

# **Processing Mobile Emissions in SMOKE: Is it worth simulating everyday onroad mobile emissions to support 8-hr ozone modeling?**

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## **ABSTRACT**

The most computationally limiting step in emissions modeling is typically the generation of onroad mobile sources. Motor vehicle emissions are influenced by meteorological variability and the processing requirements for daily motor vehicle emissions have been determined to be rate limiting under most modeling schedules. Rather than utilizing averaged meteorological data or pre-calculated motor vehicle emissions, the Visibility Improvement State and Tribal Association of the Southeast (VISTAS) / Association for Southeastern Integrated Planning (ASIP) modeling team developed an emissions processing approach that models a representative week for each month of the year in order to make the SMOKE processing time more manageable and consistent with VISTAS/ASIP modeling schedules. This representative week was selected from mid-month, to try to best represent the average temperature ranges for the month, and also adjusted to exclude holidays that would require atypical processing.

The purpose of this paper is to describe processing options for onroad mobile source emissions using the MOBILE module of the SMOKE emissions processor and to determine, based on air quality predictions and time and resource expenditure, benefits of simulating everyday for onroad mobile emissions to support 8-hr ozone modeling. We will present 12km evaluations of everyday vs. representative week emissions and associated air quality for a number of domains and discuss the benefits and limitations of the various methods relative to ozone, PM and regional haze prediction.

## INTRODUCTION

On December 17, 2004, EPA made fine particle (PM<sub>2.5</sub>) nonattainment determinations for at least one area in seven of the states participating in the Visibility Improvement State and Tribal Association of the Southeast (VISTAS) regional haze project. They are Alabama, Georgia, North Carolina, Kentucky, Tennessee, Virginia, and West Virginia. In addition, South Carolina has one three-county area that was designated as unclassifiable in the same action. EPA's Clean Air Interstate Rule (CAIR) modeling indicated that certain nonattainment areas may still be in nonattainment after full implementation of CAIR. These areas include Jefferson County, Alabama and Clayton and Fulton Counties in Georgia.

The PM<sub>2.5</sub> compliance date is April 2010 unless a state demonstrates that more time is necessary in which case up to five additional years may be granted. The nonattainment designations triggered the requirement for development of state implementation plans (SIPs) that will be due in April 2008. The draft guidance from EPA indicates that a significant requirement of PM<sub>2.5</sub> SIPs will be attainment demonstrations using, at least in part, modeling analyses to define effective emissions control strategies and confirm that attainment can be achieved after implementation of the strategies. 2009 is the modeling year for the PM<sub>2.5</sub> attainment demonstration and also is an interim analysis year for the VISTAS regional haze demonstration.

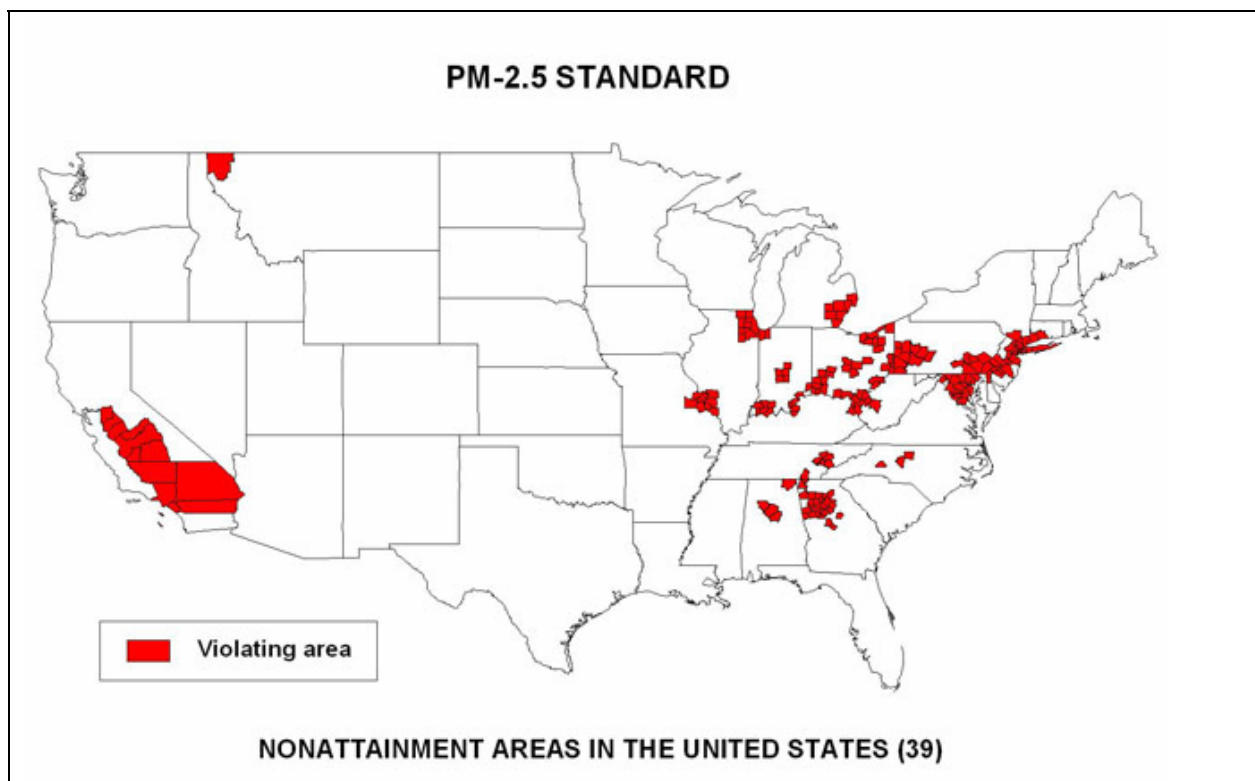
In April of 2004, EPA determined areas that were not meeting the 8-hour ozone standard. States having one or more 8-hour ozone nonattainment areas in the Southeast are Alabama, Georgia, Kentucky, North Carolina, South Carolina, Tennessee, Virginia, and West Virginia. EPA will require attainment of the 8-hour ozone standard in basic nonattainment areas by June 15, 2009 and in moderate nonattainment areas by June 15, 2010. This will require states with basic 8-hour ozone nonattainment areas to model 2008 as the SIP modeling demonstration year while moderate nonattainment areas will require 2009 as the modeling year. Given that North Carolina and Virginia have two year SIP approval processes, there is an immediate need to complete an analysis of ozone attainment using air quality modeling.

The states participating in the VISTAS project (the SESARM EPA Region 4 states plus Virginia and West Virginia from Region 3) have concluded that a collaborative process will be the most efficient approach for the collective states to develop information upon which to base the PM<sub>2.5</sub> and 8-hour ozone attainment demonstrations. The local air regulatory agencies for Jefferson County, AL, Jefferson County, KY, Mecklenburg County, NC, Forsyth County, NC, Knox County, TN, and Shelby County, TN have also become signatory parties to this collaborative effort. SESARM will coordinate among participating agencies and oversee the performance of the inventory and modeling tasks in parallel with the VISTAS regional haze project tasks.

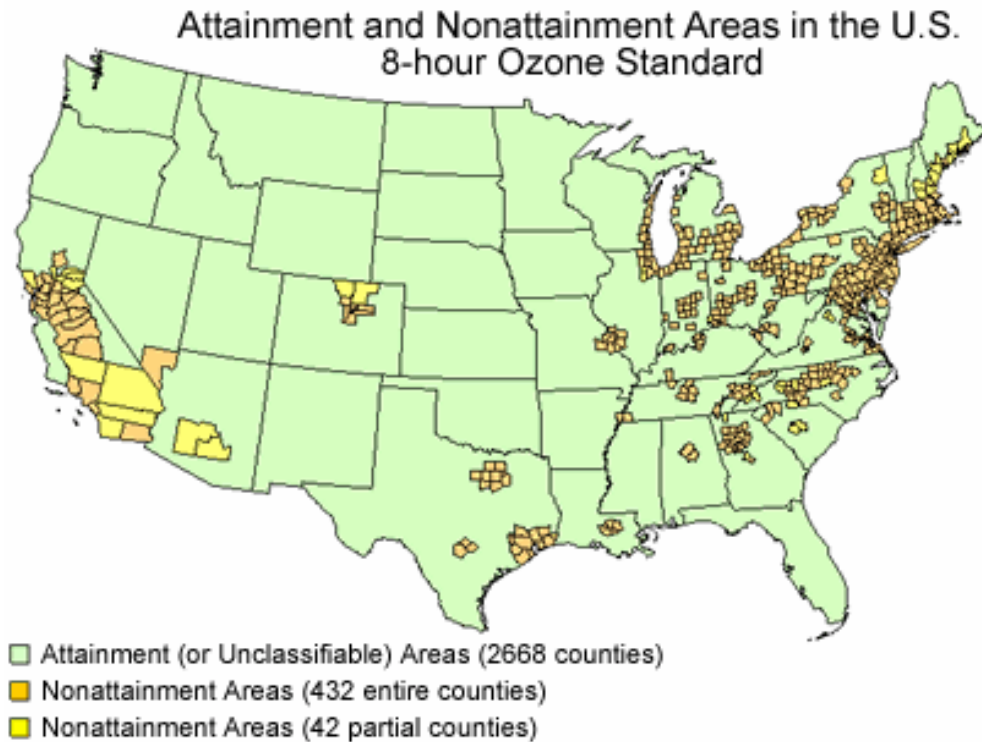
The name of this collaborative effort is the Association for Southeastern Integrated Planning (ASIP). SESARM was awarded a grant from EPA on February 8, 2005 to conduct what was originally called the fine particle SIP development support project but is now known as ASIP.

