

Air Sciences



Revised Draft Report

AIR QUALITY MODELING ANALYSIS FOR THE DENVER EARLY ACTION OZONE COMPACT:

Preliminary Photochemical Base Case Modeling and Model Performance Evaluation for the Summer '02 Denver Ozone Season and Embedded High 8-hr Ozone Episodes

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1.0 INTRODUCTION

This report describes the preliminary results of a photochemical grid modeling base case simulation and model performance evaluation carried out as part of the Denver-Northern Front Range 8-hour ozone Early Action Compact Study (Denver EAC Study). The procedures used in the Denver EAC photochemical modeling are described in detail in the modeling protocol (Tesche et al., 2003a).

BACKGROUND

As described in the ozone modeling protocol (Tesche et al., 2003a), the goal of the Denver EAC 8-hr Ozone Study is to conduct a comprehensive photochemical modeling study for the Denver-Northern Front Range Region (DNFRR) that can be used as the technical basis for 8-hr ozone SIP development. The modeling study, guided by the protocol, is specifically designed to identify the processes responsible for 8-hr ozone exceedances in the region and to develop realistic emissions reduction strategies for their control. Major objectives of the Denver EAC study include:

- Prepare an Ozone Modeling Protocol (Tesche et al., 2003a), consistent with EPA requirements, that provides direction to the 8-hr ozone modeling of the Denver-Northern Front Range. Collaborate with the CDPHE in the identification and justification of one or more 8-hr ozone modeling episodes for the Denver study;
- Construct dynamically and thermodynamically consistent MM5 meteorological inputs at appropriate grid scales for direct input to the emissions and photochemical models (McNally, Tesche and Morris, 2003);
- Produce the model-ready base-year and future-year emissions inventories suitable for input to the CAMx model and perform additional quality assurance (QA) of the emissions data sets beyond that conducted by the CDPHE (Mansell and Dinh, 2003a,b);
- Develop photochemical model base case modeling inputs for the selected modeling episode(s) and carry out base case model performance testing, diagnostic analysis, and pertinent sensitivity studies, including a check on mass consistency (this document presents a preliminary evaluation);
- Evaluate the photochemical model's performance for the selected episode(s) and compare the results with EPA's performance objectives in their draft 8hour ozone modeling guidance (EPA, 1999);
- Perform across-the-board VOC and NOx emissions reduction sensitivity simulations to explore the ozone response for the modeling episode(s);





- Perform additional future-year (2007) control scenario simulations to estimate ozone levels in the Denver region under different local control regimes (if the future year baseline modeling does not show attainment with the 8-hr NAAQS);
- Develop suitable "weight of evidence" analyses supporting the ozone attainment demonstration, consistent with EPA guidance and assist the RAQC and CDPHE in developing the technical information to support the documentation required for the Denver 8-hr ozone Early Action Compact protocol;
- Provide for a thorough and efficient transfer of modeling codes, data sets, and related information to other stakeholders in the process including the EPA Region VIII and the CDPHE; and
- Set up the full suite of models and databases developed in this study on CDPHE computers and provide on-site training in the use of the modeling system(s).

A photochemical modeling domain that covered the southwestern US using grid resolutions of 36, 12, 4 and 1.33 km was set up with the higher resolution grids (4 and 1.33 km) focused on the Denver Metropolitan Area (DMA). Figure 1-1 displays the grid nesting configuration used for the photochemical and emissions modeling. Meteorological modeling domains were slightly larger than used for the photochemical and emissions modeling and also included a large-scale 108 km grid covering North America. The MM5 meteorological, EPS2x emissions and CAMx photochemical models were selected for the Denver 8-hour ozone EAC modeling (Tesche et al., 2003a).







Figure 1-1. Denver EAC air quality 36 km (outer), 12 km (green), 4 km (red) and 1.33 km (blue) modeling domains.

MM5 METEOROLOGICAL MODELING

As part of the Denver EAC study, the PSU/NCAR Mesoscale Meteorological Model (MM5) was applied to a fifty (50) day long summer ozone period in central Colorado spanning the June 6 through July 25, 2002 timeframe (McNally, Tesche and Morris, 2003). Within this so-called Summer '02 episode, three embedded high 8-hr ozone episodes occurred in the Denver-Northern Front Range Region (DNFRR). These were: (a) Episode 1: (16-22 July 2002), (b) Episode 2: (24 June–1 July 2002), and (c) Episode 3: (8-12 June 2002). MM5 nested meteorological simulations were performed by modelers at Alpine Geophysics in technical consultation with staff at ENVIRON International Corporation (the modeling prime contractor). The Denver EAC MM5 meteorological modeling report presented results of an operational and limited scientific evaluation of the MM5 model for the Summer '02 episode and the first two intensive embedded periods¹ and assessed whether the model's performance in simulating three-dimensional fields of wind, temperature, and moisture (i.e. mixing ratio) are adequate for use in 8-hr ozone modeling over the DNFRR. The MM5's performance in Episodes 1 and 2 were compared with results from approximately fifty (50) other recent

¹ Episode 3 was dropped from the Denver EAC study due to the high influence of wildfires on air quality in the Denver area.





regional modeling studies carried out across the U.S. over the past several years using the MM5 or other contemporary prognostic models (e.g., RAMS).

The limited scientific evaluation refers to the fact that a detailed MM5 model sensitivity analysis analyzing different Planetary Boundary Layer (PBL) and Land Soil Module (LSM) schemes and other physics options was not undertaken. Instead, the science team relied on using a model configuration that has worked best in the past based on our experience in annual MM5 modeling of the continental US for 2001 and 2002 and more fine-scale MM5 modeling of the Front Range as part of the NFRAQS.

Assessment of the Adequacy of the 24 June-2 July 2002 Episode MM5 Simulation

Table 1-1 compares the 4 km and 1.33 km MM5 results for the 24 June to 1 July 2002 episode with meteorological modeling benchmarks that have been compiled through analyzing over 50 meteorological model simulations performed to support air quality modeling. Shaded cells in the table correspond to those meteorological variables that fall just outside of the benchmark ranges. On the 4 km grid for the 24 June-2 July 2002 episode the bias and gross error in surface temperature prediction and the RMSE error in surface wind speed prediction fall outside the suggested model performance benchmarks and the average results for model applications at scales ranging from 4 km to 12 km. The remaining four statistical measures are within the suggested performance ranges. The results on the 1.33 km grid are only slightly poorer when compared with the benchmarks; again, this is attributed in part to the difference in scales. McNally, Tesche and Morris (2003) concluded that the 4/1.33 km MM5 meteorological fields for the 24 June-2 July 2002 episode may be used, with appropriate review and interpretation, as input to the regional emissions and photochemical models for air quality impacts assessments for the Denver EAC study.

Episode	Tempe (degre	erature ees C)	Mixing (kg	g Ratio /kg)	Surface Winds (m/s)				
Grid Resolution	Bias	Error	Bias	Error	RMSE	IOA	WD diff		
4 km	0.65	2.75	-0.17	1.59	2.77	0.80	29		
1.33 km	1.78	2.35	-0.70	1.68	2.84	0.60	43		
Benchmark	<u>< +</u> 0.5	<u><</u> 2.0	<u>< +</u> 1.0	<u><</u> 2.0	<u><</u> 2.00	<u>></u> 0.60	<u><</u> 30		
U.S. Average	-0.2	2.0	0.0	1.8	2.00	0.71	24		

Table 1-1. Summary results for the 24 June-2 July 2002 MM5 simulation on the 4/1.33 km high resolution grids compared with the Ad Hoc performance benchmarks from ~50 recent prognostic model performance evaluations throughout the U.S. (McNally, Tesche and Morris, 2003).

Assessment of the Adequacy of the 16-22 July 2002 Episode MM5 Simulation

Table 1-2 compares the 4 km and 1.33 km MM5 results for the 16-22 July 2002 episode with the meteorological modeling benchmarks compiled based on over 50 meteorological model simulations performed primarily to support air quality modeling. Shaded cells in the table





correspond to those meteorological variables that fall just outside of the benchmark ranges. On the 4 km grid for the 16-22 July 2002 episode the gross error in surface temperature prediction, the RMSE error in surface wind speed prediction, and the mean wind direction prediction difference all fall outside the suggested model performance benchmarks and the average results for model applications at scales ranging from 4 km to 12 km. The remaining four statistical measures are within the suggested performance ranges. The results on the 1.33 km grid are only slightly poorer when compared with the benchmarks and this is attributed in part to the difference in scales. However, when considering the full set of model performance results on the 4/1.33 km grids, particularly in light of substantial challenges posed by simulating such fine scales over the Denver-Northern Front Range Region, McNally, Tesche and Morris (2003) concluded that the 4/1.33 km MM5 meteorological fields for the 16-22 July 2002 episode may be used, with appropriate review and interpretation, as input to the regional emissions and photochemical models for air quality impact assessments for the Denver EAC study.

Table 1-2. Summary results for the 16-22 June 2002 MM5 simulation on the 4/1.33 km
high resolution grids compared with the Ad Hoc performance benchmarks and ~50
recent prognostic model performance evaluations throughout the U.S. (McNally,
Tesche and Morris, 2003).

