregate the state-process MOVES data to county-process using the NMIM data and (2) compute the emissions species needed to correctly apply the temperature adjustments after SMOKE processing.

For all pollutants provided by MOVES, the disaggregation step mapped the MOVES-based SCCs/pollutants to the NMIM SCCs/pollutants and computed the county-SCC level emissions for all SCCs using the following equation:

$$\text{MOVES county-SCC} = \text{MOVES state-SCC} \times \text{NMIM county-SCC} / \text{NMIM state-SCC} \quad (1)$$

We separated out the PM_{2.5} and exhaust naphthalene emissions into the on_moves_runpm and on_moves_startpm sectors, and all other MOVES pollutants were sent to the on_noadj sector. Because MOVES contains new parking area SCCs that are not included in NMIM, we chose NMIM local road SCCs to allocate those emissions to counties. We assigned the urban local NMIM to the urban parking areas and the rural local NMIM to the rural parking areas. Finally, we used the NMIM data to disaggregate the annual California emissions to obtain monthly California data and add the road type detail of the SCC, which is needed for spatial allocation.

For the speciation pre-processing, the main issues that need to be addressed are (1) MOVES provides some, but not all, of the exhaust PM_{2.5} species, and (2) only some of the parts of PM_{2.5} get the temperature adjustment. To address these issues, we developed additional steps to calculate all PM_{2.5} species and PMC before temperature adjustment.

As shown in equation (2) below, MOVES provides total PM_{2.5}, PEC and PSO4. A remainder term, *R*, makes up the difference between the two species and the total PM_{2.5}.

$$\text{MOVES total PM}_{2.5} = \text{PEC} + \text{PSO4} + R \quad (2)$$

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:

$$R = \text{POM} + \text{PNO}_3 + \text{METAL} + \text{NH}_4 + \text{H}_2\text{O} \quad (3)$$

To correctly calculate the five $\text{PM}_{2.5}$ species needed for CMAQ, we first needed to break out the POC, PNO_3 , and PMFINE from R . Because the $\text{PM}_{2.5}$ temperature correction is applied only to the POC, PEC, and non-carbon organic matter (part of PMFINE), we needed to first calculate the species without the temperature adjustments. We named the unadjusted POC_{72} , PEC_{72} , and PMFINE_{72} , and these species were also used in the processing for the “MOVES72” case. We computed the primary nitrate based on speciation profile 92011 from the SPECIATE4.1 database (Hsu et al., 2006) using equation (4) shown below.

$$\text{PNO}_3 = \text{PEC}_{72} \times F_{\text{NO}_3} / F_{\text{EC}} \quad (4)$$

where,

F_{EC} = Fraction of elemental carbon in profile 91022 (0.20801136)

F_{NO_3} = Fraction of nitrate in profile 91022 (0.001015)

Since CMAQ’s PMFINE species is the sum of soil oxides, metals, ammonium, and water, we needed to calculate all of its components. First, the metals and ammonium are computed using equations (5) and (6). Equation (6) is based on stoichiometrical calculations.

$$\text{METAL} = \text{PEC}_{72} \times F_{\text{metal}} / F_{\text{EC}} \quad (5)$$

$$\text{NH}_4 = (\text{PNO}_3 / MW_{\text{NO}_3} + 2 \times \text{PSO}_4 / MW_{\text{SO}_4}) \times MW_{\text{NH}_4} \quad (6)$$

where,

F_{metal} = Fraction of metals in speciation profile 91022 (0.022256)

MW_{SO_4} = Molecular weight of sulfate (96.0576)

MW_{NO_3} = Molecular weight of nitrate (62.0049)

MW_{NH_4} = 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.

$$\text{POM} = 1.2 \times \text{POC} \quad (7)$$

Using this assumption and assuming that the H_2O is negligible, the equation needed for the calculation of POC_{72} is shown in equation (8) below.

$$\text{POC}_{72} = 5/6 \times (R - \text{METAL} - \text{NH}_4 - \text{PNO}_3) \quad (8)$$

From equation (7), 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 NH_4 . Thus, we computed PMFINE_{72} using equation (9) shown below.

$$\text{PMFINE}_{72} = \text{METAL} + \text{NH}_4 + 0.2 \times \text{POC}_{72} \quad (9)$$

For mobile sources, we assumed that PMC is 8.6% of the $\text{PM}_{2.5}$ mass. Equation (10) shows how we calculated it.

$$PMC_{72} = 0.086 \times (PMFINE_{72} + PEC_{72} + POC_{72} + PSO4 + PNO3) \quad (10)$$

Using these equations, we created pre-specified SMOKE input inventories in SMOKE's ORL format for the starting and running exhaust parts of the MOVES data. The exhaust naphthalene emissions without temperature adjustments came from MOVES values with the state-to-county pre-processing. The emissions species that we input to SMOKE were therefore PMC_{72} , POC_{72} , PEC_{72} , $PMFINE_{72}$, $PSO4$, $PNO3$, OTHER (sum of METAL and NH_4), and $NAPHTH_{72}$. SMOKE generated gridded, hourly speciated emissions for these species for the representative days in 2005.

Figure 4: 2005 national MOVES emissions at 72° F for onroad gasoline vehicles

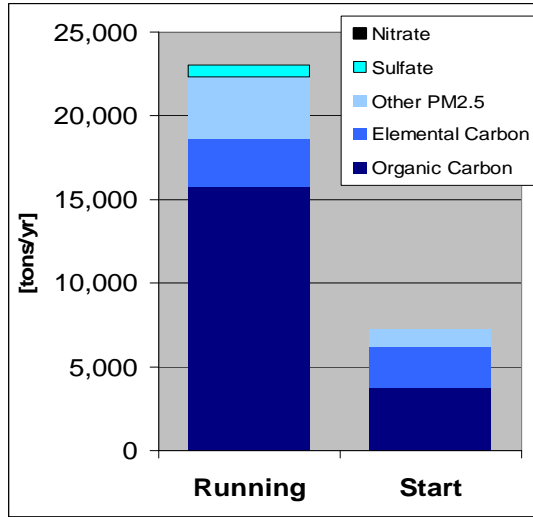


Figure 4 illustrates at the national level the speciated $PM_{2.5}$ emissions at 72° F, broken out separately for the running and start processes from MOVES. The running emissions are much larger than the start emissions, though the start emissions add significant additional emissions mass by contributing another 25% to the total emissions mass. The figure illustrates the predominance of POC in the speciation profile for both running and start emissions. The PNO_3 emissions are so small that they are imperceptible on the scale of this figure.