These states need to submit their 8-hour ozone State Implementation Plans (SIPs) to EPA by June 2007; the PM<sub>2.5</sub> SIPs are due by April 2008. Some of the states involved in the ASIP ozone/PM modeling have two-year legislative review processes. Thus, the definition of the SIP control plans is needed in early 2006. Consequently, the ASIP regional ozone and PM modeling has an aggressive schedule.

**Figure 1.** PM<sub>2.5</sub> nonattainment counties designed by EPA in December 2004.



**Figure 2.** 8-hour ozone nonattainment counties in the US designated by EPA in April 2004.



By far the most computationally limiting step in emissions modeling is typically the generation of onroad mobile sources. Motor vehicle emissions are influenced by meteorological variability and the processing requirements for daily motor vehicle emissions have been determined to be rate limiting under most modeling schedules. Rather than utilizing averaged meteorological data or pre-calculated motor vehicle emissions, the VISTAS and ASIP modeling team developed an emissions processing approach that models a representative week for each month of the year in order to make the SMOKE processing time more manageable and consistent with modeling schedule<sup>1</sup>. This representative week was selected from mid-month, to try to best represent the average temperature ranges for the month, and also adjusted to exclude holidays that would require atypical processing.

Based on the findings in the VISTAS Phase I and II modeling activities, ASIP selected the following models for use in modeling 8-hour ozone and particulate matter (PM) of size of 2.5 microns or less (PM<sub>2.5</sub>):

- **MM5<sup>2,3</sup>**: The Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Meteorological Model (MM5) is a nonhydrostatic, prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate and regional haze regulatory modeling studies.
- **SMOKE<sup>4</sup>**: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, nonroad, area, point, fire and biogenic emission sources for photochemical grid models.
- **CMAQ<sup>5,6</sup>**: EPA's Models-3/Community Multiscale Air Quality (CMAQ) modeling system is a 'One-Atmosphere' photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year.

The purpose of this paper is to describe processing options for onroad mobile source emissions using the MOBILE module of the SMOKE emissions processor and to determine, based on air quality predictions and time and resource expenditure, benefits of simulating everyday for onroad mobile emissions to support 8-hr ozone modeling. We will present 12km evaluations of everyday vs. representative week emissions and associated air quality for a number of domains and discuss the benefits and limitations of the various methods relative to ozone and regional haze prediction.

## **MOBILE6 / SMOKE PREPARATION**

For the VISTAS/ASIP 2009 annual emissions inventory modeling, SMOKE was configured to generate point, area, nonroad, highway, and biogenic source emissions. In addition, certain subcategories, such as fires and EGUs were maintained in separate source category files in order to allow maximum flexibility in producing alternate strategies. With the exception of biogenic and highway mobile source emissions that are generated using the BEIS and MOBILE6 modules in SMOKE, pre-computed annual emissions will be processed using the month, day, and hour specific temporal profiles of the SMOKE model. Area, nonroad, and point sources were modeled as a block of Thursday, Friday, Saturday, Sunday, Monday one per month (total of 60 days modeled). Biogenics were modeled for each day of the episode.

For this investigation, the onroad mobile source emissions were produced using two approaches:

- 1) Modeling every day of the annual episode, using the MM5 meteorology files for each model day. When full annual runs were executed, holidays were modeled as Sundays.

- 2) Modeling selected weeks (seven days) of each month and using these days as representative of the entire month. This selection criterion allows for the representation of day-of-the-week variability in the onroad motor vehicles, and models a representation of the meteorological variability in each month. The modeled weeks were selected from mid-month, avoiding inclusion of major holidays.

The parameters for the SMOKE runs are as follows:

Episodes:

2002 Initial Base Year, and  
2009 Future year, using 2009 inventory and modeled using the same meteorology and episode days as 2002.

Episode represented by the following weeks per month:

January 15-21  
February 12-18  
March 12-18  
April 6-22  
May 14-20  
June 11-17  
July 16-22  
August 13-19  
September 17-23  
October 15-21  
November 12-18  
December 17-23

Days modeled as holidays for annual run:

New Year's Day - January 1  
Good Friday – March 29  
Memorial Day – May 27  
July 4<sup>th</sup>  
Labor Day – September 2  
Thanksgiving Day – November 28, 29  
Christmas Eve – December 24  
Christmas Day – December 25

Output time zone:

Greenwich Mean Time (zone 0)

Projection:

Lambert Conformal with Alpha=33, Beta=45, Gamma=-97, and center at (-97, 40).

Domain:

*36 Kilometer Grid:* Origin at (-2736, -2088) kilometers with 148 rows by 112 columns and 36-km square grid cells.  
*12 Kilometer Grid:* Origin at (108, -1620) kilometers with 168 rows by 177 columns and 12-km square grid cells.

Layer structure:

The CMAQ layer structure will be 19 layers, with specific layer positions defined in the meteorology files to be provided by VISTAS meteorological contractor.

CMAQ model species:

The CMAQ configuration will be for CB-IV with PM. The model species will be: CO, NO, NO<sub>2</sub>, ALD<sub>2</sub>, ETH, FORM, ISOP, NR, OLE, PAR, TERPB, TOL, XYL, NH<sub>3</sub>, SO<sub>2</sub>, SULF, PEC, PMFINE, PNO<sub>3</sub>, POA, PSO<sub>4</sub>, and PMC.

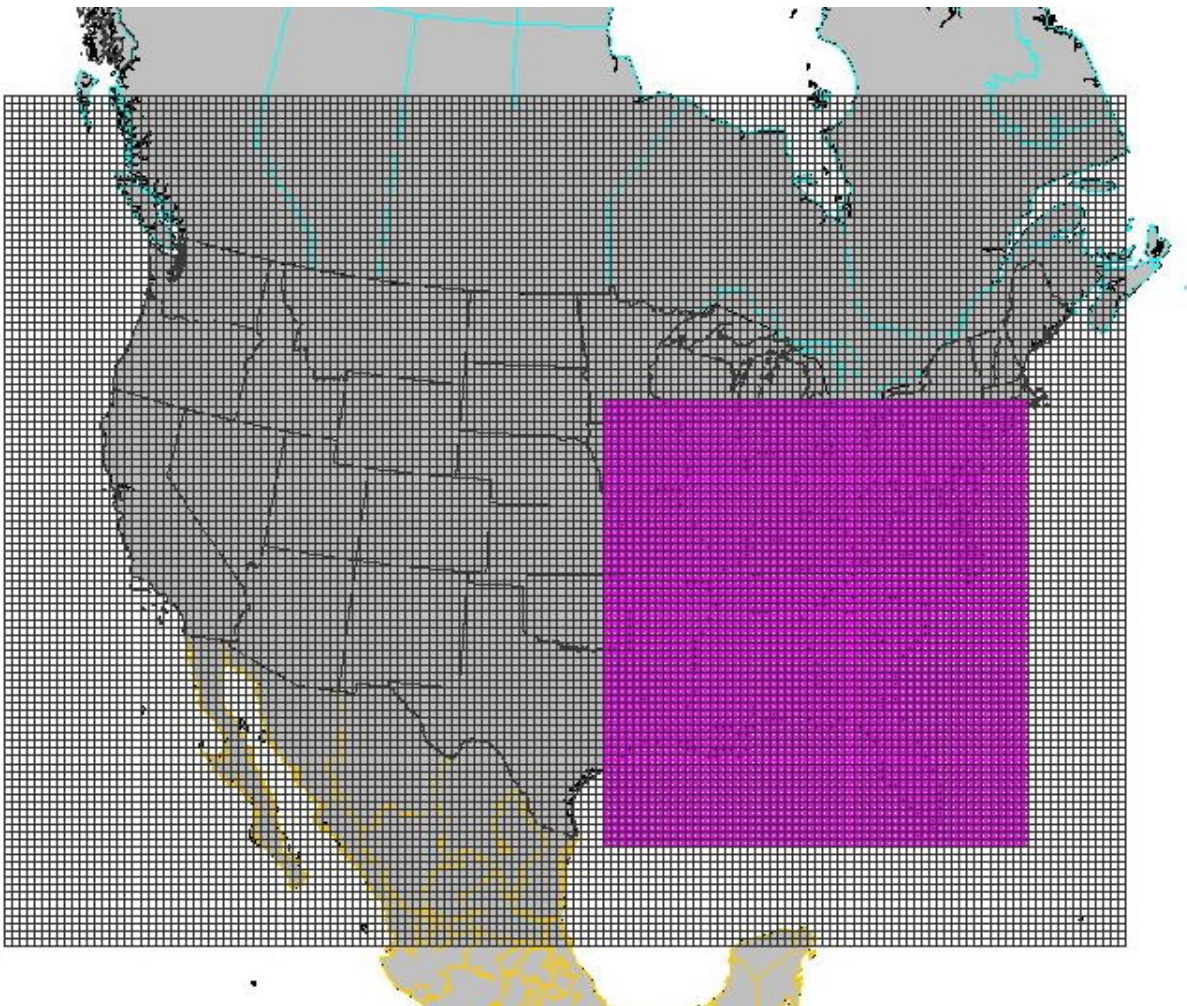
Meteorology data:

Daily (25-hour). SMOKE requires the following five types of MCIP outputs: (1) Grid cross 2-d, (2) Grid cross 3-d, (3) Met cross 2-d, (4) Met cross 3-d, and (5), Met dot 3-d.