Episode	Tempe (degre	erature ees C)	Mixing (kg/	l Ratio /kg)	Su	rface Win (m/s)	ds
Grid Resolution	Bias	Error	Bias	Error	RMSE	IOA	WD diff
4 km	0.45	2.30	-0.66	1.57	2.61	0.78	60
1.33 km	0.81	1.60	-0.59	1.47	2.53	0.57	37
Benchmark	<u>< +</u> 0.5	<u><</u> 2.0	<u>< +</u> 1.0	<u><</u> 2.0	<u><</u> 2.00	<u>></u> 0.60	<u><</u> 30
U.S. Average	-0.2	2.0	0.0	1.8	2.00	0.71	24

EMISSIONS MODELING FOR THE SUMMER '02 EPISODE

The CDPHE provided emission inventory data for 2002 for the entire State of Colorado. For the remaining states within the modeling domain (see Figure 1-1), version 2 of the EPA's 1999 National Emission Inventory (NEI99 v2) was used. These 1999 emission estimates were projected to the 2002 base year using the EPS2x growth and projection modules with growth factors developed with the EGAS model. The Colorado Oil and Gas Association (COGA) provided information regarding emissions from oil and gas operations in Weld County, including VOC speciation of "flash" emissions and ethane emissions. The New Mexico Oil and Gas Association (NMOGA) provided emission estimates for un-permitted oil and gas production wells in the northeast corner of the state. Emission data for Mexico were based on a draft inventory as used in the BRAVO modeling study (Mansell and Dinh, 2003a)

Several improvements were incorporated in EPA's NEI99 v2 emissions database based on the draft version 3 NEI database. These improvements were primarily associated with the residential fossil-fuel combustion source category, the inclusion of updated data for Midwest states developed by the Lake Michigan Air Directors Consortium (LADCO), and the inclusion of point source data for some Eastern US states. The NEI99 version 2/verison 3 data is





referred to hereafter simply as the NEI99. The data were obtained as ASCII files in IDA format. The IDA files were reformatted to AFS/AMS file format for processing with EPS2x.

A summary of the emissions data sources for the development of the modeling emissions inventory is provided in Table 1-3.

Category	Region	Data Source
Mobile	Denver Metro	CDPHE link-based, MOBILE6
	Other Colorado	CDPHE
	Outside Colorado	EPA NEI99 Version 2, MOBILE6
Off-Road	Colorado	CDPHE emissions data
	Outside Colorado	EPA NEI99 Version 2
Area	Colorado	CDPHE emissions data
	Outside Colorado	EPA NEI99 Version 2
Oil & Gas	Colorado	Included in Point Source inventory
	New Mexico	NMOGA Un-permitted data base
	Outside CO and NM	EPA NEI99 Version 2
Point	Colorado	CDPHE emissions data
	Outside Colorado	EPA NEI99 Version 2
Biogenic	Entire Domain	GloBEIS3 with BELD3 LULC data and drought adjustment

 Table 1-3.
 Summary of emissions data sources used in the Denver 8-hour ozone EAC modeling.

Point Sources

Point source data were obtained from different sources, processed separately and merged prior to modeling. The data include:

- Colorado point sources
- Other State point sources
- Mexico point sources

The point source data are processed for a typical peak ozone (PO) season weekday and weekend day. Continuous Emissions Monitoring (CEM) data was provided by the CDPHE, which are hourly episode day specific data, for major NOx sources. However, due to the scheduling and resource constraints these data were not included in the 2002 base year emissions inventory. The 2002 Colorado point source data were provided EPS2x AFS input format. For all states other than Colorado, data for criteria pollutants from the NEI99 is used.





Point source emissions for Mexico were obtained in as ASCII IDA formatted files and reformatted for processing with EPS2x.

The criteria for selecting NOx point sources for plume in grid treatment within the 4 and 1.33km modeling domains is 2 tons NOx on any episode day. For the regional emissions grid, the NOx criteria is 25 tons per day on any episode day.

On-Road Mobile Sources

On-road mobile emission sources were processed separately for the State of Colorado and all remaining states in the modeling domain and Mexico. For Colorado, link-based emissions data was provided for the Denver Metropolitan Area (DMA) as well as the Fort Collins/Greeley and Colorado Springs areas. HPMS-based VMT data provided by the CDPHE were used for the remaining counties in Colorado. All other on-road mobile emission estimates were based on the NEI99 database.

Colorado On-Road Mobile Source Emissions

Emissions were estimated for all counties in Colorado for the following episode days: June 25-July 1, 2002 and July 18-July 21, 2002. Emission factors were obtained from the US EPA's MOBILE6 model. Temperature and humidity inputs were taken from MM5 modeling (McNally, Tesche and Morris, 2003). In-use control inputs for the Denver, Fort Collins, and Colorado Springs areas were provided by the CDPHE. These parameters describe the inspection and maintenance programs as well as fuel specifications such as oxygenate content and RVP. Local VMT (fleet) mixes were also provided. For counties not included in the group above, MOBILE6 modeling was done assuming the same RVP value (as the counties above) but no other controls. Link-based activity (VMT) data for the Denver, Fort Collins, and Colorado Springs areas were provided by the CDPHE. Corresponding MOBILE6 emission factors were prepared by running the model over a range of temperatures, speeds, and humidity conditions. The M6LINC software tool was used to estimate link-specific hourly emissions by mode (start exhaust, running exhaust, running loss, resting loss, hotsoak, and crankcase). Diurnal emissions were estimated outside of M6LINC since MOBILE6 diurnal emission factors cannot be obtained at specific temperatures. These emission factors were estimated by running MOBILE6 with daily minimum and maximum temperatures (rather than for a range of specific temperatures.) Table 1-4 summarizes the link-based NOx, VOC and CO emissions for the Denver Metropolitan Area. The counties for which on-road mobile source emissions are based on transportation networks include: Adams, Arapahoe, Boulder, Denver, Douglas, Elbert, El Paso, Gilpin, Jefferson, Larimer, Teller and Weld.





Date	NOx	VOC	CO
6/25/02	235.38	197.70	1617.58
6/26/02	232.68	193.03	1623.81
6/27/02	236.13	201.10	1645.34
6/28/02	254.90	215.06	1727.42
6/29/02	193.83	171.44	1428.66
6/30/02	131.78	119.59	1058.97
7/01/02	219.86	198.45	1613.25
7/18/02	237.77	209.34	1682.98
7/19/02	248.78	219.22	1744.28
7/20/02	179.05	155.82	1371.46
7/21/02	135.11	115.76	1088.46

 Table 1-4.
 Denver Metropolitan Area link-based emission summary (tpd).

Emission Summaries

Table 1-5 summarizes the statewide and Denver Metropolitan Area (DMA) and Front Range counties emission inventory by major source category, more details are provided in Mansell and Dinh (2003a,b). Note that, with the exception of Morgan County, the on-road mobile source emissions estimates for the DMA/Front Range were not available by individual county. These sources were processed using link-based data. Total on-road link-based mobile emissions are presented in Table 1-6 for each of the episode days.

Not included in Tables 1-5 and 1-6 are the ethane emissions for Weld County or emissions from wildfires that were generated after the emission inventory reports (Mansell and Dinh, 2003a,b) and are discussed below.

	DMA/Front Range			State-wide			
Source Category	NOX	VOC	СО	NOX	VOC	CO	
Stationary Points	163.70	206.96	46.16	328.59	256.93	95.12	
Area	6.50	131.04	3.74	8.49	190.26	4.33	
On-Road Mobile	238.14	199.66	1644.66	332.51	273.48	2547.40	
Off-Road Mobile	140.85	98.80	1497.69	231.50	140.14	1865.09	
Biogenics	56.12	1025.86	134.71	254.74	7688.51	932.96	
Total	605.30	1662.32	3326.96	1155.84	8549.32	5444.89	

Table 1-5. 2002 Emission inventory summary by major source category (tons/day).





	NOx	VOC	CO
6/25/02	235.38	197.70	1617.58
6/26/02	232.68	193.03	1623.81
6/27/02	236.13	201.10	1645.34
6/28/02	254.90	215.06	1727.42
6/29/02	193.83	171.44	1428.66
6/30/02	131.78	119.59	1058.97
7/01/02	219.86	198.45	1613.25
7/18/02	237.77	209.34	1682.98
7/19/02	248.78	219.22	1744.28
7/20/02	179.05	155.82	1371.46
7/21/02	135.11	115.76	1088.46

Table 1-6.	Denver Metropolitan	Area and Weld C	County link-based	emission summary (tpd).
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Weld County, Colorado Oil and Gas Emissions

Emission estimates for oil and gas operations in Weld County, CO were also included in the base year inventory. Detailed speciation information provided by the Colorado Oil and Gas Association (COGA) was used to develop speciation profiles for these sources. Table 1-7 presents the VOC speciation data provided by COGA for the Weld County oil and gas operations. Based on these data, new speciation profiles were developed and applied to all point source records in the emission inventory with Standard Industrial Codes (SIC) of 1321. According to information provided by the Denver Regional Air Quality Council, the VOC flash emissions from these sources do not include ethane or methane, which are considered non-reactive according to the EPA. Therefore, the speciation profiles developed here did not include the fractions of methane and ethane from Table 1-7 (C1/C2).