3.4.2 Postprocessing

We developed a Python script to apply temperature adjustments to the gridded, hourly SMOKE outputs using gridded, hourly 1.5-meter temperatures from the CMAQ meteorology data files. Using the temperature curves separately for start and running emissions for gasoline vehicles (Figure 3), we interpolated the temperature adjustment factor between the one degree Fahrenheit increments and applied this adjustment for each grid cell and hour for PEC and POC. In addition, we computed $PMFINE$ and PMC because they partially depend in on the temperature-adjusted emissions. The equations for these calculations are provided in equations (11) through (14), and all equations were applied to gridded hourly emissions.

$$PEC = PEC_{72} \times TF(T) \quad (11)$$

$$POC = POC_{72} \times TF(T) \quad (12)$$

$$PMFINE = OTHER + 0.2 \times POC \quad (13)$$

$$PMC = 0.086 \times (PMFINE + PEC + POC + PSO4 + PNO3) \quad (14)$$

where,

TF = Temperature factor for either running exhaust or starting exhaust

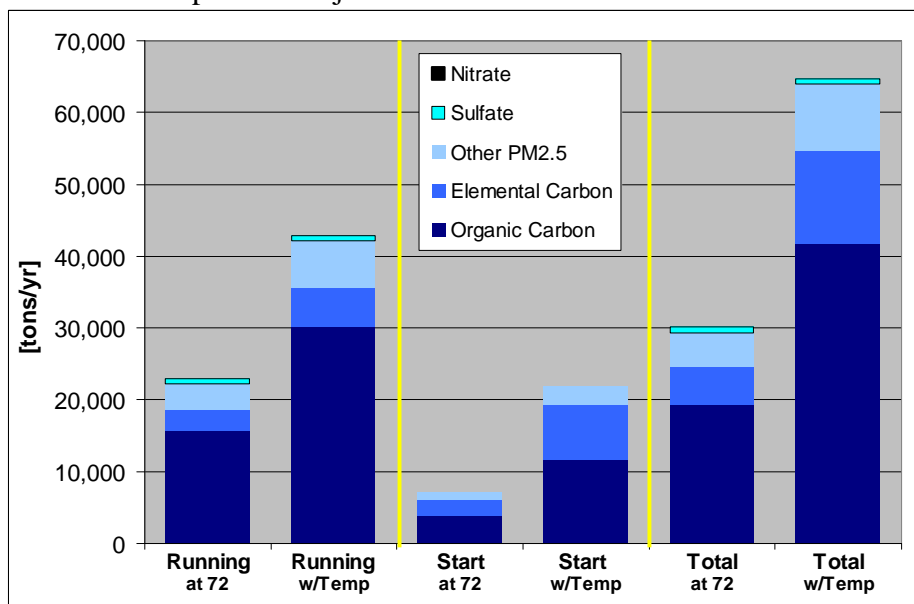
T = Gridded hourly temperature

Note that equations (13) and (14) are analogous to equations (9) and (10), but include temperature-adjusted emissions rather than their 72° F components. The temperature adjustments are used only for temperatures less than 72° F and only down to -20° F. Adjustments for temperatures below -20° F are the same as the adjustment at -20° F.

In addition to applying the temperature adjustments to the gridded emissions, we also applied them to reports from SMOKE that had pre-adjusted emissions sums by state/county FIPS code, SCC, and grid cell. This additional step allowed us to apply the grid-specific temperature adjustment factors to the county-SCC level emissions, so that temperature-adjusted county-SCC emissions could be computed for reporting, summary, and analysis purposes. Since this step is optional and not in the directly line of processing needed to support air quality modeling, it can be skipped or done later to reduce processing times.

Figure 5 illustrates the impact of the temperature adjustments on the onroad gasoline emissions from MOVES. The bars at the far left show the running emissions before and after temperature adjustments. These adjustments impact organic and elemental carbon the most, with a smaller impact on the PMFINE species (labeled “Other PM2.5”). The middle two bars show the impact on the start process and the final two bars show the impact on the total PM_{2.5} from exhaust onroad gasoline vehicles, excluding motorcycles.

Figure 5: 2005 48-state speciated PM_{2.5} MOVES emissions for onroad gasoline vehicles (excluding motorcycles) before and after temperature adjustments