Elevated sources:

All sources will be treated by SMOKE as potentially elevated. No plume-in-grid sources will be modeled. Wildfire emissions will be handled as point sources.

**Figure 3.** 36-km national unified RPO domain and VISTAS 12-km domain.



## DEVELOPMENT OF ONROAD MOTOR VEHICLE SOURCE EMISSIONS

The MOBILE6 module of SMOKE was used to develop the onroad mobile source emissions estimates for CO, NOX, PM, and VOC emissions. The MOBILE6 parameters, vehicle fleet descriptions, and VMT estimates are combined with gridded, episode-specific temperature data to calculate the gridded, temporalized emission estimates. The MOBILE6 emissions factors are based on episode-specific temperatures predicted by the meteorological model. Further, the MOBILE6 emissions factors model accounts for the following:

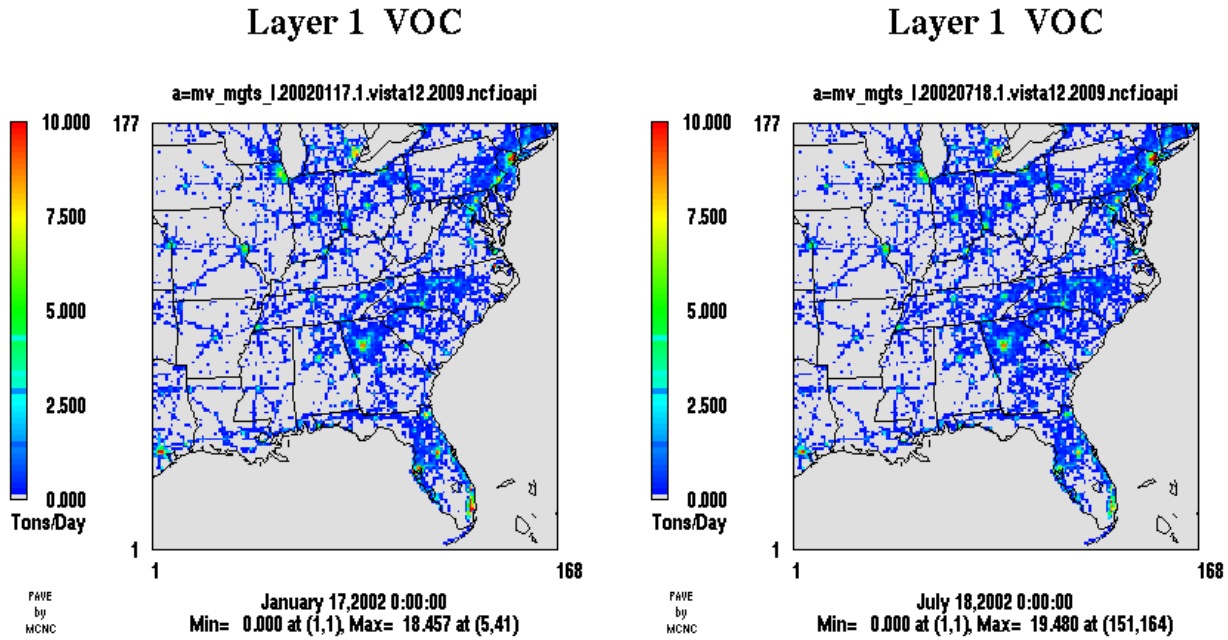
- Hourly and daily minimum/maximum temperatures;
- Facility speeds;
- Locale-specific inspection/maintenance (I/M) control programs, if any;
- Adjustments for running losses;
- Splitting of evaporative and exhaust emissions into separate source categories;
- VMT, fleet turnover, and changes in fuel composition and Reid vapor pressure (RVP).

The primary input to MOBILE6 is the MOBILE shell file. The MOBILE shell contains the various options (e.g. type of inspection and maintenance program in effect, type of oxygenated fuel program in effect, alternative vehicle mix profiles, RVP of in-use fuel, operating mode) that direct the calculation of the MOBILE6 emissions factors. The shells used in these runs were based on VISTAS/ASIP BaseF modeling inputs<sup>7</sup>. The options for all MOBILE6 parameters were held constant between the annual and representative week runs.

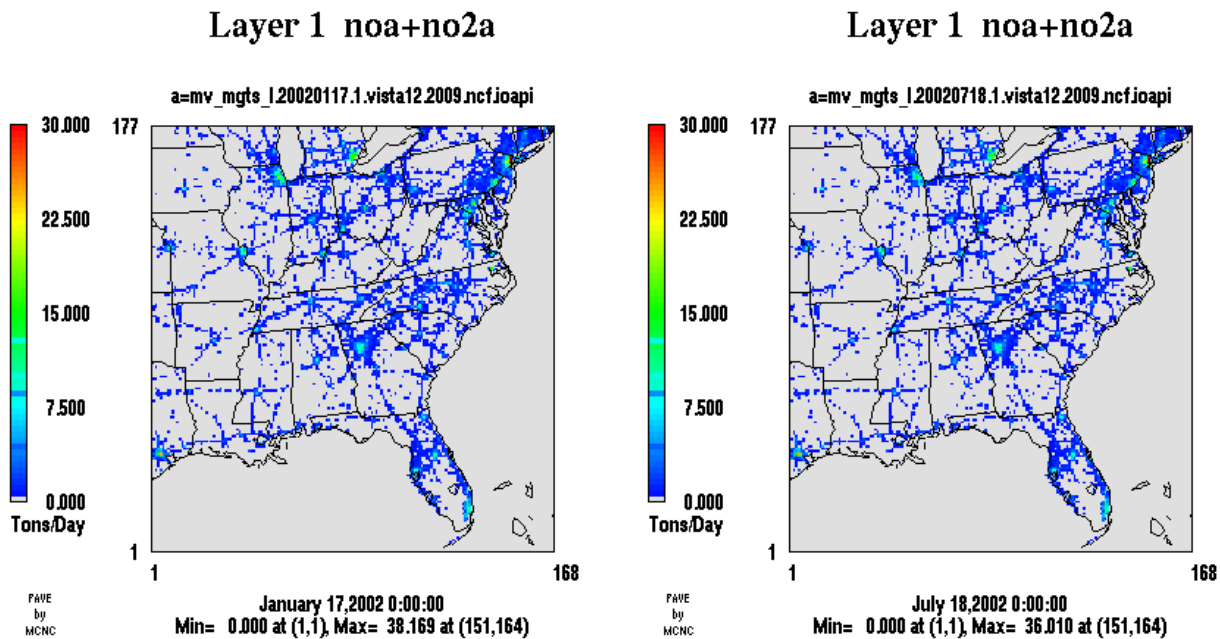
Daily results of these model runs for a winter (January 17) and summer (July 18) day are represented in Figures 4 through 6 below. These data provide a comparison of the magnitude difference between ozone and particulate matter precursor species for each of these seasonally different episodes. As can be seen in these figures, the variable inputs (temperature, VMT, seasonal fuels) associated with each month's run have an impact on the overall emissions generated for the onroad mobile source category. It is through modeling these differences with CMAQ for both ozone and PM that we have based our conclusions.

Each of the onroad mobile source emissions runs conducted with the MOBILE6 module of SMOKE were performed on a dual Athlon MP 2600+ with 1.5 G RAM. With this configuration, the modeling team experienced run times of approximately sixty-three (63) minutes per run day on the 12km domain. Using this estimate, the representative week processing would require a total of 5,292 minutes (12 months x 7 days x 63 minutes per run day) or about 88.2 hours (3.5 days) of CPU runtime to generate the files necessary to simulate the annual episode. In comparison, actually running each day's onroad mobile source emissions using the same configuration would require 22,995 minutes (365 days x 63 minutes per run day) or about 383.25 hours (16 days) of CPU run time.

**Figure 4.** Daily VOC emissions as generated with the MOBILE6 module of SMOKE for a winter (January 17) and summer (July 18) episode day.