	All Samples		
Compound	Total	Avg (lb/hr)	PCT - Wt
H2S	0.000	0.000	
02	0.000	0.000	
CO2	0.664	0.027	2.90
N2	0.011	0.000	
C1	2.334	0.093	10.19
C2	3.769	0.151	16.45
C3	6.539	0.262	28.55
i-C4	2.001	0.080	8.74
n-C4	3.591	0.144	15.68
i-c5	1.237	0.049	5.40
n-C5	0.995	0.040	4.34
C6	0.482	0.019	2.10
C7	0.697	0.028	3.04
C8	0.110	0.004	0.48
C9	0.030	0.001	0.13
C10+	0.004	0.000	0.02
Benzene	0.043	0.002	0.19
Toluene	0.063	0.003	0.28
Eth-Benze	0.000	0.000	0.00
Xylenes	0.014	0.001	0.06
n-C6	0.311	0.012	1.36
224-Tri-MP	0.021	0.001	0.09
Total	0.000	0.916	100.00
	Percent wt	based on total emissi	ons (lb/hour)

 Table 1-7.
 Raw oil & gas speciation data from COGA.





The total VOC flash emissions (Condensate Tank SIC 1321) in the point source inventory in Weld County amount to approximately 129 tons/day. Applying the speciation profiles based on the COGA-specific gas profile information results in the CB4 speciated VOC emissions presented in Table 1-8. The resulting speciated VOC emissions presented in Table 1-8 are considered more appropriate than those resulting from use of the default speciation profiles for the current emission inventory as they are based on local data.

1	able i e. eeen openine en openine en and gas ennesions for werd eeunty (tens/day).									
	Source Category	VOC	OLE	PAR	OL	XYL	FORM	ALD2	ISOP	
	Condensate Tank SIC 1321	128.96	0.0	111.83	0.6124	0.1350	0.0	0.0	0.0	

Table 1-8.	COGA-specific	CB4 speciated	oil and gas emiss	sions for Weld	County (tons/day).
			0		

Ethane emissions associated with the flash VOC emissions sources in Weld County were added to the existing VOC emissions. Based on the speciation information provided, 30 tons per day of ethane emissions were added. The CB-IV speciation profile assumes that a 0.4 fraction of the ethane is split as the CB-IV PAR (parifin) species on a molar basis. As the molecular weight of ethane is 30.07 and the molecular weight of PAR is assumed to be 16 then this results in an additional 6.39 tons per day of PAR emissions in the air quality modeling emissions inputs ($6.39 = 0.04 \times 30 / 30.07 \times 16$).

Wildfire Emissions

Emissions estimates for wildfires were provided by the CDPHE for each day of the June/July 2002 episode. The data were processed as point sources following the methodology used in the WRAP modeling efforts as described in Air Sciences, 2002.

A summary of NOx, VOC and CO emissions by day for each of the June/July 2002 episode days is provided in Table 1-9. These values represent total emissions in tons per day for the entire modeling domain.



Table 1-9. Summary of wildfire emissions (tpd).							
	Wildfire Emissions Summary (tons/day)						
Date	NOx	VOC	CO				
6/4/02	35.35	77.56	1648.03				
6/5/02	61.98	135.99	2889.69				
6/6/02	65.48	143.67	3053.09				
6/7/02	21.30	46.73	992.99				
6/8/02	3062.92	6719.79	143000.00				
6/9/02	732.38	1606.96	34100.00				
6/10/02	1261.78	2768.25	58800.00				
6/11/02	1071.52	2350.87	50000.00				
6/12/02	400.09	877.81	18700.00				
6/13/02	207.44	455.14	9671.41				
6/14/02	143.72	315.30	6700.18				
6/15/02	337.27	739.96	15700.00				
6/16/02	371.52	815.06	17300.00				
6/17/02	140.27	307.78	6539.71				
6/18/02	246.38	540.55	11500.00				
6/19/02	1042.43	2287.08	48600.00				
6/20/02	947.45	2078.62	44200.00				
6/21/02	1393.21	3056.56	65000.00				
6/22/02	1648.12	3616.15	76800.00				
6/23/02	3697.70	8112.82	172000.00				
6/24/02	2401.81	5269.53	112000.00				
6/25/02	1237.10	2714.12	57700.00				
6/26/02	1495.87	3281.90	69700.00				
6/27/02	1591.24	3491.05	74200.00				
6/28/02	1045.22	2293.18	48700.00				
6/29/02	1181.59	2592.33	55100.00				
6/30/02	1951.80	4282.18	91000.00				
7/1/02	1120.90	2459.29	52300.00				
7/2/02	970.32	2128.78	45200.00				
7/3/02	1040.66	2283.16	48500.00				
7/4/02	763.81	1675.79	35600.00				
7/5/02	235.43	516.51	11000.00				
7/6/02	134.64	295.38	6277.16				
7/7/02	125.97	276.39	5873.18				
7/8/02	96.11	210.89	4481.53				
7/9/02	39.54	86.77	1844.06				
7/10/02	25.11	55.09	1170.86				
7/11/02	48.32	106.00	2252.37				
7/12/02	82.57	181.14	3849.39				
7/13/02	183.21	401.93	8541.42				
7/14/02	595.91	1307.33	27800.00				
7/15/02	353.34	775.20	16500.00				
7/16/02	806.12	1768.59	37600.00				
7/17/02	498.13	1092.92	23200.00				
7/18/02	160.32	351.70	7473.30				
7/19/02	88.17	193.43	4110.65				
7/20/02	49.64	108.91	2314.63				
7/21/02	7.07	15.53	329.68				



2.0 MODEL PERFORMANCE EVALUATION APPROACH

To date, ten (10) CAMx base case sensitivity configurations have been analyzed for the Summer '02 period for the two Denver 8-hour ozone episodes. These base case sensitivity simulations were performed using slight variations in meteorological and emission inputs and grid resolution that were updated during the course of the study.

The CAMx base case sensitivity simulations performed to date are as follows:

<u>Run 1:</u> Preliminary Base Case for the June 7 through July 22, 2002 period on the 36/12 km regional grid.

<u>Run 2</u>: Preliminary Base Case simulation for the June 25 – July 1, 2002 episode on a 36/12/4 km grid.

<u>Run 2a</u>: Preliminary Base Case simulation for the July 18-21, 2002 episode on a 36/12/4 km grid.

<u>Run 3</u>: Preliminary Base Case simulation for the June 25 – July 1, 2002 episode on a $\frac{36}{12}/\frac{4}{1.33}$ km grid.

<u>Run 3a</u>: Preliminary Base Case simulation for the July 18-21, 2002 episode on a 36/12/4/1.33 km grid.

<u>Run 4</u>: Same as 36/12 km Run 1 only limit mixing heights to 2,000 m AGL and add Kvpatch minimum to layer 1.

<u>Run 5</u>: Same as 36/12 km Run 1 only with reprocessed emissions to include VOC speciation profiles provided by COGA for Flash VOC emissions in Weld County and to correct some Colorado mobile source emissions where 2007 emissions were mistakenly provided in the 2002 inventory.

Run 5a: Run 5 only on a 36/12/4 km grid and for the June 25 – July 1, 2002 episode.

<u>Run 5b</u>: Run 5 only on a 36/12/4 km grid and for the July 18-21, 2002 episode. <u>Run 6</u>: Restructured vertical layer configuration. Run aborted after little improvement in model performance seen in first part of episode.

<u>Run 7</u>: Same as Run5 (36/12 km) only with minimum 100 m nighttime and 1,500 m afternoon maximum mixing (PBL) heights and increased VOC boundary conditions on northern boundary.

<u>Run 7a</u>: Run7 configuration for the June 25-July 1, 2002 episode using the 36/12/4 km grid.

<u>Run 7b</u>: Same as Run7a only with no clouds or wet deposition inputs to CAMx. <u>Run 8</u>: Same as Run7 (36/12 km) only including ethane emissions for oil and gas operations in Weld County.

<u>Run 8a</u>: Run8 configuration using the 36/12/4 km grid and the June 2002 episode. <u>Run 9</u>: Same as Run 8 (36/12 km) also including wildfire emissions.

Run9a: With wildfires for the June 2002 episode using the 36/12/4 km grid.

<u>Run9b</u>: With wildfires for the July 2002 episode using the 36/12/4 km grid.

Run 10: Same as Run 9 (36/12 km) without the PBL patch.

<u>Run10a</u>: With wildfires and no PBL patch for the June 2002 episode using the 36/12/4 km grid.

<u>Run10b</u>: With wildfires and no PBL patch for the July 2002 episode using the 36/12/4 km grid.



The CAMx model using a 36/12 km grid requires 1.5 to 3 CPU hours per simulation day. Thus, the 46 day June 7 through July 22, 2002 Summer '02 episode requires a little over 3 CPU days to complete. Using the 36/12/4 km grid, the CAMx model requires approximately 11 CPU hours per simulation day to run. Thus, using the 36/12 km grid for the entire Summer '02 episode and the June 2002 and July 2002 episodes at 36/12/4 km resolution requires approximately 8 CPU days. Running the two episodes at the 1.33 km grid resolution requires an additional 8 CPU days to complete. The initial CAMx model simulations using the 4 km and 1.33 km grid resolutions (i.e., Run 2 and Run 3) produced very similar model performance. Thus, due to schedule constraints additional sensitivity simulations focused on running on the 36/12/4 km grid.