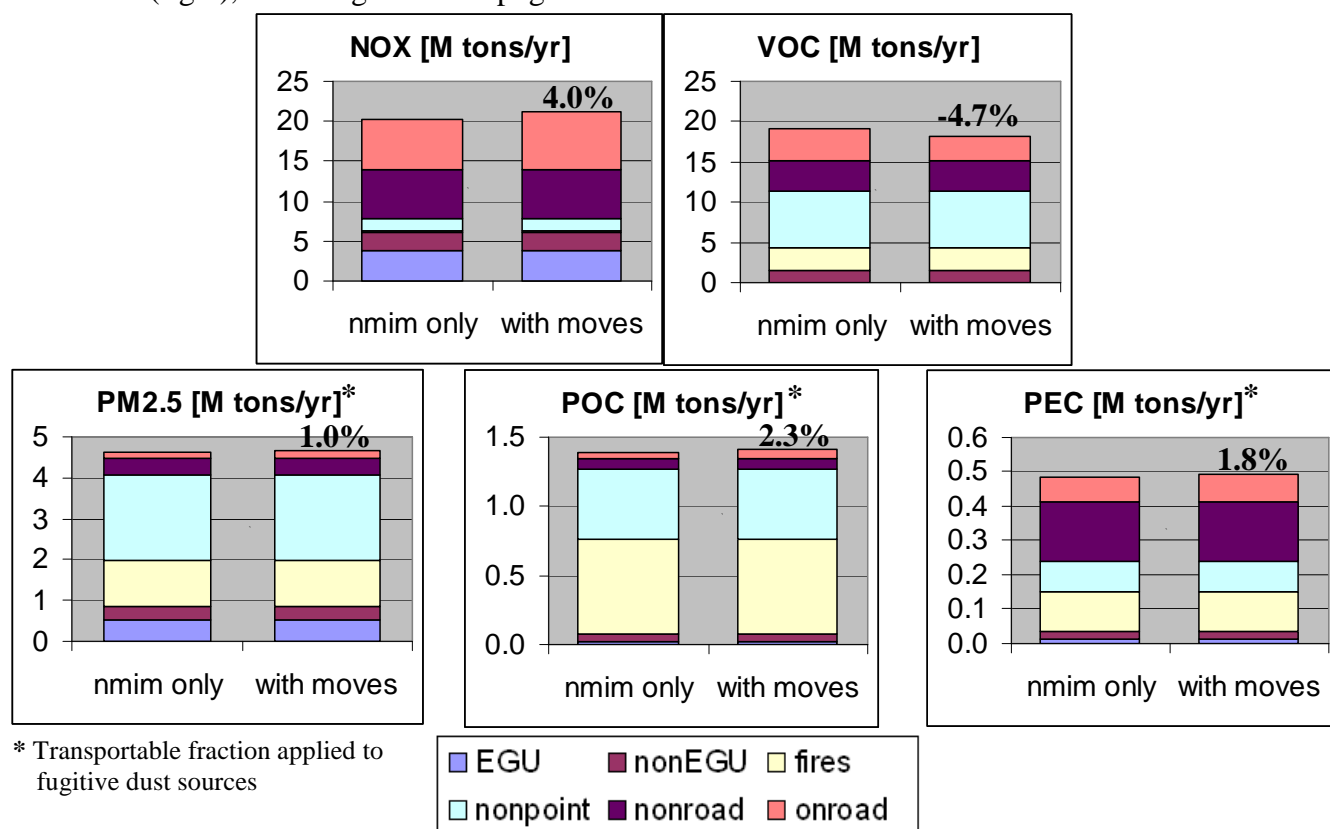
4 RESULTS

4.1 Emissions results

We compared the impact of the MOVES-based emissions to that of the NMIM emissions including all anthropogenic emissions sources. The emissions using MOVES instead of NMIM are significantly different, and different in ways that are likely to impact air quality modeling results. Although the MOVES emissions were generated using national defaults for most settings other than VMT, we believe that these emission estimates represent a significant improvement over previous emissions estimates.

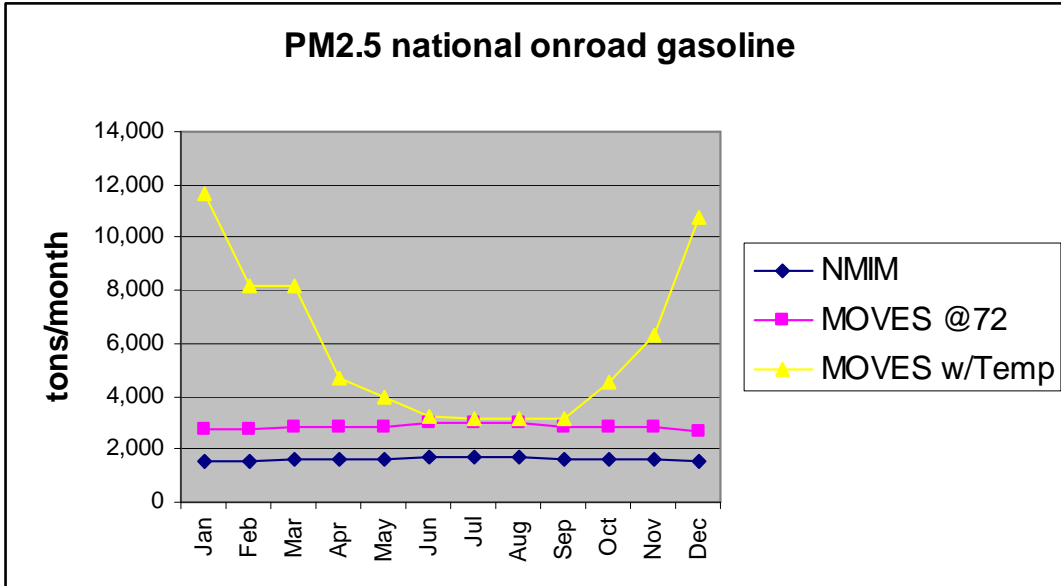
As shown in Figure 6, the national anthropogenic emissions inventory in 2005 either increased or decreased, depending on the pollutant. For NO_x emissions, the MOVES case was 28% higher than the NMIM case for the entire onroad sector (including only the gasoline and not the diesel increases), resulting in a 4% increase in national NO_x emissions across all sectors. For VOC emissions, the MOVES case was 22% lower than the NMIM case for the onroad sector, resulting in a 4.7% decrease in national VOC emissions across all sectors. The PM_{2.5}, POC, and PEC emissions all had a more modest impact at the national level because the onroad mobile emissions are still a relatively small portion of the total emissions of those pollutants. For example, though POC increased by 95% in the onroad mobile sector, the increase across all sectors was only 2.3%. The national increases in PM_{2.5} and PEC were 1% and 1.8% respectively. These national, annual numbers downplay the significance of the PM emissions changes. As we will show, the impact is much more significant in northern urban regions during cold months, where both the temperature corrections and the greater proportion of emissions from mobile sources in those areas result in much larger impacts.

Figure 6: Comparison of national inventories using NMIM only (left) versus MOVES onroad gasoline (right), including all anthropogenic emissions sources.



Focusing on the impacts changes by month, Figure 7 shows higher PM_{2.5} emissions in the winter, spring, and fall in the MOVES case as compared to the NMIM and MOVES72 cases. The figure illustrates that the MOVES changes *other than* the temperature adjustments increase the emissions by about 80%. In October through May, the temperature adjustments increase the emissions above the NMIM values from 83% in July to 658% in January.

Figure 7: Monthly distribution of onroad gasoline PM_{2.5} emissions for the three modeled cases.