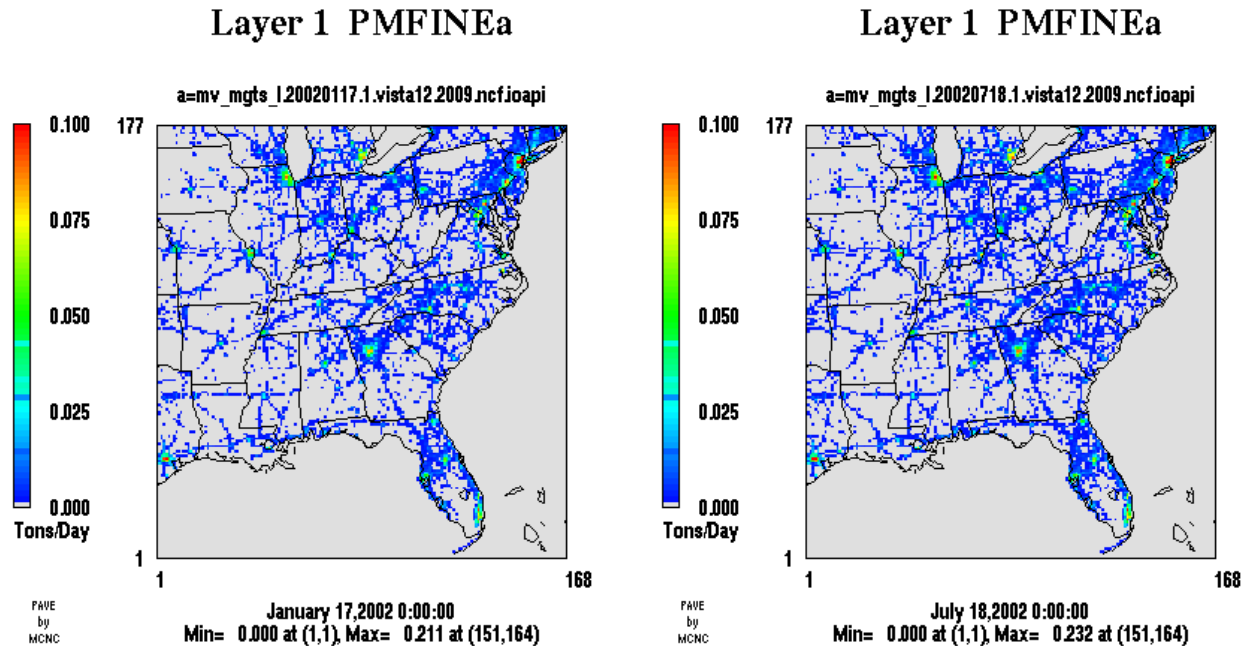


**Figure 5.** Daily NO<sub>x</sub> emissions as generated with the MOBILE6 module of SMOKE for a winter (January 17) and summer (July 18) episode day.





**Figure 6.** Daily PM-fine emissions as generated with the MOBILE6 module of SMOKE for a winter (January 17) and summer (July 18) episode day.



## EMISSIONS SUMMARY

The reconstructed emissions based on the representative week run were calculated by mapping each day of week (Mon, Tue, Wed, etc.) from the modeled month to the same day of week generated in the representative week run. In the case of holidays, these days were mapped to representative week Sundays. An example of this mapping for the January episode is presented in Table 1. Note that although the emissions were generated for calendar year 2009, the meteorology is based on 2002. Table 2 presents a comparison of January emissions as generated using the everyday MOBILE6 module run for each VISTAS/ASIP State and these emissions as reconstructed from the representative week MOBILE6 module runs. In comparison, Table 3 presents these emissions for the month of July.

**Table 1.** Representative day mapping for January episode (Highlighted representative week).

Modeled Date	Representative Day	Modeled Date	Representative Day	Modeled Date	Representative Day
1/1/2002*	1/20/2002	1/11/2002	1/18/2002	1/22/2002	1/15/2002
1/2/2002	1/16/2002	1/12/2002	1/19/2002	1/23/2002	1/16/2002
1/3/2002	1/17/2002	1/13/2002	1/20/2002	1/24/2002	1/17/2002
1/4/2002	1/18/2002	1/14/2002	1/21/2002	1/25/2002	1/18/2002
1/5/2002	1/19/2002	1/15/2002	1/15/2002	1/26/2002	1/19/2002
1/6/2002	1/20/2002	1/16/2002	1/16/2002	1/27/2002	1/20/2002
1/7/2002	1/21/2002	1/17/2002	1/17/2002	1/28/2002	1/21/2002
1/8/2002	1/15/2002	1/18/2002	1/18/2002	1/29/2002	1/15/2002
1/9/2002	1/16/2002	1/19/2002	1/19/2002	1/30/2002	1/16/2002
1/10/2002	1/17/2002	1/20/2002	1/20/2002	1/31/2002	1/17/2002
		1/21/2002	1/21/2002		

\* Modeled holiday

**Table 2.** January 2009 onroad mobile emissions comparison.

<b>January 2009 Emissions (Everyday Calculation)</b>							
<b>State</b>	<b>VOC</b>	<b>NOx</b>	<b>CO</b>	<b>SO2</b>	<b>PM-10</b>	<b>PM-2.5</b>	<b>NH3</b>
Alabama	6,567	8,774	105,011	51	266	174	500
Florida	28,354	26,686	336,541	171	834	529	1,736
Georgia	15,558	17,935	224,920	100	509	328	999
Kentucky	5,321	8,618	102,603	47	250	165	453
Mississippi	3,928	5,999	61,323	31	191	130	312
North Carolina	13,590	18,406	231,897	104	489	311	988
South Carolina	5,372	7,934	92,169	44	240	159	429
Tennessee	8,729	12,954	142,906	67	356	238	609
Virginia	7,377	11,708	156,617	72	311	190	716
West Virginia	2,025	3,177	41,742	18	91	59	168
	<b>96,821</b>	<b>122,190</b>	<b>1,495,728</b>	<b>705</b>	<b>3,536</b>	<b>2,283</b>	<b>6,910</b>

<b>January 2009 Emissions (Representative Day Calculation)</b>							
<b>State</b>	<b>VOC</b>	<b>NOx</b>	<b>CO</b>	<b>SO2</b>	<b>PM-10</b>	<b>PM-2.5</b>	<b>NH3</b>
Alabama	6,394	8,765	102,800	51	266	174	500
Florida	28,852	26,476	333,248	171	833	529	1,736
Georgia	15,337	17,867	218,990	100	509	328	999
Kentucky	5,023	8,679	104,247	47	250	165	453
Mississippi	3,710	6,012	60,454	31	191	130	312
North Carolina	12,605	18,383	225,563	104	489	311	988
South Carolina	5,226	7,911	89,001	44	240	159	430
Tennessee	8,011	13,000	141,962	67	356	238	609
Virginia	7,005	11,735	155,321	72	311	190	715
West Virginia	1,941	3,194	42,096	18	91	59	168
	<b>94,104</b>	<b>122,021</b>	<b>1,473,682</b>	<b>705</b>	<b>3,536</b>	<b>2,283</b>	<b>6,909</b>

<b>January 2009 Emissions (Difference as Percent)</b>							
<b>State</b>	<b>VOC</b>	<b>NOx</b>	<b>CO</b>	<b>SO2</b>	<b>PM-10</b>	<b>PM-2.5</b>	<b>NH3</b>
Alabama	-2.6%	-0.1%	-2.1%	0.0%	0.0%	0.0%	0.0%
Florida	1.8%	-0.8%	-1.0%	0.0%	0.0%	0.0%	0.0%
Georgia	-1.4%	-0.4%	-2.6%	0.0%	0.0%	0.0%	0.0%
Kentucky	-5.6%	0.7%	1.6%	0.0%	0.0%	0.0%	0.0%
Mississippi	-5.5%	0.2%	-1.4%	0.0%	0.0%	0.0%	0.0%
North Carolina	-7.2%	-0.1%	-2.7%	0.0%	0.0%	0.0%	0.0%
South Carolina	-2.7%	-0.3%	-3.4%	0.0%	0.0%	0.0%	0.0%
Tennessee	-8.2%	0.4%	-0.7%	0.0%	0.0%	0.0%	0.0%
Virginia	-5.0%	0.2%	-0.8%	0.0%	0.0%	0.0%	0.0%
West Virginia	-4.1%	0.6%	0.8%	0.0%	0.0%	0.0%	0.0%
	<b>-2.8%</b>	<b>-0.1%</b>	<b>-1.5%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>

**Table 3.** July 2009 onroad mobile emissions comparison.

<b>July 2009 Emissions (Everyday Calculation)</b>							
<b>State</b>	<b>VOC</b>	<b>NOx</b>	<b>CO</b>	<b>SO2</b>	<b>PM-10</b>	<b>PM-2.5</b>	<b>NH3</b>
Alabama	5,968	8,654	61,362	58	278	175	584
Florida	21,715	27,067	208,947	190	864	531	1,971
Georgia	15,833	17,965	133,828	114	533	332	1,162
Kentucky	5,289	8,196	56,333	53	262	166	537
Mississippi	3,934	6,013	38,674	36	200	130	376
North Carolina	12,975	17,340	130,042	120	512	311	1,171
South Carolina	5,316	7,859	57,163	51	251	160	512
Tennessee	8,797	12,446	81,289	75	368	237	712
Virginia	7,064	11,221	87,946	82	331	195	832
West Virginia	2,038	3,006	23,429	21	96	61	205
	<b>88,930</b>	<b>119,768</b>	<b>879,013</b>	<b>800</b>	<b>3,695</b>	<b>2,299</b>	<b>8,063</b>