EPA MODEL PERFORMANCE EVALUATION GUIDELINES AND GOALS

EPA has published draft 8-hour ozone modeling guidelines (EPA, 1999) that is used as a basis, in part, for judging the adequacy of the Denver base case simulation. As discussed in the Denver 8-hour ozone EAC Modeling Protocol (Tesche et al., 2003), model performance evaluation consists of as a series of tests that become more stringent as one moves through the model performance process. We are using the EPA draft 8-hour modeling guidelines as an initial test of model performance. These tests focus primarily on ozone model performance. After applying the EPA's performance tests to the model, the model performance moves on toward more stringent tests that will include comparisons of ozone precursors with available data, comparisons of VOC speciation, ozone indicator comparisons as available, and further diagnostic tests. If the model does not achieve a level of performance in the initial tests, then corrective action and further diagnostic tests are usually performed to identify the problem(s) and corrections needed. Such corrective action can range from simple adjustments, like accounting for drought stress in biogenic emissions and dry deposition or eliminating wet scavenging due to uncertain convective cloud systems, to more intensive tests that may include rerunning the meteorological model or identifying and quantifying missing or improperly characterized emissions in the inventory.

There are two main components in EPA's draft 8-hour ozone guidance operational ozone model performance that are used as an initial test of model performance: (1) Big Picture Assessment Using Graphics; and (2) Ozone Metrics.

Big Picture Assessment Using Graphics

EPA's draft 8-hour ozone guidance lists four graphic displays that are used to obtain a big picture of model performance:

• <u>Tile plots of observations and predictions</u>: These are used to understand the spatial differences and displacements of the predicted and observed ozone concentrations and to compliment the ozone metrics. For example, an ozone plume that is displaced a little from the ozone monitor may produce degraded ozone performance metrics but may still be a reliable tool for control strategy evaluation if the correct sources and processes are being simulated to produce accurate peak ozone that is just displaced from the monitor. These plots can be used to assess model performance upwind and





downwind of the Denver urban area to assist in interpreting performance issues due to transport versus local photochemical production.

- <u>Tile plots of differences in observations and predictions</u>: Combined with the tile plots of absolute predicted and observed concentrations above this plot may provide some insight into performance under low and high ozone concentrations. Given the limited ozone network in the Denver area, the same information from this plot can be obtained by the absolute concentrations plots.
- <u>Scatter plots and quantile-quantile (Q-Q) plots</u>: Scatter plots provide a measure of how well the model is replicating the observed ozone concentrations at or in the vicinity of the monitor. Q-Q plots provide a measure of how well the model is reproducing the frequency distribution of the observed ozone concentrations.
- <u>Time series plots</u>: Time series plots of predicted and observed hourly ozone concentrations provide a stringent test of how well the model replicates the observed hourly ozone at the same time and location as the observed value. Problems with temporal timing in the model are readily apparent in a time series plot.

Ozone Metrics

EPA's draft 8-hour ozone guidance identifies several ozone metrics to be applied to the model along with performance goals that should be met. Table 2-1 lists EPA's performance tests, performance goals and comments on how the model will be tested using these tests in the Denver 8-hour ozone EAC modeling. EPA recommends using performance measures of bias and gross error that are expressed as a percent. Two types of bias and gross error are recommended, normalized and fractional, they differ in that the first the difference in the predicted and observed value is normalized by the observed value whereas the second it is normalized by the average of the predicted and observed value. If $c_e(x_i,t)$ and $c_o(x_i,t)$ are the estimated and observed hourly or n-hour (e.g., n=8) ozone concentration at a monitor x_i at time t, then the Mean Normalized Bias Error (MNBE), Mean Fractional Bias (MFBE), Mean Absolute Normalized Gross Error (MANGE) and Mean Absolute Fractional Gross Error (MAFGE) are defined as follows:

$$MNBE = \frac{l}{N} \sum_{i=1}^{N} \frac{(c_{e}(x_{i},t) - c_{o}(x_{i},t))}{c_{o}(x_{i},t)} \ge 100\%$$

MFBE =
$$\frac{1}{N} \sum_{i=1}^{N} \frac{(c_e(x_i, t) - c_O(x_i, t))}{\frac{1}{2} (c_e(x_i, t) + c_O(x_i, t))}$$

$$MANGE = \frac{1}{N} \sum_{i=1}^{N} \frac{|c_{e}(x_{i}, t) - c_{o}(x_{i}, t)|}{c_{o}(x_{i}, t)} \ge 100\%$$

MAFGE =
$$\frac{1}{N} \sum_{i=1}^{N} \frac{(c_e(x_i, t) - c_o(x_i, t))}{\frac{1}{2} (c_e(x_i, t) + c_o(x_i, t))}$$

Here t represents time and can me the time of the daily maximum 1-hour or N-hour ozone concentrations, in which case the sum is also over days, or may represent hourly or running N-hour ozone concentrations, in which case the sum is also over hours.

and how they are applied (EPA, 1998).						
Test(s)	Goals/Objectives	Comment				
"bias pred/obs mean 8-hr (& 1-hr) daily maxima near each monitor" ¹	"~20% most monitors (8-hr comparisons only)" ¹	 EPA's draft modeling guidance does not define "near each monitor". After discussing this issue with EPA "near" was defined to mean the same block of grid cells near the monitor used in EPA's attachment test (e.g., 7 x 7 for 5 km grid). There are three ways we defined "near" for this metric: (1) Select the maximum predicted daily maximum 8-hr ozone concentrations "near" the monitor; (2) Select the predicted values closest in value to the observed value (best fit) "near" the monitor; and (3) Select the predicted value at the monitor (spatially paired). 				
"fractional bias pred/obs mean 8-hr (& 1-hr) daily maxima near each monitor" ¹	"~20% most monitors (8-hr comparisons only)" ¹	Define "near" the three ways described above.				
"correlation coefficients, all data, temporally paired means, spatially paired means" ¹	"moderate to large positive correlations" ¹	Apply to three data sets described above.				
"bias (8-hr daily max and 1-hr obs/pred), all monitors" ¹	"~5-15%" ¹					
"gross error (8-hr daily max and 1-hr obs/pred), all monitors" ¹	"~30-35%" ¹					
Partition data base into upwind, center city and downwind sites and repeat analysis		Get better ideas of level of model agreement based on upwind/downwind stratification and whether there is any obvious pattern of the model performance.				
"Scatter plots & Q-Q plots of 8-he and 1-hr metrics"		Applied to three sets of databases listed above.				

Table 2-1 EPA's draft 8-hour ozone modeling guidance ozone performance tests and goals

1 "Draft Guidance on the use of Models and other Analysis in Attainment Demonstrations of the 8-Hour Ozone NAAQS" (EPA, 1999)

Additional Measures of Model Performance

Once the model performance tests listed above are applied, additional performance tests may be applied depending on schedule and resource constraints. The application of these performance tests have not yet been undertaken so are not discussed in this document but they include:

- Comparisons of secondary species (e.g., NO2, NOy, NOx, NOz).
- Comparisons of ozone precursors (NOx, VOC, CO and VOC speciation).
- Comparisons of ratios of co-varying species (VOC or VOC/CO, VOC species/CO, VOC/NOx, etc.).
- Spatially averaged predictions of the above or of primary species.
- Comparison of modeling results with Observation Based Models (OMB) (e.g., CMB, multivariate models, extent parameter, etc.).
- Comparison of weekday versus weekend day effects.
- Ratios of key indicator species (e.g., O3/NOy, O3/NOz, O3/HNO3, H2O2/HNO3).
- Retrospective analysis.

Of these, the comparison of the model ozone precursors and VOC speciation is ongoing, whereas the rest are beyond the present scope of the Denver EAC.

PRELIMINARY MODEL PERFORMANCE EVALUATION FOR INITIAL CONFIGURATION

The initial configuration of the CAMx model included running at the three grid resolutions (36/12, 36/12/4 and 36/12/4/1.33 km) using the first set of processed emissions that did not include the COGA VOC speciation data for the Weld County flash emissions and included 2007 Vehicle Miles Traveled (VMT) data for El Paso County Colorado that were mistakenly labeled as 2002. The ozone model performance for these initial simulations (i.e., Run1, Run2a, Run2b, Run3a and Run3b) was documented in an October 12, 2003 memorandum (Morris and Mansell, 2003) and at the October 17, 2003 Modeling Review Panel (MRP) meeting at the Denver RAQC's office in Denver, Colorado.

The preliminary Denver 8-hour ozone Base Case simulation for the June/July 2002 episodes achieves EPA's draft 8-hour ozone modeling guidance performance goal of estimating predicted daily maximum 8-hour ozone concentrations near the monitor to within " 20% of the observed value at most monitors. However, more detailed analysis of model performance reveals several performance issues that should be addressed in order to have a more reliable



ozone modeling tool for 8-hour ozone planning. Some of the major performance issues identified are as follows (Morris and Mansell, 2003):

- The model exhibits a spatial displacement of the elevated ozone concentrations further away from the Denver Metropolitan Area (DMA) than observed.
- Overstatement of the afternoon ozone suppression in the Denver Metropolitan Area (DMA) on most days.
- Underestimation of ozone transport into the Denver Metropolitan Area (DMA).
- Underestimation of the amount of local photochemical production due to local emissions.
- Overstatement or misallocation of local convective activity during some days of the episode.
- Other as yet unidentified performance issues.