Focusing more closely on the regions where the PM increases from MOVES occur, Figures 8a through 8c show the spatial variability of organic carbon for the MOVES minus the NMIM emissions across the sum of the emissions from *all anthropogenic sources* in January. Figure 8a shows the NMIM-based emissions and Figure 8b shows the MOVES-based emissions. Figure 8c shows the absolute difference between the two cases. These figures illustrate that the largest impacts are in the northern urban areas, though impacts still exist everywhere but California. The absence of changes in California is artificial and results from our traditional and continued use of California-supplied inventories, which do not include these temperature impacts.

Figure 8a: January POC from NMIM case

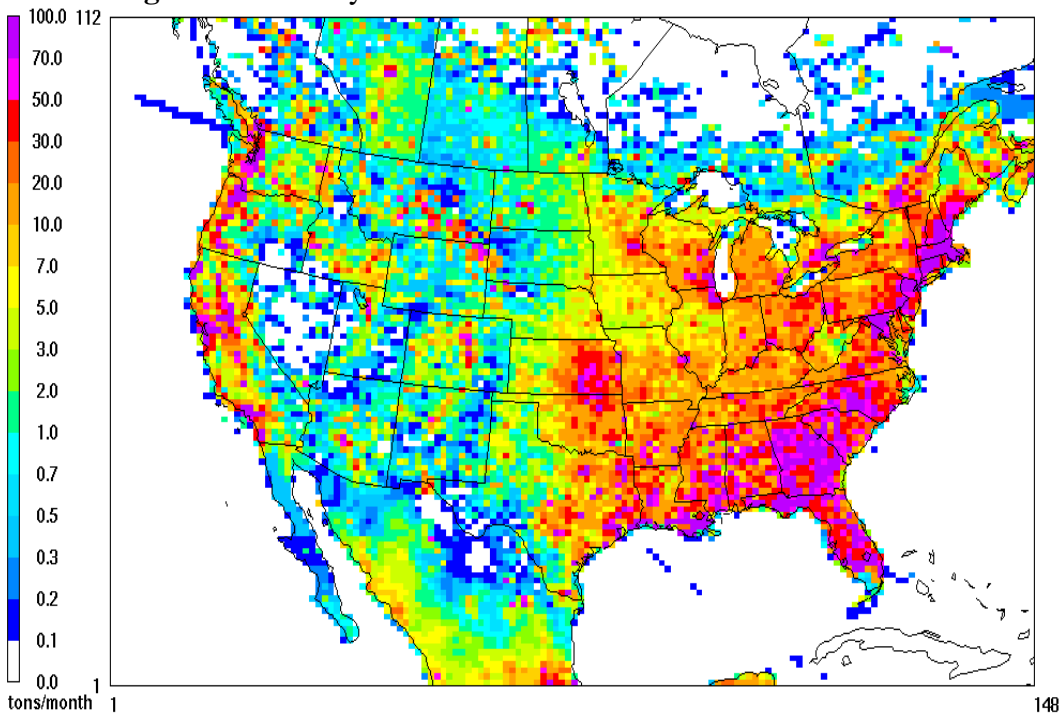


Figure 8b: January POC from MOVES case

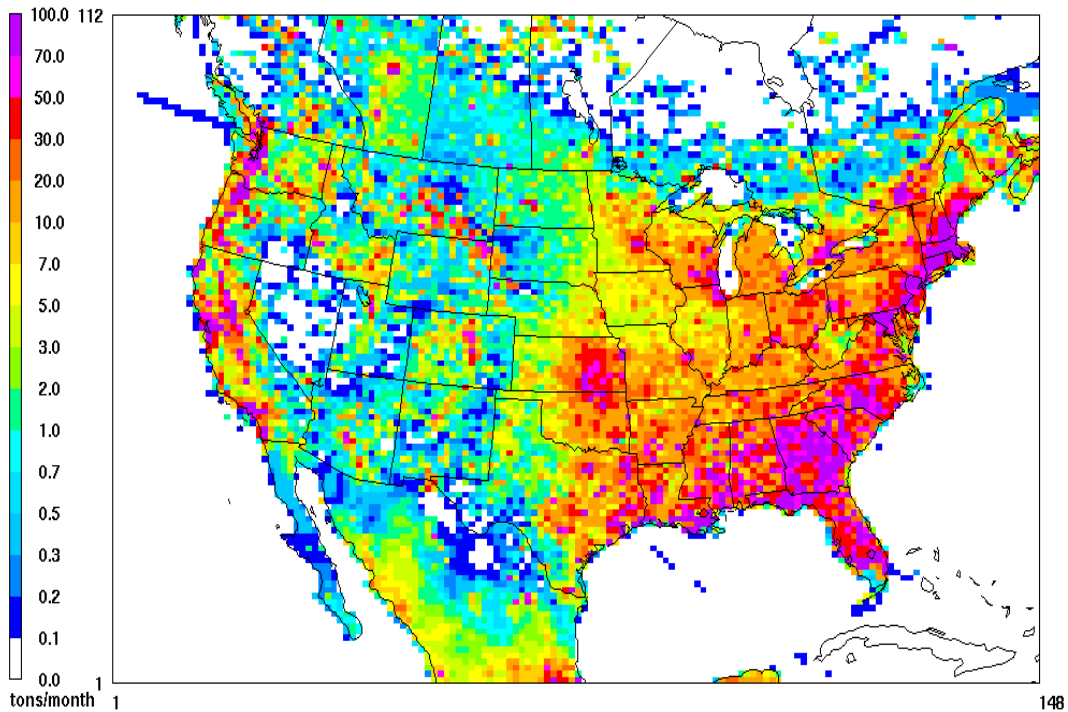
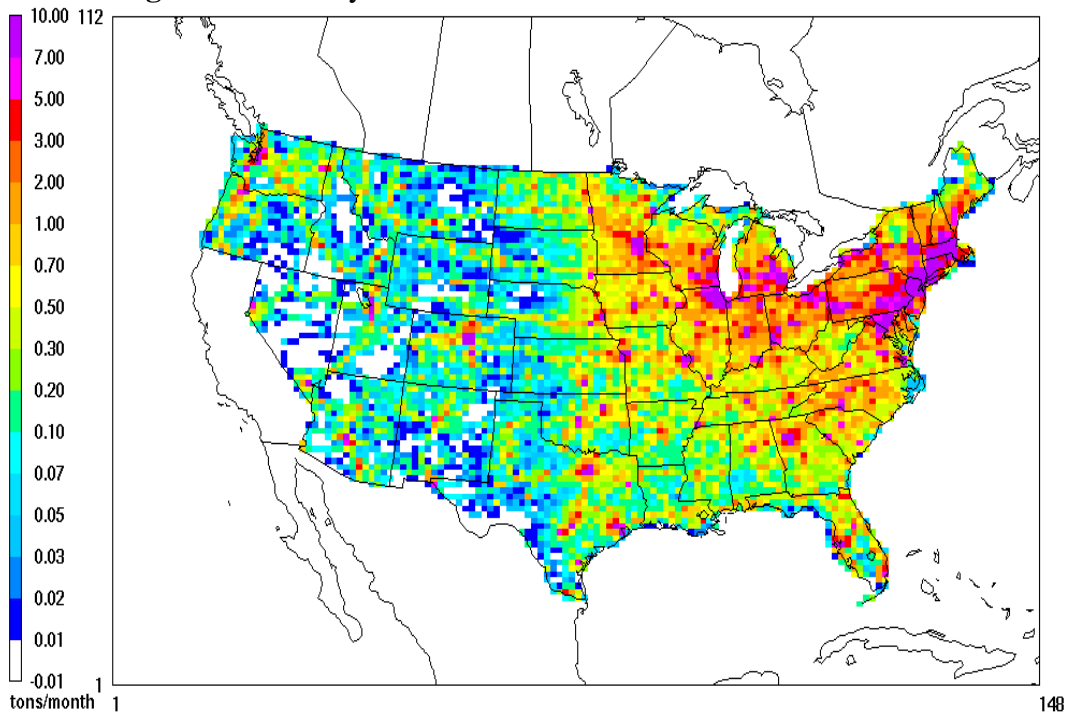
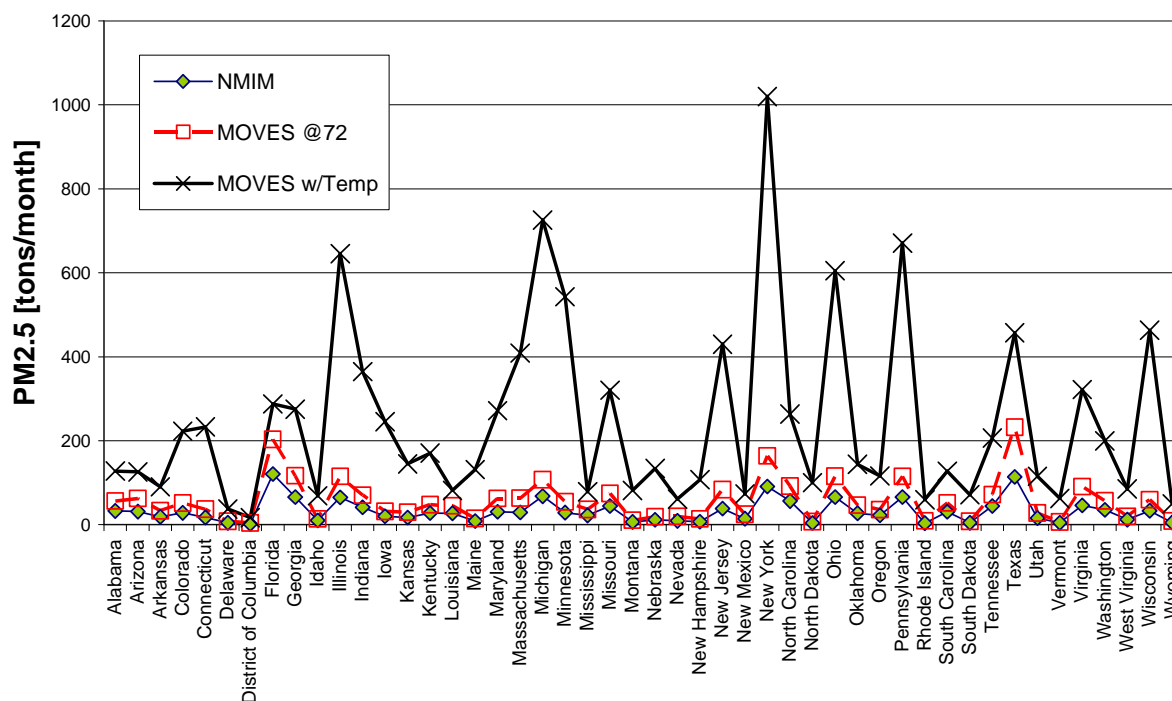