<b>July 2009 Emissions (Representative Day Calculation)</b>							
<b>State</b>	<b>VOC</b>	<b>NOx</b>	<b>CO</b>	<b>SO2</b>	<b>PM-10</b>	<b>PM-2.5</b>	<b>NH3</b>
Alabama	6,017	8,682	61,581	58	278	175	585
Florida	22,006	27,217	210,901	190	864	531	1,971
Georgia	16,252	18,091	135,119	114	533	332	1,163
Kentucky	5,274	8,196	56,184	53	262	167	537
Mississippi	3,960	6,023	38,911	36	200	130	376
North Carolina	13,160	17,394	130,728	120	512	311	1,171
South Carolina	5,449	7,903	57,867	51	251	160	512
Tennessee	8,798	12,454	81,930	75	368	237	712
Virginia	7,104	11,248	87,523	82	331	195	832
West Virginia	2,047	3,010	23,419	21	96	61	205
	<b>90,068</b>	<b>120,218</b>	<b>884,162</b>	<b>800</b>	<b>3,695</b>	<b>2,299</b>	<b>8,063</b>

<b>July 2009 Emissions (Difference as Percent)</b>							
<b>State</b>	<b>VOC</b>	<b>NOx</b>	<b>CO</b>	<b>SO2</b>	<b>PM-10</b>	<b>PM-2.5</b>	<b>NH3</b>
Alabama	0.8%	0.3%	0.4%	0.0%	0.0%	0.0%	0.0%
Florida	1.3%	0.6%	0.9%	0.0%	0.0%	0.0%	0.0%
Georgia	2.6%	0.7%	1.0%	0.0%	0.0%	0.0%	0.0%
Kentucky	-0.3%	0.0%	-0.3%	0.0%	0.0%	0.0%	0.0%
Mississippi	0.7%	0.2%	0.6%	0.0%	0.0%	0.0%	0.0%
North Carolina	1.4%	0.3%	0.5%	0.0%	0.0%	0.0%	0.0%
South Carolina	2.5%	0.6%	1.2%	0.0%	0.0%	0.0%	0.0%
Tennessee	0.0%	0.1%	0.8%	0.0%	0.0%	0.0%	0.0%
Virginia	0.6%	0.2%	-0.5%	0.0%	0.0%	0.0%	0.0%
West Virginia	0.5%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%
	<b>1.3%</b>	<b>0.4%</b>	<b>0.6%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>	<b>0.0%</b>

These aggregate emission summaries would lead one to believe that on an extended episode scale (like those required for PM or regional haze modeling), the use of representative week onroad mobile source emissions would be appropriate. However, in modeling either 1-hr or 8-hr ozone, there is enough of a temperature variability and therefore apparent ozone precursor emissions delta on an hour-to-hour basis that this same assumption could not be made without accompanying air quality simulations.

## **AIR QUALITY MODELING**

The VISTAS/ASIP modeling team has applied the CMAQ Version 4.5 O<sub>3</sub>/PM<sub>2.5</sub> photochemical grid modeling system. The VISTAS/ASIP modeling team implemented a comprehensive evaluation of the meteorological<sup>8</sup>, emissions and air quality models. The CMAQ model performance evaluation indicated an underestimation of 8-hour ozone maximums during the summer. The model demonstrated reasonably good performance for sulfate, winter overestimation bias and summer underestimation bias for nitrate and reasonably good performance for elemental carbon (EC), albeit with lots of scatter and low correlation. However, organic carbon (OC) was underestimated with the summer OC underestimation bias being quite severe. After an intense focused analysis of the OC underestimation issue, the VISTAS/ASIP modeling team identified processes important to the formation of secondary organic aerosols (SOA) that were not included in the CMAQ SOA module that may be important to OC in the Southeastern U.S.<sup>9</sup> Consequently, VISTAS/ASIP enhanced the CMAQ SOA module by adding several new processes. This enhancement, called “SOAmods”, was implemented in CMAQ Version 4.5 and exhibited much improved OC model performance over the standard CMAQ SOA treatment<sup>10</sup>. A complete description of the modeling methods, configurations and performance are described elsewhere<sup>1,7</sup>.

CMAQ was applied using both of the mobile emissions modeling methods described above. Recall, all emissions and air quality model inputs and configurations were held constant, with the exception of the mobile source emissions. This will allow us to isolate the air quality impacts of using the representative week mobile emissions versus the “actual” daily modeled mobile emissions. While the VISTAS/ASIP modeling is conducted on both 36-km National RPO and 12-km “VISTAS/ASIP” modeling domains as shown in Figure 3, this study focuses on evaluations of the 12-km air quality modeling results only.

Using each of the mobile emissions databases (daily and the representative week) generated for the January and July study periods, we performed future-year air quality simulations for 2009 using CMAQ. We then post-processed the air quality model results to qualitatively evaluate the magnitude, location, and spatial extent of the differences in predicted ozone and PM<sub>2.5</sub> concentrations due to the different mobile emissions modeling methodologies. Spatial plots were generated for each day simulated, including:

- 1) daily maximum 8-hour ozone difference plots;
- 2) maximum 1-hour ozone maximum difference plots; and,
- 3) daily PM<sub>2.5</sub> difference plots.

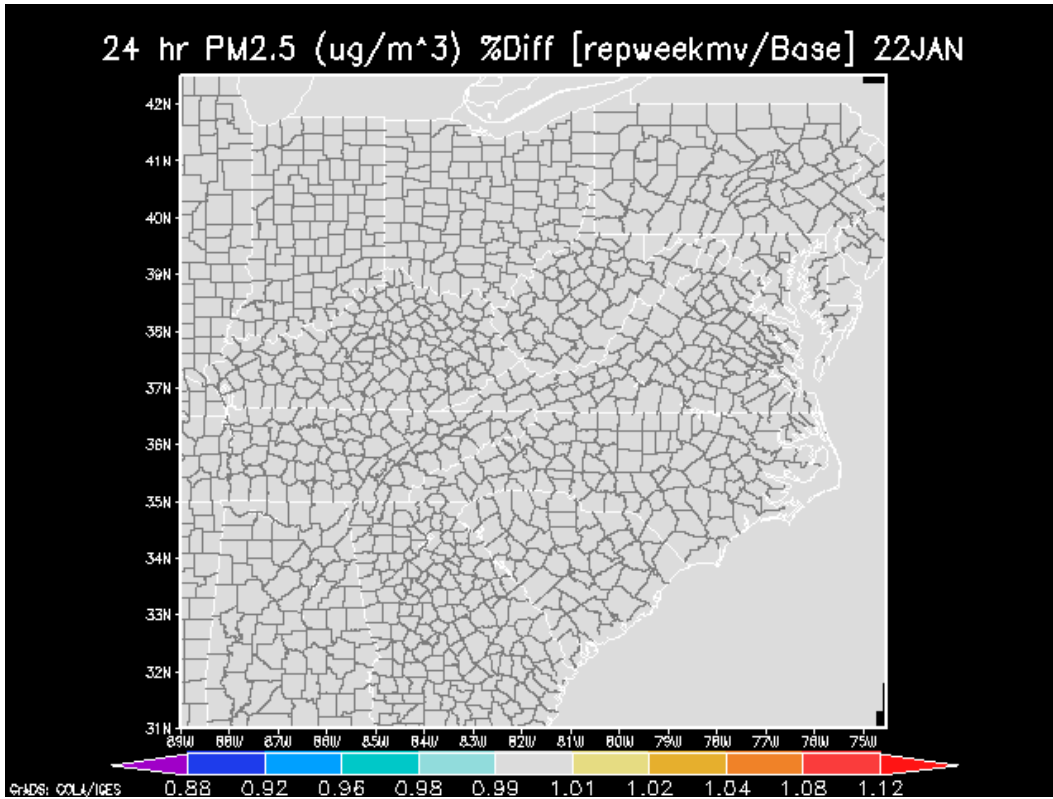
## RESULTS

Our examination of the two air quality simulations began with the daily differences in PM<sub>2.5</sub> concentrations. Figures 7 and 8 represent the percent difference in the daily PM<sub>2.5</sub> concentrations between the air quality simulations with representative week mobile emissions and the daily mobile emissions for one winter day (January 22<sup>nd</sup>) and one summer day (July 9<sup>th</sup>). No change is seen in either plot indicating daily PM<sub>2.5</sub> concentrations changed less than one percent. Absolute differences in daily PM<sub>2.5</sub> concentrations are shown in Figures 9 and 10 for the same two days (January 22<sup>nd</sup> and July 9<sup>th</sup>). Again, no change is seen in either plot indicating daily PM<sub>2.5</sub> concentrations changed less than 0.2 µg/m<sup>3</sup>. In fact, all of the fourteen days modeled (seven winter days and seven summer days) show no differences as high as 0.2 µg/m<sup>3</sup>.