Causes for many of these phenomena may include:

- Understated mixing in the Denver area.
- Overstated maximum afternoon mixing heights.
- Understated VOC emissions inventory or understated VOC reactivity (local and/or regional).
- Overstated local NOx emissions.
- Understated ozone and/or VOC boundary conditions (BCs).
- Wind direction and wind speed errors.
- Other causes.

Recommendations from Preliminary Model Performance Evaluation

As part of the development of SIP quality photochemical modeling databases it is fairly typical that the initial photochemical grid model Base Case simulation uncovers issues in the meteorological and emission fields that should be improved. The rerunning of the meteorological model with alternative Planetary Boundary Layer (PBL) or Land Surface Module (LSM) schemes, other physics options, and/or with different levels of Four Dimensional Data Assimilation (FDDA) to generate more representative meteorological inputs is routinely performed as part of the development of a SIP quality modeling database. The



photochemical model is also a good diagnostic tool for identifying uncertainties and/or omissions in the emissions database or inappropriate boundary conditions (BCs). Morris and Mansell (2003) recommended several potential actions aimed at improving meteorological, emissions and boundary conditions inputs that would likely lead to improved model performance. However, most of these activities were beyond the current schedule constraints of the Denver 8-hour ozone EAC. Thus, a series of short-term improvements were recommended that may realize improved model performance as follows:

- (1) Update the VOC boundary conditions in the north over land areas of the US to be more representative of continental air mass;
- (2) Impose a minimum nighttime mixing height of 100 m AGL and a minimum afternoon maximum mixing height of 1,500 m AGL to limit MM5 nighttime and daytime cloud induced mixing artifacts.
- (3) Add wildfire emissions to the modeling database.
- (4) Add a placeholder VOC emissions inventory to account for missing VOC emissions from oil and gas operations as reported by Katzenstein and co-workers (2003) that occur mainly to the southeast of the DMA.

Run 8 was performed that included the updated northern boundary VOC boundary conditions and minimum PBLpatch (items 1 and 2 above). Run9 included the same two updates as Run8 along with wildfire emissions (items 1, 2 and 3 above). When it was determined that the PBLpatch had little effect on the estimated ozone concentrations Run 10 base case configuration was performed that included the northern VOC BC and wildfire updates, but without the PBLpatch update. Work is continuing on the develop of the placeholder emissions inventory with other resources to account for missing emissions from oil and gas operations, as suggested by Katzenstein and co-workers (2003), but such an update will not be possible within the current Denver EAC schedule.





3.0 REVISED MODEL PERFORMANCE EVALUATION

Below we discuss the ozone model performance for the updated base case sensitivity simulations for Run8 (BC and PBLpatch updates), Run9 (BC, PBLpatch and wildfire updates), and Run10 (BC and wildfire updates). Model performance using the recently collected CDPHE VOC speciation data is ongoing.

A preliminary ozone model performance evaluation for the June 2002 and July 2002 Denver 8hour ozone episodes was presented previously (Morris and Mansell, 2003). These results suggested that better model performance was obtained for the June 2002 than July 2002 episode. Given the schedule constraints of the Denver EAC, it was decided to initially focus more on improving model performance for the June 2002 episode, although results for the July 2002 episode are also presented. Furthermore, given the similarities of the ozone performance when using the 4 km and 1.33 km grids, the doubled run times when using the 1.33 km grid along with the limited time available resulted in revised base case modeling being performed on just the 36/12/4 km grid.

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Revised base case sensitivity simulation was performed updating the VOC northern boundary conditions (BCs) and adding a minimum nighttime and afternoon patch to the MM5 estimated Planetary Boundary Layer (PBL) heights (PBLpatch) (i.e., Run8). Another base case sensitivity simulation was performed that included wildfires as well as the updated BCs and PBLpatch (Run9). When it was realized that the PBLpatch made little difference in the ozone model performance, it was decided to go back to using the PBL heights out of the MM5 model and Run10 that includes the updated BCs and wildfire emissions became the current base case simulation.

Appendices A, B and C contain spatial plots of estimated and observed daily maximum 8-hour ozone concentrations in the Denver area using 4 km resolution for the June 2002 episode and, respectively, Run8a (BC, PBLpatch), Run9a (BC, PBLpatch, wildfires) and Run10a (BC, wildfires) model configurations. Table 3-1 shows that, with the exception of June 29th, the effect of the PBLpatch on the peak estimated 8-hour ozone concentration was minimal, typically ~0.1 ppb (Run9a vs. Run10a). The effects of the wildfires on the 8-hour ozone peak was usually more pronounced, but always small (< 4 ppb).



dase case sensitivity simulations.							
Date	Run8a	Run9a	Run10a				
June 25, 2002	63.4	65.8	66.2				
June 26, 2002	69.4	69.9	70.0				
June 27, 2002	70.7	70.9	71.0				
June 28, 2002	72.8	73.0	73.1				
June 29, 2002	72.9	73.0	75.1				
June 30, 2002	75.4	76.9	77.0				
July 1, 2002	86.1	89.5	89.6				

Table 3-1. Summary of estimated maximum 8-hour ozone concentrations in the Denver vicinity for the Run8a (BC, PBLpatch), Run9a (BC, PBLpatch, wildfires) and Run10a (BC, wildfires) base case sensitivity simulations.

Spatial Distribution of Daily Maximum 8-Hour ozone Concentrations

Appendices A, B and C display the spatial distribution of estimated and observed daily maximum 8-hour ozone concentrations for the June 2002 episode and, respectively, Run8a, Run9a and Run10a. Since the basic model performance attributes of the three sensitivity runs are similar and Run10a has been adopted as the new base case, the following discussion focuses on model performance for Run10a (Appendix C).

<u>June 25, 2002</u>: On June 25, 2002, the peak observed 8-hour ozone concentration was 81 ppb at the Rocky Flats monitor. Nearby the Rocky Flats monitor was an observed 8-hour ozone value of only 68 ppb at Boulder on this day. The model estimates values of 55-60 ppb at these two locations. Northwest of the Rocky Flats monitor on the border of Boulder and Larimer Counties the model is estimating the peak daily maximum 8-hour concentration of 66 ppb. In the immediate Denver metropolitan area the peak observed 8-hour ozone concentrations is 75 ppb at the NREL monitor where the model estimates values in the 55-60 ppb range. The other Denver monitors have lower observed 8-hour ozone concentrations (58-68 ppb) that agree somewhat with the predictions (45-60 ppb). However, the model appears to estimate a higher level of suppression of ozone in downtown Denver (68 ppb observed vs. < 50 ppb predicted) that is likely due to NOx suppression of ozone formation that could be due to insufficient mixing, understated VOC emissions, overstated NOx emissions, understated photolysis rates (e.g., overstated clouds), and/or other factors.

<u>June 26, 2002</u>: The peak observed 8-hour ozone concentration on June 26, 2002 was 81 ppb in Weld County where ~ 55 ppb was estimated. The maximum observed 8-hour ozone concentrations in the Denver area was 79 ppb south of Denver at the Chatfield monitor. At this location the model estimates values in the 60-65 ppb. The peak estimated 8-hour ozone concentration on this day was 70 ppb and occurs to the west-southwest of the Chatfield monitor. Elevated (65-70 ppb) daily maximum 8-hour ozone concentrations are estimated to occur to the southwest, west and northwest of the DMA that is supported by high observed values at the monitors around the DMA. Again, the model is overstating the effects of the local suppression of ozone due to NOx emissions in the downtown Denver area that may be due, in part, to some the same reasons discussed for the previous day.

June 27, 2002: On June 27, 2002, the spatial displacement of the estimated elevated 8-hour ozone concentrations from the Denver area is not as great as on the previous days and





consequently better model performance is estimated. The maximum observed 8-hour ozone concentrations in the Denver area (76 ppb at Chatfield) is underestimated by the model (55-60 ppb). However, the high observed values at Boulder (74 ppb) and NREL (72 ppb) are reproduced fairly well (60-70 ppb). The peak estimated 8-hour ozone concentration on June 27th is 71 ppb and occurs between the NREL (72 ppb) and Boulder (74 ppb) monitors. The observed elevated 8-hour ozone concentrations at sites away from the DMA, such as 69 ppb in Fort Collins and 74 ppb in Colorado Springs, indicate a regional ozone buildup on this day that is not reproduced by the model.

<u>June 28, 2002</u>: A peak observed 8-hour ozone concentration of 83 ppb occurs at the Chatfield monitor south of Denver on this day. The model also estimates elevated ozone concentrations south of Denver with a value of 73 ppb adjacent to and immediately south of the Chatfield monitor. The ozone suppression area within the downtown Denver areas appears to be overstated by the model, which likely accounts for the spatial displacement of the estimated peaks occurring further downwind (i.e. away from DMA) than observed.

June 29, 2002: On June 29 a peak observed 8-hour ozone concentrations of 90 ppb occurred at the Rocky Flats monitoring site where values of 65-70 ppb are estimated. Immediately adjacent to the 90 ppb observed value at Rocky Flats is a 78 ppb observed value at the Boulder monitor. The model will have difficulty estimating this 12 ppb gradient that occurs so close together. North of the Rocky Flats monitor the estimated 8-hour ozone concentrations of 75 ppb occur. In general, the model is estimating the magnitude of the observed 8-hour ozone concentrations on this day much better than on many of the previous days. The ozone "hole" over metropolitan Denver is not as pronounced and there is better agreement with the downtown observed 8-hour ozone concentrations.