Figure 8c: January MOVES POC less NMIM POC - absolute difference



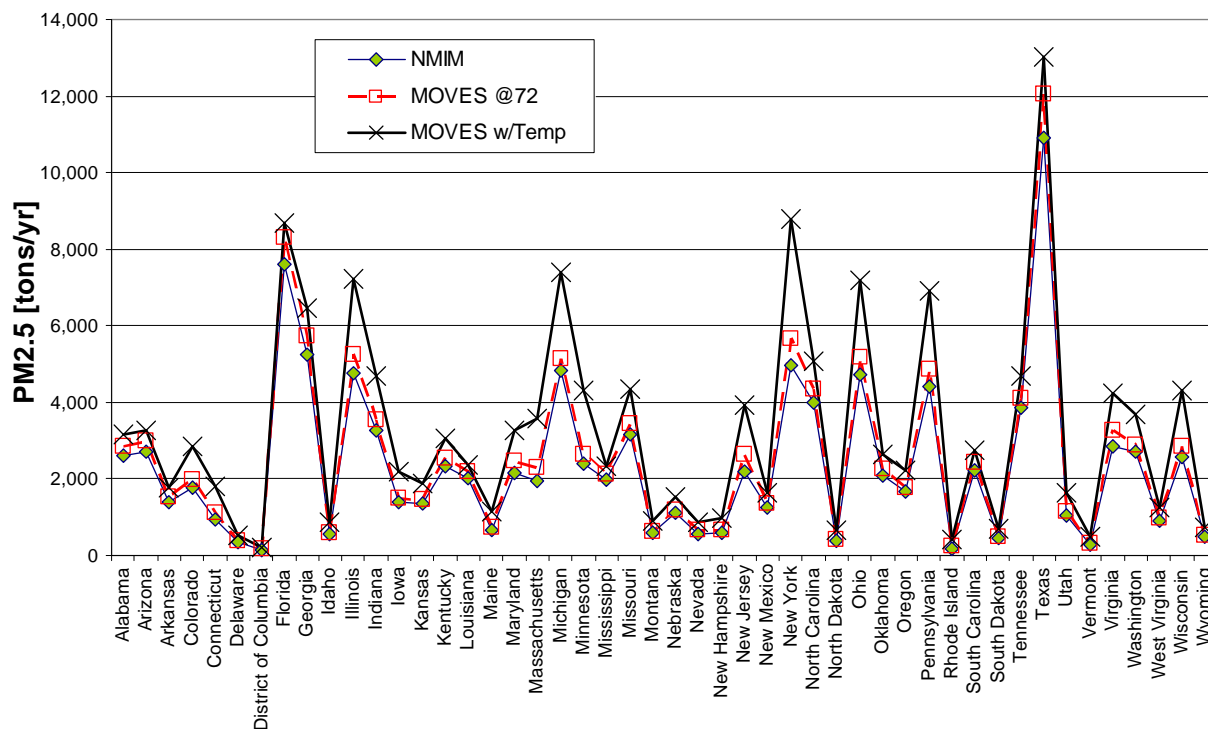
We also compared state total differences for the onroad gasoline emissions by state for the three cases, as shown in the January monthly emissions totals in Figure 9. This figure demonstrates that colder states show more impact than warmer states. For example, the NMIM-based and MOVES72-based emissions in Georgia and Illinois are nearly identical prior to temperature adjustment. However, after temperature adjustment the Illinois emissions are more than double those in Georgia.

Figure 9: January 2005 PM_{2.5} emissions from onroad gasoline sources, comparing MOVES with NMIM values by state



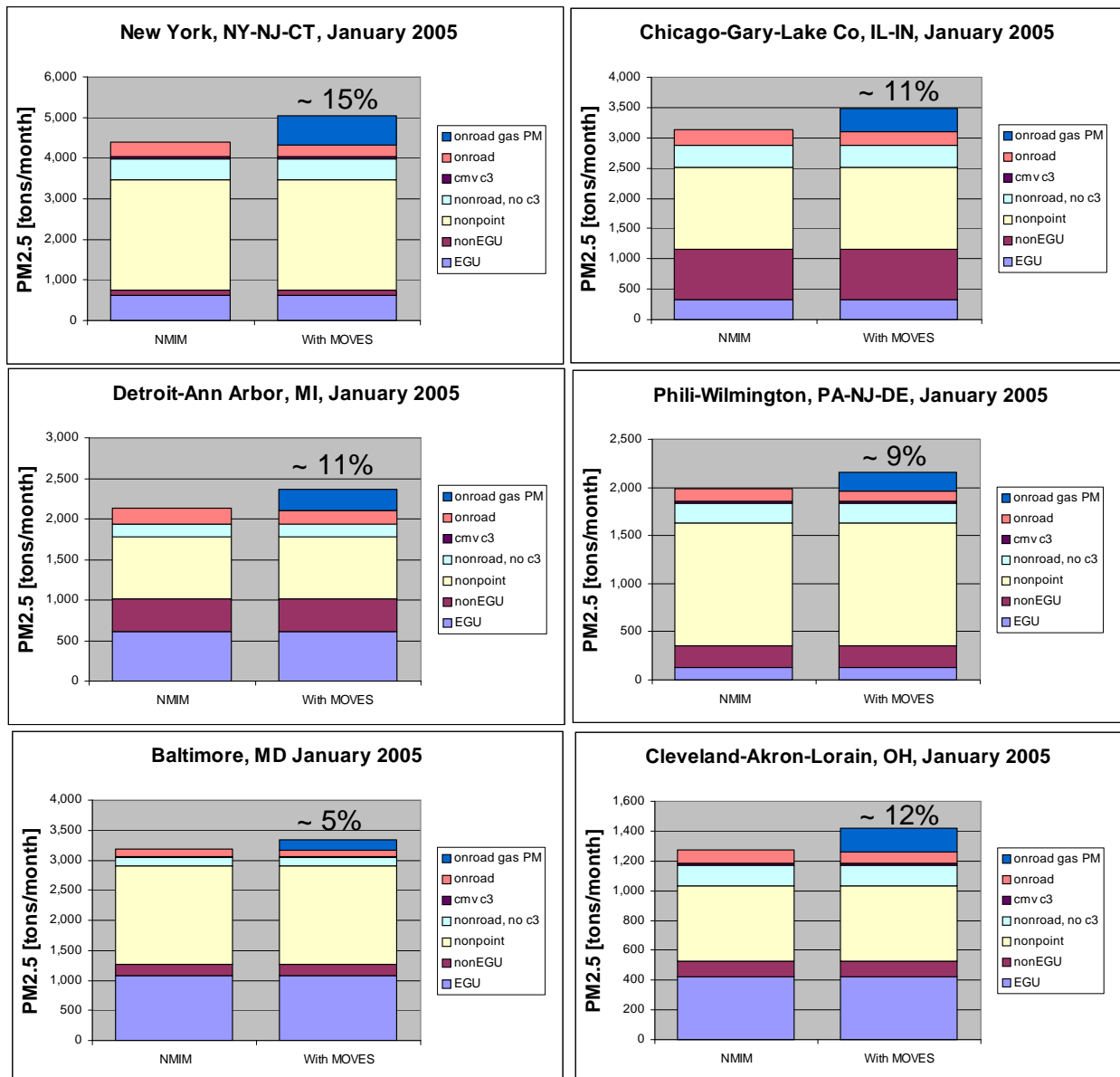
January is likely to show the largest impact (on average), according to the national impacts shown in Figure 7. Once the other months are included and an annual impact is computed by state, the total increases are less dramatic. Figure 10 illustrates this point below.