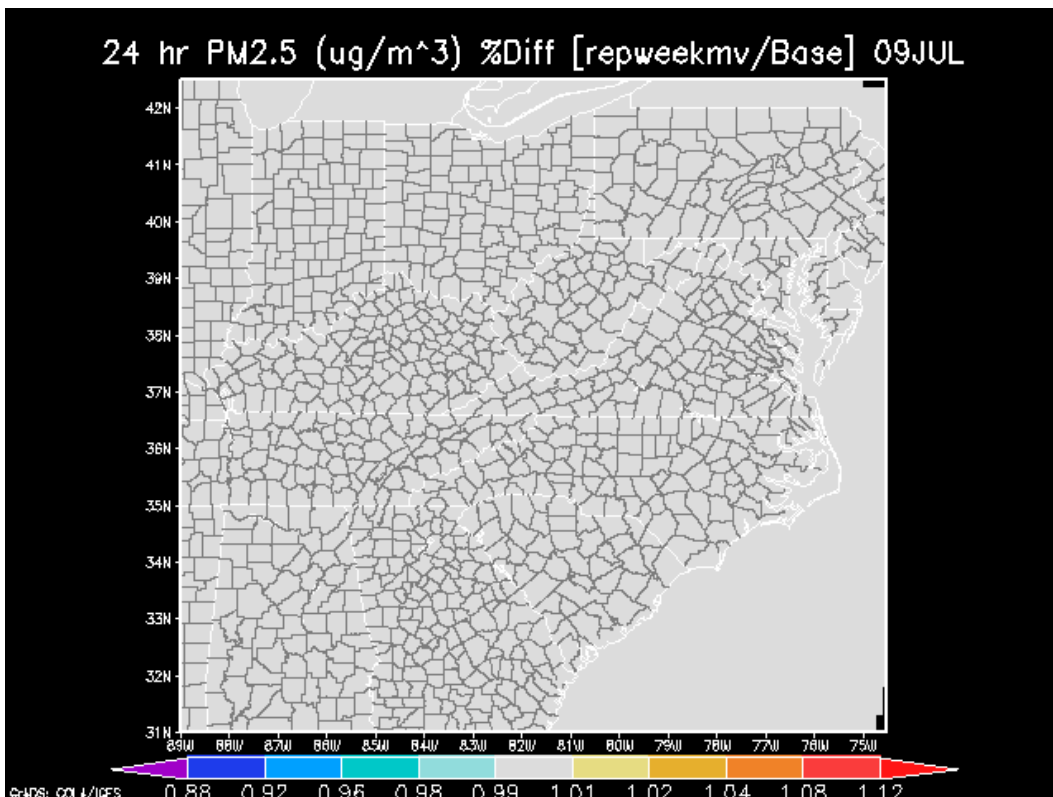
We next examined the results of the two air quality simulations with the daily differences in maximum 8-hour ozone concentrations. Figures 11 and 12 present the percent difference in the daily maximum 8-hour ozone concentrations for one winter day (January 28<sup>th</sup>) and one summer day (July 15<sup>th</sup>). In most areas for the winter day, daily maximum 8-hour ozone concentrations changed less than one percent. In a few urban corridors, namely, near Chicago, IL, Atlanta, GA and Baltimore, MD, changes of one percent are noted. Near Philadelphia, PA, changes of up to two percent are noted. However, this was the only day of the seven wintertime days simulated that showed a daily maximum 8-hour ozone difference as high as one percent anywhere in the modeling domain. It should also be noted that predicting wintertime ozone concentrations is not usually an interest because most, if not all high ozone events in the middle latitudes of the northern hemisphere occur during the summertime. Therefore the remainder of the ozone analysis will focus on summertime differences. On the summer day, July 15<sup>th</sup>, presented in Figure 12, no changes are seen indicating daily maximum 8-hour ozone concentrations changed less than one percent. In fact, all seven of the summer days modeled showed no changes as high as one percent.

Absolute differences in daily maximum 8-hour ozone concentrations are shown in Figure 13 for July 15<sup>th</sup>. Again, no change as high as 0.5 ppb (0.0005 ppm) was noted on this day or any of the seven summer days modeled. In addition to the 8-hour ozone metrics discussed above, differences in 1-hour ozone maximums were examined. As shown in Figure 14 and 15, only two days during the seven day summertime period simulated showed differences in 1-hour ozone maximums as high as 0.5 ppb (0.0005 ppm).

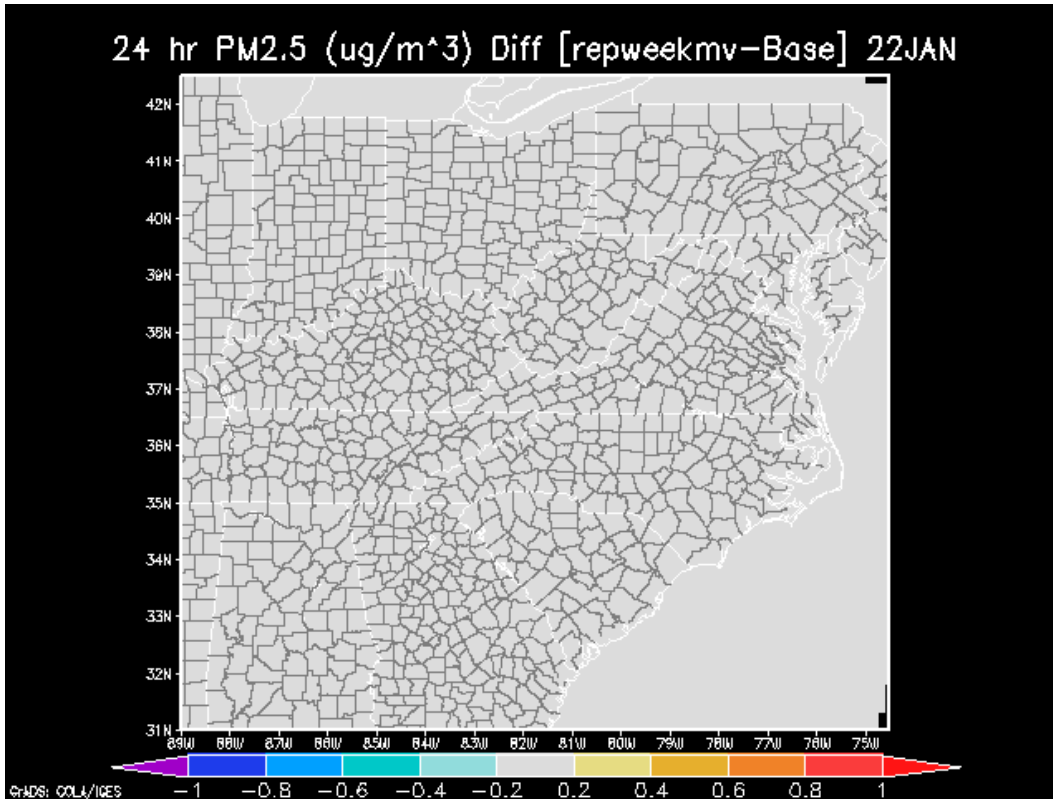
**Figure 7.** Percent difference in 24-hour PM<sub>2.5</sub> concentrations for January 22nd (Representative week mobile emissions versus daily mobile emissions).



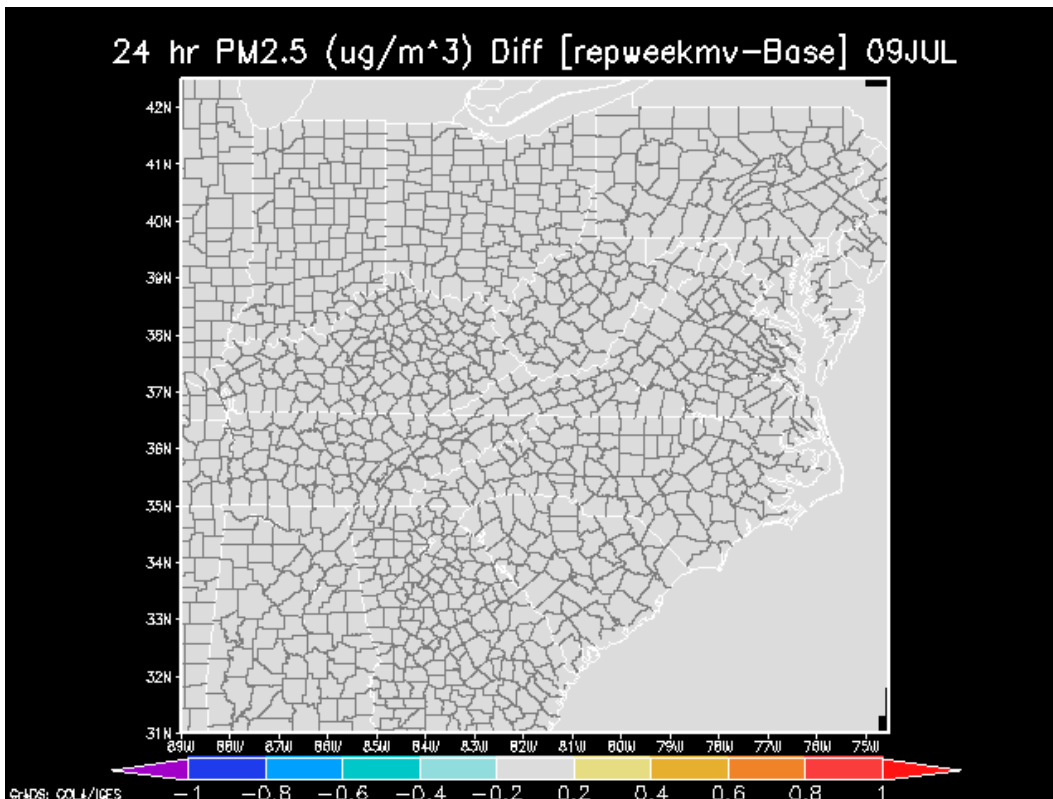
**Figure 8.** Percent difference in 24-hour PM<sub>2.5</sub> concentrations for July 9<sup>th</sup> (Representative week mobile emissions versus daily mobile emissions).