<u>June 30, 2002</u>: On June 30, 2002, the model estimates a cloud of elevated (75-85 ppb) 8-hour ozone concentrations with a southeast to northwest orientation just west of Denver. The observations support the occurrence of such an elevated cloud with observed values of 76, 70, 81, 89 and 81 ppb oriented along the same southeast to northwest axis. However, the estimated ozone cloud occurs a couple grid cells further west than observed. Thus, at the location of the observed peak (89 ppb at Rocky Flats) the model estimates values in the 65-70 ppb range, whereas further west values as high as 75 occur. However, the model exhibits good agreement with the observed values at the Chatfield (78 ppb) and NREL (81 ppb) monitors. In addition, the model agrees with the observations that the highest 8-hour ozone concentrations on this day occur at the Rocky Mountain National Park monitor (94 ppb), just the modeled peaks are \sim 15 ppb lower than observed. The local ozone suppression in the downtown Denver area estimated by the model (55-65 ppb) appears to be overstated based on the observed values (68-72 ppb).

<u>July 1, 2002</u>: The model estimates the highest 8-hour ozone concentrations of the June 2002 episode on this day with a peak of 90 ppb occurring immediately to the southwest of the NREL monitor where 91 ppb was observed. Elevated estimated ozone in excess of 80 ppb occurs west of Denver that occurs close to the high values at Chatfield (95 ppb), NREL (91 ppb) and Rock Flats/Boulder (89/71 ppb).





Statistical 8-Hour Ozone Model Performance Evaluation

As noted in Chapter 2, the EPA draft 8-hour ozone guidance has developed model performance goals for 8-hour ozone concentrations (EPA, 1999). These performance goals compare observed daily maximum 8-hour ozone concentrations with estimated values "near the monitor". As discussed in Section 2, we have developed three approaches for defining "near the monitor". For two of the approaches we define "near" as the same NX by NY array of cells centered on the monitor as used in EPA's 8-hour ozone attainment test (e.g., 7 x 7 for 5 km grid) and the two tests differ in only which estimated value is selected from this array of cells. For the third test, we select the estimated value at the monitor.

<u>Maximum</u>: Select the maximum estimated daily maximum 8-hour ozone concentration near the ozone monitor for each day. This is the same approach used in EPA's 8-hour ozone attainment test.

Best Fit: Select the estimated 8-hour ozone concentrations near the monitor that matches the observed value best.

Spatially Paired: Select the estimated 8-hour ozone concentrations at the monitoring location.

As noted previously, the Spatially Paired comparison of predicted and observed daily maximum ozone concentrations is an overly strict interpretation of the EPA draft guidance "near the monitor", but it does represent a particularly stringent test of model performance so is included in our analysis.

Run10a Estimated Maximum 8-Hour Ozone Concentration Near the Monitor Compared with EPA's <" 20% Performance Goal

Figure 3-1 displays a scatter plot and quantile - quantile plot of the predicted and observed daily maximum 8-hour ozone concentrations for the June 25 through July 1, 2002 Denver episode using the <u>maximum</u> estimated 8-hour ozone concentration near the monitor. Of the 85 predicted and observed 8-hour ozone concentrations pairs in the greater Denver area, 96% of the monitor-days lie within EPA's <" 20% performance goal. The three monitor-days that lie outside of EPA's <" 20% performance goal are as follows:

- Weld County on June 26, 2002 where the observed 81 ppb is underestimated by the model by -29% (57 ppb). As seen in Appendix A, there is an elevated ozone cloud west of the Weld County monitor where the observed values at the Rocky Mountain National Park and Fort Collins monitors achieving the EPA performance goal (-17% and -14%, respectively). As noted previously, the model is failing to account for a regional ozone buildup on this day, which is reflected by the underprediction tendency at the monitors away from the DMA.
- El Paso County (Colorado Springs) on June 28, 2002 where the observed value (74 ppb) is underestimated by -23% (57 ppb). As shown in Appendix C, there is an elevated cloud of ozone concentrations between Fort Collins and the DMA that appears





to be too low. Again, increases in the regional ozone background would improve performance in Fort Collins on this day.

• Boulder on July 1, 2002 where the observed value (71 ppb) is overestimated by 24% (89 ppb) using the maximum estimated 8-hour ozone concentration near the monitor. Again, by looking in Appendix C the actual estimated 8-hour ozone concentration at the Boulder monitor is 80 ppb, an 11% overprediction tendency that achieves EPA's performance goal.

In conclusion, using the maximum estimated 8-hour ozone concentrations near the monitor the Run10a base case simulation achieves EPA's performance goal of within < 20% at over 95% of the monitor-days during the June 2002 episode so therefore satisfies EPA's performance test of "~20% most monitors" (EPA, 1999).



Figure 3-1. Estimated and observed daily maximum 8-hour ozone concentrations in the Denver Metropolitan Area and vicinity using the <u>maximum</u> estimated 8-hour ozone concentration near the monitor for the June 2002 episode and the Run10a base case simulation (with updated BCs, no PBLpatch and with wildfires).





Run10a Estimated Best Fit 8-Hour Ozone Concentration Near the Monitor Compared with EPA's <" 20% Performance Goal

Figure 3-2 displays a scatter plot and quantile-quantile plot of the estimated and observed daily maximum 8-hour ozone concentrations using the <u>best fit</u> estimated value near the monitor. The model estimates daily maximum 8-hour ozone concentrations that match the observed value within EPA's <" 20% performance goal near the monitor at 98% of the monitor-days. The two monitor-days that fall outside of the <" 20% performance goal are the June 26, 2002 Weld County and June 28, 2002 El Paso County (Fort Collins) events discussed above. Thus, at all monitors in the DMA proper, EPA's 8-hour performance goal is being met. Thus, again using the best fit estimated ozone near the monitor the Run10a base case simulation achieves EPA's 8-hour ozone performance goal.



Figure 3-2. Estimated and observed daily maximum 8-hour ozone concentrations in the Denver Metropolitan Area and vicinity using the <u>best fit</u> estimated 8-hour ozone concentration near the monitor for the June 2002 episode and the Run10a base case simulation (with updated BCs, no PBLpatch and with wildfires).





Run10a Estimated Spatial Paired 8-Hour Ozone Comparisons

Figure 3-3 displays scatter plot and quantile-quantile plot of the estimated and observed daily maximum 8-hour ozone concentrations that are <u>spatially paired</u> at the monitor. Although EPA's "near the monitor" <" 20% performance goal does not apply for the spatially paired performance metric, it is useful to make the comparison for a more stringent test of model performance. The underestimation tendency of the estimated daily maximum 80-hour ozone concentrations at the locations of the ozone monitors that are apparent in the spatial maps comparisons (Appendix C) are also seen in Figure 3-3. At most monitor-days the model daily maximum 8-hour ozone estimates are below the observed values. As noted above, this is due to a spatial displacement of the estimated ozone plume further from the Denver urban core than observed. Even with this most stringent definition of "near the monitor", over half (~60%) of the monitor-days achieve EPA's <" 20% performance goal.



Figure 3-3. Estimated and observed daily maximum 8-hour ozone concentrations in the Denver Metropolitan Area and vicinity using the <u>spatially paired</u> estimated 8-hour ozone concentration near the monitor for the June 2002 episode and the Run10a base case simulation (with updated BCs, no PBLpatch and with wildfires).





Daily 8-Hour Ozone Model Performance Statistics

Tables 3-2, 3-3 and 3-4 display the daily average normalized and fractional bias and gross error model performance evaluation statistical measures (Tesche et. al., 2003a) for daily maximum 8-hour ozone concentrations from the Run10a base case simulation and the June 25 through July 1, 2002 Denver 8-hour ozone episode using the maximum, best fit and spatially paired definition of "near the monitor", respectively. The EPA draft 8-hour ozone guidance (EPA, 1999) has adopted the same model performance goals for hourly ozone bias and gross error as in the 1-hour guidance (EPA, 1991)

- Bias <" 15%
- Gross Error <" 35%

Note that the adoption of the hourly ozone performance goals for daily maximum 8-hour ozone concentrations is actually inconsistent because one includes the diurnal and spatial variations in ozone (hourly), whereas the others just includes the spatial variations (daily maximum 8-hour). This makes the EPA performance goals for daily maximum 8-hour ozone a more stringent test. It is unclear in EPA's draft 8-hour ozone guidance whether they intended this test to be more stringent than the 1-hour ozone performance goals. Thus, below we calculate the 8-hour ozone bias and gross error performance measures two ways, for daily maximum 8-hour ozone concentrations using the three definitions of near the monitor discussed previously and for running 8-hour ozone concentrations using just the spatially paired predicted and observed values, that is similar to the hourly ozone performance statistical measures.

Summary Daily Maximum 8-Hour Ozone Modeling Performance

When using the <u>maximum</u> estimated daily maximum 8-hour ozone concentration (Table 3-2), the normalized bias and normalized gross error achieves the two performance goals, although on June 26^{th} the normalized bias (-14%) comes close to the performance goal (<" 15%). The fractional bias and gross error achieves EPA's performance goals on all days except June 26, 2002 when the <" 15% performance goal is barely exceeded (-15.2%)

When using the <u>best fit</u> estimated daily maximum 8-hour ozone comparison (Table 3-3), EPA's bias and error performance goals are achieved on all days except for the fractional bias on June 26^{th} where the <" 15% performance goal is barely exceeded (-15.4%).