Figure 10: Annual 2005 PM_{2.5} emissions from onroad gasoline sources, comparing MOVES with NMIM values by state



Focusing in on specific nonattainment areas, Figure 11 shows the January anthropogenic PM_{2.5} emissions before and after the addition of the MOVES case's temperature-adjusted PM_{2.5} onroad gasoline emissions. As illustrated by the figure, PM_{2.5} emissions across all sectors increased from 5% to 15% in January. These increases are due to both the increases from MOVES unadjusted emissions and the temperature adjustments. While not shown, the increases in POC in January are more pronounced, with increases across all sectors as follows: New York (31%), Chicago (38%), Detroit (44%), Philadelphia (18%), Baltimore (13%), and Cleveland (34%).

Figure 11: Impact on January PM_{2.5} anthropogenic emissions of MOVES-based onroad mobile for six PM_{2.5} nonattainment areas in 2005.



4.2 Impact on MOVES and temperature adjustments on modeled air quality

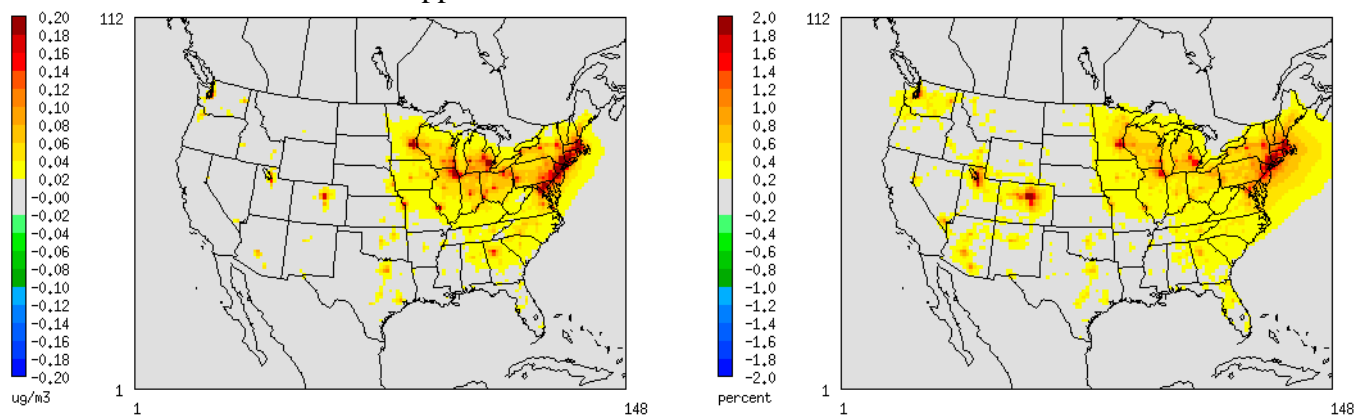
We completed the three simulations of the Community Multiscale Air Quality (CMAQ) model to assess the impacts of the MOVES-based PM_{2.5} emissions from on-road gasoline vehicles on base case air

pollutant concentrations. The three modeling cases were identical 2005 base year simulations, except for their treatment of onroad gasoline sources.

Our approach allowed us to assess the full impacts of the MOVES emissions relative to previous estimates of on-road gasoline vehicle emissions, as well as to isolate the impacts from the temperature adjustments relative to the other changes discussed in Section 2.2. The annual simulations were performed over a 36-km resolution model domain that covers the 48-State portion of the U.S. shown in Figure 1. We used the most recent public release of the model, CMAQ version 4.7 (Roselle *et al.*, 2008) for the analysis.

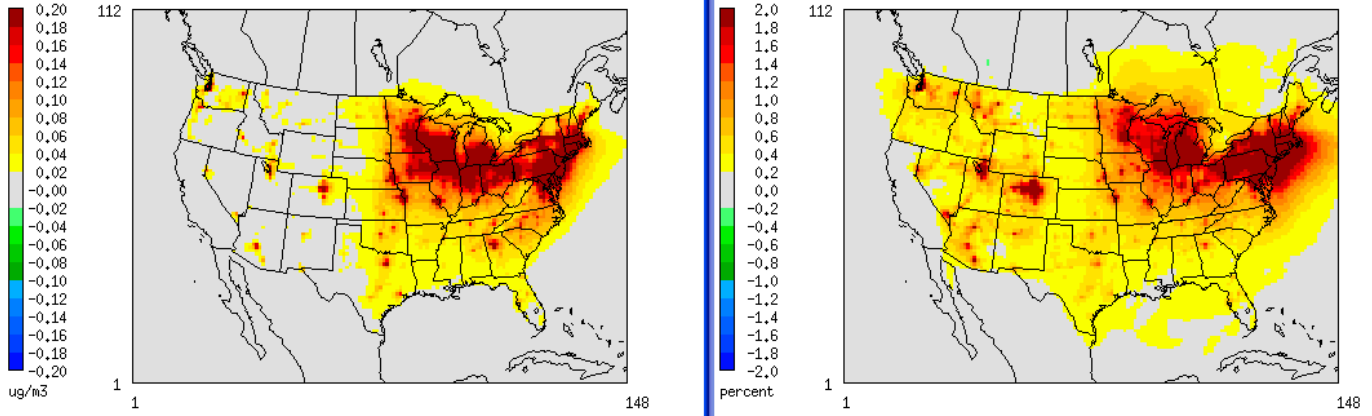
Figure 12 shows the absolute and percentage changes in annual average $PM_{2.5}$ concentrations over the U.S. as a result of the increased emissions from the MOVES-based approach. The figure shows annual average $PM_{2.5}$ increases of at least $0.02 \mu\text{g}/\text{m}^3$ (0.2 percent) are simulated over large parts of the U.S. in the MOVES case. The increases are largest in major metropolitan areas across the northern portion of the U.S. where mobile emissions are large and temperatures can be below 72°F during many periods of the year. $PM_{2.5}$ concentrations are increased by up to 0.2 to $0.4 \mu\text{g}/\text{m}^3$ in locations such as Minneapolis, Chicago, Detroit, and the Washington, DC to Boston corridor.

Figure 12: Absolute (left) and percent (right) change in 2005 base case annual average $PM_{2.5}$ concentrations resulting from switch to MOVES-based emissions from previous MOBILE6/NMIM approach.