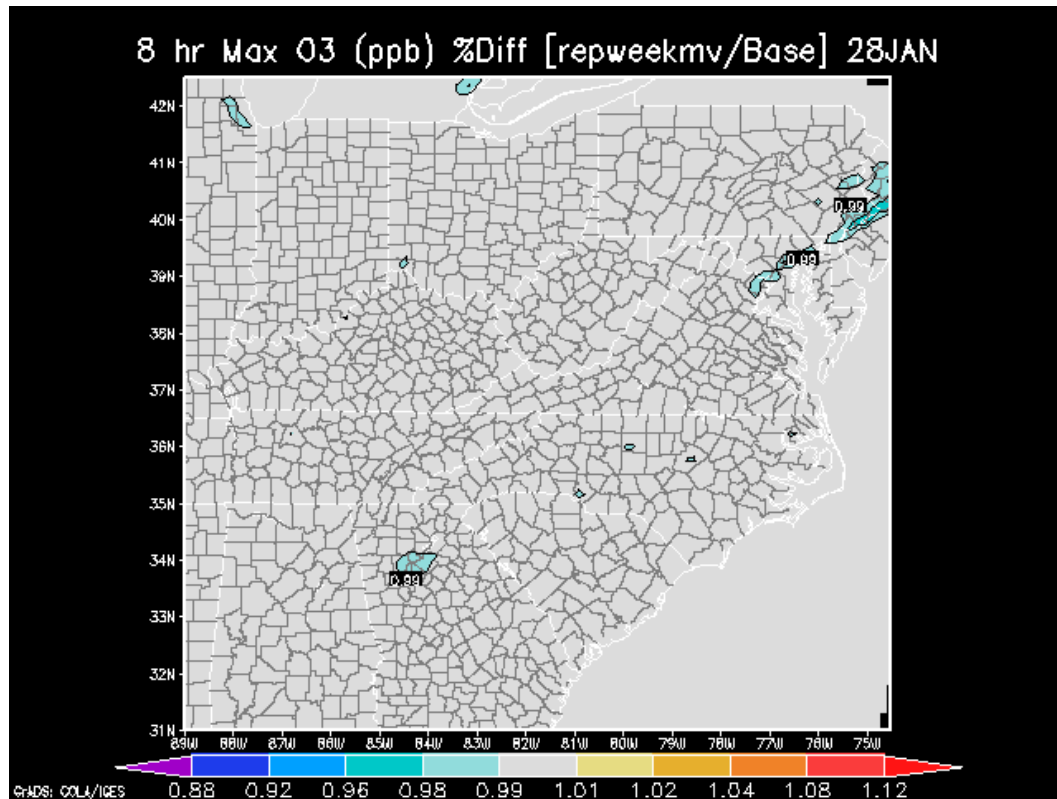
**Figure 9.** Absolute differences in 24-hour PM<sub>2.5</sub> concentrations for January (Representative week mobile emissions versus daily mobile emissions).



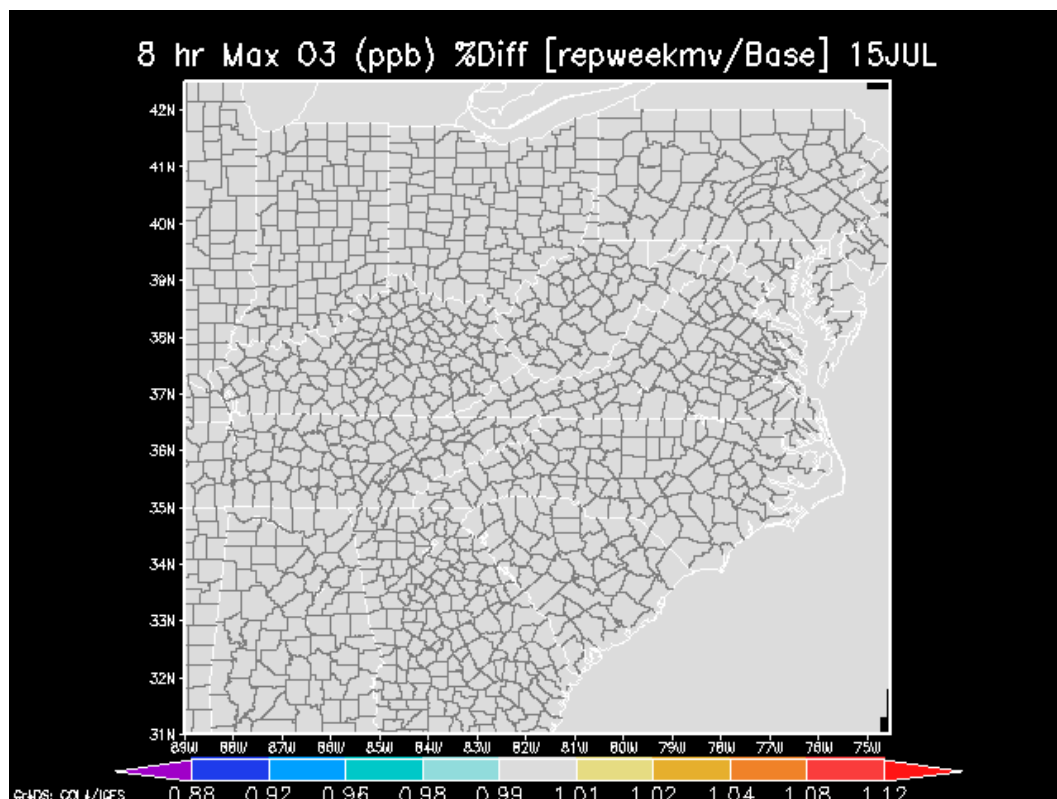
**Figure 10.** Absolute differences in 24-hour PM<sub>2.5</sub> concentrations for July 9<sup>th</sup> (Representative week mobile emissions versus daily mobile emissions).



**Figure 11.** Percent differences in daily 8-hour maximum ozone concentrations for January 28th (Representative week mobile emissions versus daily mobile emissions).



**Figure 12.** Percent differences in daily 8-hour maximum ozone concentrations for July 15<sup>th</sup> (Representative week mobile emissions versus daily mobile emissions).





**Figure 13.** Absolute differences in daily 8-hour maximum ozone concentrations for July 15<sup>th</sup> (Representative week mobile emissions versus daily mobile emissions).

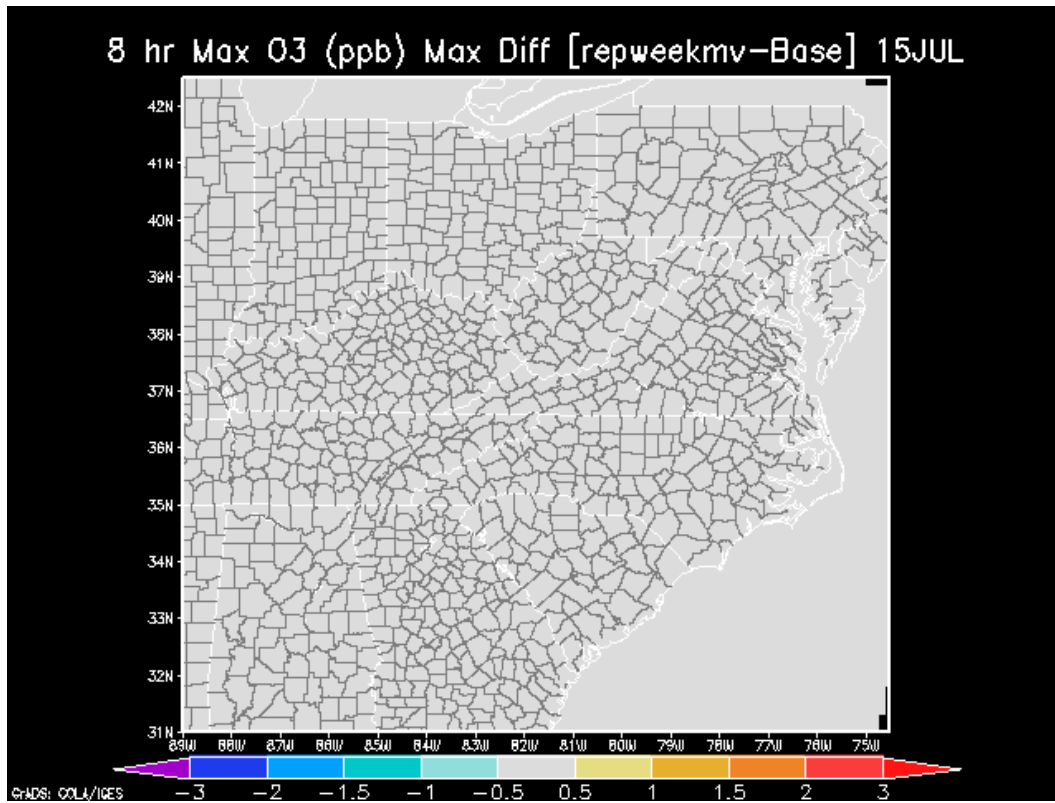


Figure 14. Absolute differences in 1-hour maximum ozone concentrations for July 12<sup>th</sup>.