When examining the <u>spatially paired</u> daily maximum 8-hour performance comparisons, the spatial alignment performance problems identified in the spatial maps comparisons (Appendix C) are also clearly present in the performance statistics. Although the normalized and fractional gross error achieves the EPA <35% performance goal on all days, the normalized and fractional bias indicate an underprediction tendency that is greater than -15% on all days except June 30 and July 1.





Date	Avg Obs	Avg Pred	Norm Bias	Fract Bias	Norm Error	Fract Error
EPA Goal			<i>_</i> "15%	<i>"</i> 15%	_، 35%	_, 35%
June 25	66.84	62.15	-6.32	-6.78	7.27	7.72
June 26	73.62	63.19	-13.86	-15.19	14.37	15.69
June 27	71.15	66.68	-5.45	-6.30	9.92	10.57
June 28	70.47	65.74	-6.23	-6.75	8.70	9.14
June 29	73.53	69.75	-4.57	-4.99	6.88	7.24
June 30	76.37	72.29	-4.73	-5.08	6.21	6.53
July 1	79.74	83.57	5.59	4.95	9.16	8.62

Table 3-2. Daily maximum 8-hour ozone model performance for the June 2002 episode and the Run10a base case simulation using the maximum estimated value near the monitor.

Table 3-3.	Daily maximum 8-hour ozone model performance for the June 2002 episode and the
Run10a ba	se case simulation using the best fit estimated value near the monitor.

Date	Avg Obs	Avg Pred	Norm Bias	Fract Bias	Norm Error	Fract Error
EPA Goal			_ِ "15%	_، "15%	_. 35%	_, 35%
June 25	66.84	61.86	-6.82	-7.28	6.82	7.28
June 26	73.62	63.03	-14.11	-15.43	14.12	15.44
June 27	71.15	65.24	-7.71	-8.46	7.76	8.51
June 28	70.47	64.96	-7.46	-7.94	7.48	7.96
June 29	73.53	68.93	-5.77	-6.17	5.83	6.23
June 30	76.37	71.79	-5.45	-5.78	5.51	5.85
July 1	79.74	78.25	-1.72	-1.77	1.91	1.96

Table 3-4.	Daily ma	aximum 8-ł	nour ozon	e model	perform	ance for	the June	2002 epis	sode and the
Run10a ba	ise case s	simulation	using the	<u>spatially</u>	paired e	estimated	d value n	ear the mo	onitor.

Date	Avg Obs	Avg Pred	Norm Bias	Fract Bias	Norm Error	Fract Error
EPA Goal			_ِ "15%	_، "15%	_. 35%	_. 35%
June 25	66.84	55.72	-15.98	-17.80	15.98	17.80
June 26	73.62	54.68	-25.57	-29.78	25.57	29.78
June 27	71.15	58.41	-17.43	-19.55	17.43	19.55
June 28	70.47	58.57	-16.47	-18.29	16.47	18.29
June 29	73.53	61.77	-15.66	-17.18	15.66	17.18
June 30	76.37	65.34	-13.97	-15.36	14.03	15.42
July 1	79.74	71.05	-10.08	-11.37	12.88	14.05

Summary of Running 8-Hour Ozone Model Performance

Table 3-5 displays the daily model performance statistics for bias and gross error and the Run10a base case using running 8-hour ozone concentrations that are <u>spatially paired</u>. The average observed and predicted values in Table 3-5 are for all spatially paired predicted and observed 8-hour running averages in the Denver area, whereas the bias and gross error performance statistics are just for those pairs in which the observed value exceeds a 40 ppb threshold. EPA's bias and gross error performance goals are met on 4 of the 7 episode days





during the June 2002 episode. The underestimation tendency on June 26-28 results in both the normalized and fractional bias not meeting the <" 15% performance goal, although the gross error performance goal of < 35% is met on all days.

Date	Avg Obs	Avg Pred	Norm Bias	Fract Bias	Norm Error	Fract Error
EPA Goal			_ِ "15%	₂ "15%	_، 35%	_, 35%
June 25	44.3	42.0	-10.3	-12.5	16.9	18.3
June 26	37.3	47.6	-24.1	-30.9	28.9	35.1
June 27	41.0	50.3	-20.2	-24.4	21.4	35.5
June 28	40.7	48.3	-18.3	-21.9	-20.5	-23.9
June 29	46.1	48.0	-10.0	-11.9	15.3	16.7
June 30	47.3	51.5	-12.3	-14.4	15.8	17.6
July 1	49.2	54.5	-12.1	-14.2	15.9	17.8

Table 3-5. Running 8-hour ozone model performance for the June 2002 episode and the Run10a base case simulation using the <u>spatially paired</u> predictions and observations.

Scatter Plots and Time Series Comparisons

Time series of predicted and observed hourly and 8-hour average ozone concentrations are shown in Appendices E and F, respectively. The model does a good job in reproducing the diurnal variations in the hourly and 8-hour ozone concentrations. However, the peak 1-hour and N-hour ozone concentrations are underestimated by the model, which is partly due to the spatial displacement of the estimated ozone peaks further away from the DMA than observed.

Figures 3-4 and 3-5 display scatter plots of spatially and temporally paired predicted and observed hourly and 8-hour ozone concentrations at monitors in the DMA and vicinity. The predictions and observations span a wide range of ozone concentrations, with the observed ozone peaks underestimated due to the spatial displacement discussed previously. The model estimated 1-hour and 8-hour ozone concentrations are well corrected with the observations (R2²>0.5).













DENVER JULY 2002 8-HOUR OZONE EPISODE

Appendix D compares spatial maps of predicted and observed daily maximum 8-hour ozone concentrations for the July 18-21, 2002 Denver ozone episode.

<u>July 18, 2002</u>: The maximum observed 8-hour ozone concentration on July 18, 2002 is 82 ppb at the NREL monitor immediately west of the Denver urban core. The maximum estimated value is 73 ppb to the southwest of Denver (Appendix D). Both the NREL (82 ppb) and Rocky Flats (78 ppb) monitors indicate elevated ozone should be further west and north than estimated. The local ozone suppression in the downtown Denver area is overstated by the model (< 50 ppb) compared to the observations (64-70 ppb).

<u>July 19, 2002</u>: On July 19, 2002 the model again estimates that the estimated elevated ozone cloud is displaced from the monitoring network to the southwest. The elevated observed values to the northwest of the city at Rocky Flats (93 ppb) and Boulder (87 ppb) are





underestimated by the model (55-65 ppb). As are the observed values at the NREL monitor (92 ppb observed vs. 55-65 ppb estimated) and Chatfield monitor (89 ppb observed \sim 70 ppb estimated) monitors. The ozone suppression in the Denver area is greatly overstated on this day with estimated values of < 50 ppb occurring where 84 ppb ozone is observed.

<u>July 20, 2002</u>: The model greatly underestimated the observed 8-hour ozone concentrations on this day. A peak value of only 69 ppb is estimated to the south of an 83 ppb value observed at Chatfield. At the NREL monitor, where a 92 ppb 8-hour ozone value is observed, the estimated values are only in the 55-65 ppb range. Again, this is partly due to overstating the suppression of ozone in the Denver area with estimated values of < 50 ppb occurring where an 84 ppb is observed.

<u>July 21, 2002</u>: Slightly better model performance is seen on July 21 compared to the previous days with an elevated cloud of 8-hour ozone concentrations of 65-70 ppb estimated immediately southwest of Denver where observed values of 81, 66 and 79 ppb occur. Ozone appears to be underestimated by 5-15 ppb across the network on this day.

Statistical 8-Hour Ozone Model Performance Evaluation

The daily maximum 8-hour ozone model performance for the July 2002 episode and Run 10a are examined using the same maximum, best fit and spatially paired approach as used for the June 2002 episode (Figure 3-6, 3-7, and 3-8).

Using the <u>maximum</u> estimated value near the monitor, the estimated daily maximum 8-hour ozone values fall mostly below the observed values. Of the 48 predicted and observed daily maximum 8-hour ozone pairs, two-thirds fall within EPA's < 20% performance goal. The quantile-quantile plot indicates a 20% underestimation tendency on the upper end of the estimated and observed frequency distribution.

The results for the <u>best fit</u> comparison of estimated and observed daily maximum ozone concentrations near the monitor is similar as seen for the maximum comparisons. 67% of the monitor-days achieve the <" 20% performance goal, although almost all have an underestimation tendency.

Comparison of the <u>spatially paired</u> estimated and observed daily maximum ozone concentrations confirm that the model has both a spatial alignment and magnitude problem in 8-hour ozone predictions for this episode. Of the 48 valid monitor-day daily maximum 8-hour ozone concentrations, only 11 monitor days (23%) achieve the < "20% performance goal.






Figure 3-6. Estimated and observed daily maximum 8-hour ozone concentrations in the Denver Metropolitan Area and vicinity using the <u>maximum</u> estimated 8-hour ozone concentration near the monitor for the July 2002 episode and the Run10a base case simulation (with updated BCs, no PBLpatch and with wildfires).







Figure 3-7. Estimated and observed daily maximum 8-hour ozone concentrations in the Denver Metropolitan Area and vicinity using the <u>best fit</u> estimated 8-hour ozone concentration near the monitor for the July 2002 episode and the Run10a base case simulation (with updated BCs, no PBLpatch and with wildfires).