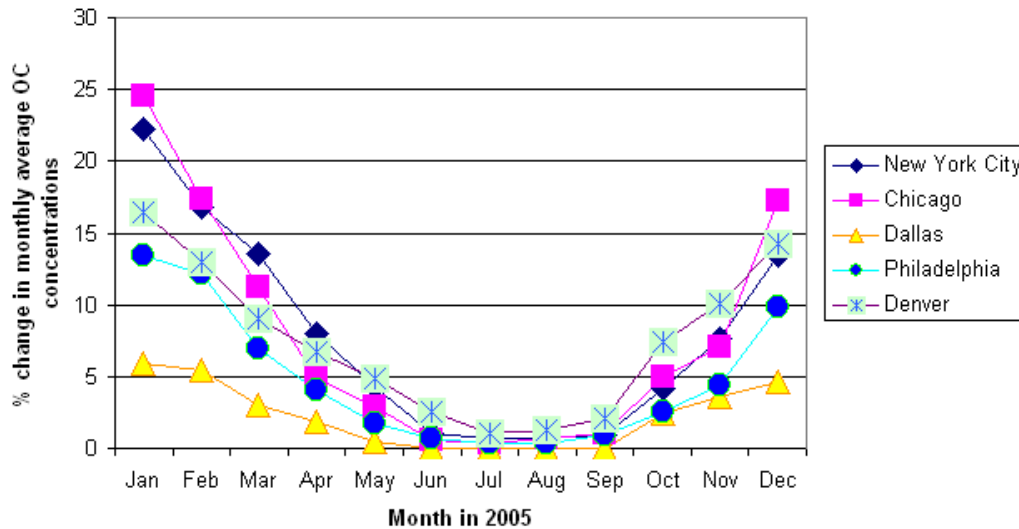
As expected, the impact on annual averages are driven primarily by air quality changes in the winter months when temperatures are colder and the resulting $PM_{2.5}$ adjustments are larger. Figure 13 shows the same absolute and percentage changes in $PM_{2.5}$ but for a January monthly average as opposed to an annual average. During this period, monthly averages can be as much as $1.0 \mu\text{g}/\text{m}^3$ higher with the MOVES-based emissions. The modeling showed that the majority of the impacts in using the MOVES-based emissions estimates were due to the temperature adjustments rather than the other changes in MOVES.

Figure 13: Absolute (left) and percent (right) change in January 2005 base case average PM_{2.5} concentrations in MOVES case as compared to NMIM case.



The CMAQ-predicted PM_{2.5} increases are driven by increases in predicted elemental carbon (EC) and organic carbon (OC); sulfates and nitrates are not appreciably impacted. For EC and OC, the fractional increases can be much larger than what was seen when PM_{2.5} was totaled. Figure 14 shows the percentage increase in monthly average OC concentrations for several major U.S. cities over the year. Monthly OC concentrations can be increased by as much as 20-25% in locations like New York City. Similar to Figure 7, this plot shows that the temperature adjustments have very little impact on model base year concentrations during the warm season.

Figure 14: Percent change in monthly average organic carbon concentrations from using temperature-adjusted PM_{2.5} rather than unadjusted at five PM_{2.5} nonattainment areas.



The full model performance evaluation for the 2005 base case simulation with MOVES-based emissions is ongoing. Recent EPA model evaluations (EPA, 2008) have shown that our CMAQ applications have underestimated OC concentrations. For instance in the modeling that supported the final rule on the “Control of Emissions from New Nonroad Spark-Ignition Engines”, organic carbon concentrations were consistently underestimated by 25 to 50 percent over all networks and at all locations. The expectation is that model performance for OC will be improved as a result of including the emissions revisions discussed in this paper.

5 CONCLUSIONS

In conclusion, the methods and analyses describe here illustrate several key points both about emissions changes and air quality predictions as a result of onroad gasoline MOVES-based emissions. First on the emissions, the MOVES-based inventories are significantly different than MOBILE6-based inventories for NO_x, VOC, PM_{2.5}, and naphthalene. Second, the PM_{2.5} temperature adjustment approach described here provides a credible, efficient approach for applying MOVES-based temperature adjustments without significantly adding to total emissions processing time for regional modeling applications. The approach of using gridded temperatures provides consistency with the meteorology used in the air quality modeling simulations and also captures temperature gradients that could occur across counties, particularly when using finer grid resolutions. Third, the PM_{2.5} temperature adjustments add significantly to the total PM_{2.5} emissions in urban areas, particularly in northern regions of the U.S. Examination of the nonattainment areas with the largest impact showed increases in PM_{2.5} emissions across all sectors from between 5% and 15%. For these same areas, POC across all sectors increased from 13% to 44%.

For the air quality results, first the MOVES-based PM_{2.5} emissions increase modeled base case air quality PM_{2.5} concentrations by up to 1.0 µg/m³ in highly-populated urban areas of the U.S. in the winter time, as compared to MOBILE6-based emissions only. Analysis of the air quality results using MOVES emissions without the temperature adjustment showed that the majority of the air quality changes were due to the temperature adjustments as opposed to the other MOVES-based emissions updates.

Our approaches have two major limitations, which are caveats on these conclusions. First, the national defaults used as inputs for MOVES (except for state-to-county allocation of VMT) do not provide as accurate MOVES-based emissions values as using local-specific MOVES inputs. Thus, conclusions provided for specific areas may not reflect local differences in onroad mobile vehicle mix, age distributions, and other factors. This caveat also allowed us a similar temperature curve approach for all PM_{2.5} and naphthalene adjustments, which would be more difficult with local-specific inputs used for each county. Second, since we ran MOVES at the state rather than the county level, we added additional uncertainties to our results. While this limitation is ameliorated to some extent by the use of state-to-county ratios from NMIM/MOBILE6, using county-specific MOVES runs would provide different results.

Nevertheless, this work represented a good estimate of the impacts of moving from an NMIM/MOBILE6 approach to a MOVES approach for PM_{2.5} emissions. We anticipate additional results from this work at a later time, including ozone impacts of the NO_x emissions changes and revised CMAQ model performance evaluations using the MOVES-based inventories. Further work is needed to incorporate diesel MOVES impacts and develop feasible temperature adjustment approaches to use when using local-specific MOVES inputs.

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KEYWORDS

MOVES

NMIM

SMOKE

PM2.5

Air quality modeling