### Layer 1 $\max(\max(\text{O3k}) - \max(\text{O3e}))$

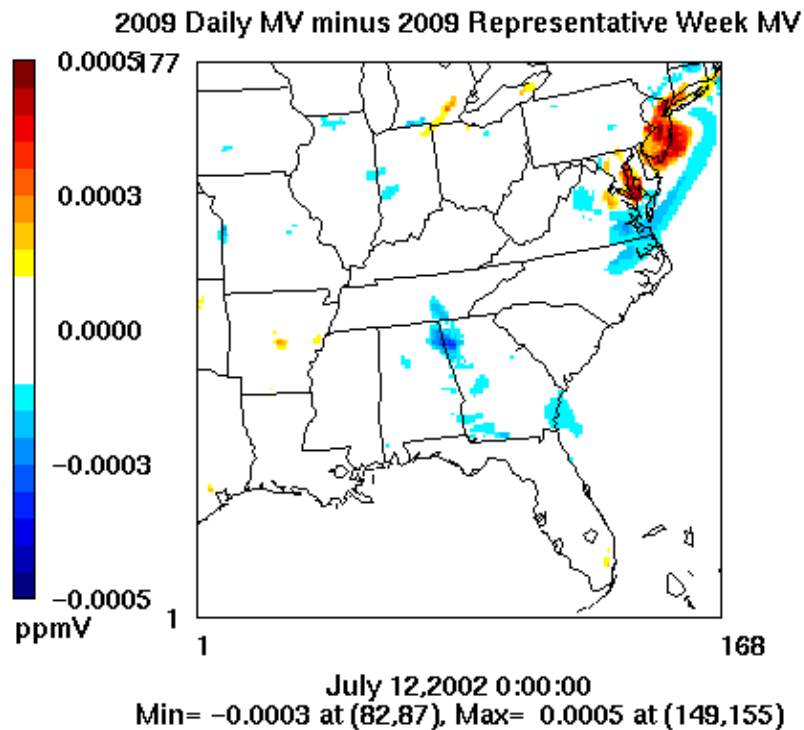
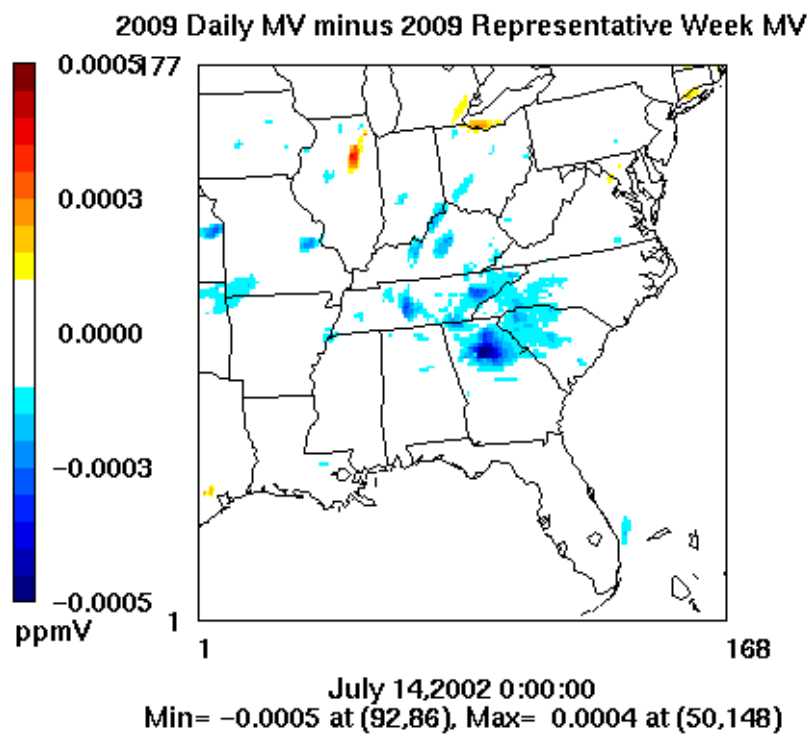


Figure 15. Absolute differences in 1-hour maximum ozone concentrations for July 14<sup>th</sup>.

### Layer 1 $\max(\max(\text{O3m}) - \max(\text{O3g}))$



## CONCLUSIONS

U.S. EPA attainment demonstration modeling guidance<sup>11,12</sup> notes that in some cases it may be useful to evaluate how the response of an air quality model to emissions changes varies as a function of alternative model inputs or model algorithms. These types of tests can be used to assess the robustness of a base case or control strategy modeling evaluation. As an example, EPA remarks that States/Tribes could consider the effects of assumed boundary conditions on predicted effectiveness of a control strategy. If the model response does not differ greatly over a variety of alternative plausible configurations, this increases confidence in the model results.

The parameters for these sensitivity tests can include, but are not limited to: different chemical mechanisms, finer or coarser grid resolution, meteorological inputs from alternative, credible meteorological model(s), different initial/boundary conditions, and *multiple sets of reasonable emission projections*. Sensitivity tests can and should be applied throughout the modeling process, not just when model performance is being evaluated.

The modeling team's research in using *reasonable alternate sets of onroad emission projections* has determined that the use of representative week onroad mobile emissions for each month of our episodes within our 12km modeling domain predicts ozone and particulate matter concentration differences from annual, everyday onroad mobile modeling which could be considered insignificant from an air quality modeling standpoint. The small differences in the air quality results in combination with the length of time necessary to conduct daily onroad mobile runs using the MOBILE6 module of SMOKE has resulted in the project team's recommendation that representative week onroad mobile emissions methodology be carried forward in the VISTAS regional haze modeling and the ASIP PM<sub>2.5</sub> and 8-hour ozone modeling.

## REFERENCES

1. "Draft Modeling Protocol For Association for Southeastern Integrated Planning (ASIP) – Emissions and Air Quality Modeling to Address 8-Hour Ozone and PM<sub>2.5</sub> Nonattainment in the Southeastern United States"; Prepared for ASIP by ENVIRON, Alpine Geophysics and University of California, Riverside, January 31, 2006.
2. Dudhia, J. "A Non-hydrostatic Version of the Penn State/NCAR Mesoscale Model: Validation Tests and Simulation of an Atlantic Cyclone and Cold Front", *Mon. Wea. Rev.*, 1993, Vol. 121. pp. 1493-1513.
3. Grell, G. A., J. Dudhia, and D. R. Stauffer. "A Description of the Fifth Generation Penn State/NCAR Mesoscale Model (MM5). NCAR Tech. Note, 1994. NCAR TN-398-STR, 138 pp.
4. University of North Carolina at Chapel Hill, *Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System*, <http://cf.unc.edu/cep/empd/products/smoke/index.cfm>.
5. Byun, D.W., and J.K.S. Ching. "Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System", EPA/600/R-99/030. 1999.
6. Pleim J. et al. "New Developments in CMAQ Model Physics", Presented at the 4<sup>th</sup> Annual CMAS Models-3 User's Conference, September 26-28, 2005, Friday Center Chapel Hill North Carolina.

7. VISTAS Phase II Modeling website, <http://pah.cert.ucr.edu/vistas/vistas2/> .
8. Abraczinskas, M.A., Olerud, D.T., Sims, A.P. “Characterizing Annual Meteorological Modeling Performance for Visibility Improvement Strategy Modeling in the Southeastern U.S.”, Presented at the 3<sup>th</sup> AMS Joint Conference on the Applications of Air Pollution Meteorology with the Air and Waste Management Association, Vancouver, BC, 2004.
9. Morris, R.E., McNally, D.E., Tesche, T.W., Tonnesen, G., Boylan, J.W., Brewer, P. “Preliminary Evaluation of the Community Multiscale Air Quality Model for 2002 over the Southeastern United States”. 2005. J. Air & Waste Manag. Assoc. 55:1694-1708
10. Morris, R.E.; Koo, B.; Yarwood, G.; McNally, D.E.; Tesche, T.W.; Tonnesen, G.S.; Boylan, J.; Brewer, P. “Model Sensitivity Evaluation for Organic Carbon Using Two Multi-Pollutant Air Quality Models that Simulate Regional Haze in the Southeastern United States”, Atmos. Environ. Submitted for publication.
11. *Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-hour Ozone NAAQS*, U.S. Environmental Protection Agency Office of Air Quality Planning and Standards Emissions, Monitoring, and Analysis Division Air Quality Modeling Group Research Triangle Park, North Carolina, 2005; EPA-454/R-05-002.
12. *Guidance for Demonstrating Attainment of Air Quality Goals for PM<sub>2.5</sub> and Regional Haze*, Draft Report, U.S. Environmental Protection Agency, Research Triangle Park, NC. 2001.

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## **KEYWORDS**

ASIP

MOBILE

Modeling

Onroad Mobile

Ozone

Particulate Matter

Regional Haze

Regional Planning Organization

SMOKE

VISTAS