Figure 3-8. Estimated and observed daily maximum 8-hour ozone concentrations in the Denver Metropolitan Area and vicinity using the <u>spatially paired</u> estimated 8-hour ozone concentration near the monitor for the July 2002 episode and the Run10a base case simulation (with updated BCs, no PBLpatch and with wildfires).





4.0 CONCLUSIONS

UPDATES TO BASE CASE SIMULATIONS

Based on a preliminary model performance evaluation (Morris and Mansell, 2003), four short-term activities were identified that may improve model performance:

- (1) Update the VOC boundary conditions in the north over land areas of the US to be more representative of continental air mass;
- (2) Impose a minimum nighttime mixing height of 100 m AGL and a minimum afternoon maximum mixing height of 1,500 m AGL to limit MM5 nighttime minimum and daytime cloud induced limited mixing artifacts.
- (3) Add wildfire emissions to the modeling database.
- (4) Add a placeholder VOC emissions inventory to account for missing VOC emissions suspected to be from oil and gas operations as reported by Katzenstein and co-workers (2003) that occur in Texas/Oklahoma/Kansas and eastern Colorado and New Mexico.

The northern boundary VOC boundary conditions below the afternoon mixing heights were increased from approximately 22 ppbC to 50 ppbC to account for presence of enhanced VOC emissions due primarily to biogenic emission. The major increase in the BCs is in isoprene concentrations that increase from 0.1 to 3.6 ppb (0.5 to 18 ppbC) to account for higher biogenic emissions in this region. It should be noted that there were no increases in formaldehyde (HCHO) boundary conditions due to this change. The increases in the northern VOC boundary conditions had little affect on ozone concentrations in the DMA. This update to the base case simulation is believed to be more technically credible and consistent with other ozone SIP modeling so was retained in the base case configuration.

The implementation of a patch to the MM5 estimated planetary boundary layer (PBL) depths to eliminate potentially too low nighttime minimum and force a daytime maximum values of 1,500 m AGL did little to improve model performance. As the PBLpatch was somewhat arbitrary and may not be appropriate in all situations, it was dropped from further consideration in our base case configuration.

The addition of wildfires to the base case simulation resulted in slight increases in ozone concentrations in the DMA. As wildfires were present during the Summer '02 episode, accounting for emissions from wildfires was deemed more technically correct, so they were retained in our base case.

The results from Katzenstein and co-workers study that suggest there are large levels of VOC emissions that were suspected to be due to oil and gas operations primarily from the Texas, Oklahoma and Kansas areas, but also eastern New Mexico and Colorado. Current work is ongoing in other studies to provide a preliminary characterization of these emissions to



develop a "place holder" inventory. Although such missing VOC emissions may explain or at least reduce the underestimation tendency in the Denver Summer '02 episode modeling, the Denver 8-hour ozone EAC schedule precludes their incorporation into the study. The schedule constraints, and the fact that such emissions are likely better characterized in Weld County, Colorado based on the information provided by COGA, requires us to defer this update until resources are available.

MODEL PERFORMANCE CONCLUSIONS

The general tendency of the Run10 base case model configuration simulation of the Summer '02 period is to underestimate the observed ozone concentrations. This underestimation is more pronounced for the July 2002 episode than the June 2002 episode.

For the June 2002 episode, the Run10a base case simulation estimated daily maximum 8-hour ozone concentrations that achieved EPA's performance goal of < 20% at over 95% of the ozone monitor-days. The two monitor-days that did not achieve this performance goal occur outside of the DMA (Weld County and Fort Collins). The statistical model performance measures for ozone using the maximum and best fit comparisons mostly achieve EPA's performance goals for the June 2002 episode. However, it is our conclusion that the model is working well enough for the June 2002 episode that if used with appropriate interpretation and caution can provide valuable control strategy evaluation information that, when used with other information, can aid in determining whether a selected control plan would achieve attainment of the 8-hour ozone standard in 2007.

For the July 2002 episode we have less confidence in the results. Whereas the June 2002 episode exhibited estimated elevated ozone concentrations of similar magnitude (i.e., within "20%) of the observed daily maximum 8-hour ozone concentrations at all the key ozone monitors in the DMA, the same is not true for the July 2002 episode. Several of the key DMA monitor-days exhibiting underpredictions that exceed EPA's <" 20% performance goal.

Thus, at this time we recommend proceeding with the 2007 attainment demonstration modeling with the June 2002 episode, but use the July 2002 episode only for corroborative analysis.





5.0 REFERENCES

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Appendix A

Estimated and Observed Daily Maximum 8-Hour Ozone Concentrations (ppb) for the 36/12/4 km Run9a Base Case CAMx Simulation (With Updated North VOC BCs, and Patched Minimum PBL Heights) June 25 – July 1, 2002 Episode



CAMx Daily Maximum 8hr O3 June25, 2002 36/12/4 Denver Base Case with Gridded Emissions Update. Run 8a



CAMx Daily Maximum 8hr O3 June26, 2002 36/12/4 Denver Base Case with Gridded Emissions Update. Run 8a



CAMx Daily Maximum 8hr O3 June27, 2002 36/12/4 Denver Base Case with Gridded Emissions Update. Run 8a



CAMx Daily Maximum 8hr O3 June28, 2002 36/12/4 Denver Base Case with Gridded Emissions Update. Run 8a



CAMx Daily Maximum 8hr O3 June29, 2002 36/12/4 Denver Base Case with Gridded Emissions Update. Run 8a



CAMx Daily Maximum 8hr O3 June30, 2002 36/12/4 Denver Base Case with Gridded Emissions Update. Run 8a



CAMx Daily Maximum 8hr O3 July01, 2002 36/12/4 Denver Base Case with Gridded Emissions Update. Run 8a

Appendix B

Estimated and Observed Daily Maximum 8-Hour Ozone Concentrations (ppb) for the 36/12/4 km Run9a Base Case CAMx Simulation (With Updated Northern VOC BCs, Patched Minimum PBL Heights and Wildfires) June 25 – July 1, 2002 Episode



CAMx Daily Maximum 8hr O3 June25, 2002 36/12/4 Denver Base Case with Fire Emissions. Run 9a



CAMx Daily Maximum 8hr O3 June26, 2002 36/12/4 Denver Base Case with Fire Emissions. Run 9a



CAMx Daily Maximum 8hr O3 June27, 2002 36/12/4 Denver Base Case with Fire Emissions. Run 9a



CAMx Daily Maximum 8hr O3 June28, 2002 36/12/4 Denver Base Case with Fire Emissions. Run 9a



CAMx Daily Maximum 8hr O3 June29, 2002 36/12/4 Denver Base Case with Fire Emissions. Run 9a



CAMx Daily Maximum 8hr O3 June30, 2002 36/12/4 Denver Base Case with Fire Emissions. Run 9a



CAMx Daily Maximum 8hr O3 July01, 2002 36/12/4 Denver Base Case with Fire Emissions. Run 9a

Appendix C

Estimated and Observed Daily Maximum 8-Hour Ozone Concentrations (ppb) for the 36/12/4 km Run10a Base Case CAMx Simulation (With Updated Northern VOC BCs and Wildfires) June 25 – July 1, 2002 Episode



CAMx Daily Maximum 8hr O3 June25, 2002 36/12/4 Denver Base Case Run 10a



CAMx Daily Maximum 8hr O3 June26, 2002 36/12/4 Denver Base Case Run 10a



CAMx Daily Maximum 8hr O3 June27, 2002 36/12/4 Denver Base Case Run 10a



CAMx Daily Maximum 8hr O3 June28, 2002 36/12/4 Denver Base Case Run 10a



CAMx Daily Maximum 8hr O3 June29, 2002 36/12/4 Denver Base Case Run 10a



CAMx Daily Maximum 8hr O3 June30, 2002 36/12/4 Denver Base Case Run 10a



CAMx Daily Maximum 8hr O3 July01, 2002 36/12/4 Denver Base Case Run 10a

Appendix D

Estimated and Observed Daily Maximum 8-Hour Ozone Concentrations (ppb) for the 36/12/4 km Run10a Base Case CAMx Simulation (With Updated Northern VOC BCs and Wildfires) July 18 – July 21, 2002 Episode



CAMx Daily Maximum 8hr O3 July18, 2002 36/12/4 Denver Base Case Run 10b



CAMx Daily Maximum 8hr O3 July19, 2002 36/12/4 Denver Base Case Run 10b



CAMx Daily Maximum 8hr O3 July20, 2002 36/12/4 Denver Base Case Run 10b



CAMx Daily Maximum 8hr O3 July21, 2002 36/12/4 Denver Base Case Run 10b
Appendix E

Time Series of Estimated and Observed Hourly Ozone Concentrations (ppb) for the 36/12/4 km Run2 and Run10a Base Case CAMx Simulation June 25 – July 1, 2002 Episode









-693.570 21.623

80590006: Jefferson









Appendix F

Time Series of Estimated and Observed 8-Hour Ozone Concentrations (ppb) for the 36/12/4 km Run2 and Run10a Base Case CAMx Simulation June 25 – July 1, 2002 Episode



Denver Base Case run2 and run10a 8hr Ozone 04km





Denver Base Case run2 and run10a 8hr Ozone 04km

