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Implementation of the Piecewise Parabolic Method for Vertical Advection in Comprehensive Air Quality Model with Extensions (CAMx)

Final Report

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LIST OF ACRONYMS AND ABBREVIATIONS

3-D	Three-dimensional
ACM2	Asymmetric Convective Mixing, version 2
AM	Ante-meridian
AMET	Atmospheric Model Evaluation Tool
AQS	Air Quality System
BC	Boundary conditions
CAMx	Comprehensive Air quality Model with extensions
CB6r5	Carbon Bond version 6, release 5
CHS	CAMx hybrid scheme
CPA	Chemical Process Analsyis
CST	Central Standard Time
DDM	Decoupled Direct Method of sensitivity analysis
EBI	Euler Backward Iterative solver
EPA	Environmental Protection Agency
GEOS-Chem	Goddard Earth Observing System Chemical global model
GHz	Gigahertz
HCHO	Formaldehyde
IC	Initial conditions
IofA	Index of Agreement
IPR	Integrated Process Rates
IRR	Integrated Reaction Rates
Ix	Inorganic iodine
km	Kilometer
m	Meter
Mn-M	Mean modeled
Mn-O	Mean observation
MDA8	Maximum Daily Average 8-hour
MPI	Message Passing Interface
NMB	Normalized mean bias
NME	Normalized mean error (unsigned, or gross)
NO	Nitric oxide
NO_2	Nitrogen dioxide
NO_3	Nitrate radical
NOx	Nitrogen oxides
NOAA	National Oceanic and Atmospheric Administration
O_3	Ozone
O&G	Oil and gas
OH	Hydroxyl radical
OMP	Open Multi-Processing
OSAT	Ozone Source Apportionment Tool
PA	Process Analysis
ppb, ppbv	Parts per billion by volume
PM	Post-meridian
ppm	Parts per million by volume
PPM	Piecewise Parabolic Method
RTRAC	Reactive Tracers
SA	Source Apportionment
SIP	State Implementation Plan
TCEQ	Texas Commission on Environmental Quality
US	United States
UTC	Universal Time Coordinate
VOC	Volatile organic compounds
WRF	Weather Research and Forecasting model

EXECUTIVE SUMMARY

The Texas Commission on Environmental Quality (TCEQ) has noted that the Comprehensive Air quality Model with extensions (CAMx) tends to over predict stratospheric ozone concentrations at altitudes above 10-12 km with larger vertical gradients than observed. Overstating deep vertical transport can lead to overestimates of stratospheric ozone intrusion into the troposphere and potentially to ground level. Ramboll previously investigated the overprediction of upper-tropospheric ozone by testing increased vertical resolution and an alternative vertical advection scheme called the Piecewise Parabolic Method (PPM). The PPM possesses high-order accuracy and reduces numerical diffusion, thereby improving accuracy. Since PPM offers several benefits with no downside to the original CAMx hybrid scheme (CHS), Ramboll recommended implementing PPM into CAMx permanently as a vertical advection option.

This project involved extended testing of the PPM vertical advection solver for the CAMx core model and its Probing Tools: Source Apportionment (SA), Decoupled Direct Method (DDM), Process Analysis (AP), and Reactive Tracers (RTRAC). Ramboll conducted multiple tests of CAMx using the TCEQ's 2019 modeling platform, ensuring that the Probing Tools perform correctly using PPM and comparing model results and performance between model runs using the original CHS and PPM advection solvers.

CAMx Core Model Results

Ramboll ran CAMx for the month of August using the TCEQ 2019 modeling platform. We compared simulated ozone profiles against available ozonesonde measurements and compared simulated surface ozone patterns against observed concentrations recorded at monitoring sites in the El Paso area. Highlights from core model tests are:

- Model runtimes differed by only 1% using the two advection schemes.
- Simulated vertical ozone profiles were not sensitive to the choice of vertical advection scheme.
- CAMx-predicted vertical ozone profiles on the US west coast were well-replicated, which is most likely reflecting the boundary conditions derived from global modeling.
- CAMx-predicted vertical ozone profiles in Colorado and El Paso exhibited tropospheric under predictions and stratospheric over predictions, the latter of which is likely caused by continued numerical diffusion from the use of thick model layers above ~10 km.
- Use of the Weather Research and Forecasting (WRF) model's hybrid vertical coordinate in the 2019 modeling platform likely mitigated numerical diffusion in the upper layers relative to that previously reported by Ramboll using the 2012 platform.
- Surface hourly ozone differences between the two advection schemes were not large on average, but episodically differed as much as -50 to +10 ppb in complex terrain, with the largest negative differences usually occurring at night and the largest positive differences occurring during the day, both apparently associated with convection and the different treatments of surface boundary conditions used in CHS and PPM.
- Simulated surface ozone exhibited an underprediction bias and poorly correlated agreement with measured ozone at monitoring sites in El Paso and Dona Ana Counties, however ozone performance was not appreciably different using the two advection schemes.

CAMx Probing Tool Results

Ramboll applied the Ozone Source Apportionment Tool (OSAT) using TCEQ's 2019 modeling platform tracking ozone contributions in El Paso from four source areas by two sectors and initial/boundary conditions (IC/BC). The other three Probing Tools were applied using Ramboll's distributed 2016 2-day test case (June 10-11, 2016). Highlights from Probing Tool tests are:

- All Probing Tool results exhibited negligible to minor sensitivity to the choice of vertical advection scheme, with the largest differences occurring mostly during nighttime hours during convective conditions in complex terrain as seen for the core model tests summarized above.
- To complete the 31-day OSAT simulation, the CHS run took an average of 3.7 hours per day, while the PPM run took an average of 3.5 hours per day (almost 6% faster).
- In El Paso, OSAT differences arising from the two advection solvers were relatively small and short-lived. The largest differences were associated with initial/boundary contributions due to their larger ozone contributions, longer transport distances, vertically deeper distribution, and complex terrain features traversed between the boundaries and El Paso.
- Except for IC/BC, Mexico contributed the most to simulated ozone at the El Paso Chamizal monitor, followed by Texas, then other US states and other tracked sources. Model underpredictions render the estimated absolute contributions to be inaccurate but the relative contributions are probably more robust.
- For DDM, both CHS and PPM runs took an average of 1.0 hour per day to complete the 2-day test case simulation. Model runtimes differed by less than 1% using the two advection schemes.
- DDM estimated ozone sensitivity to biogenic emissions. Sensitivity differences arising from PPM vertical advection were largest at night and in areas of complex terrain. These patterns were consistent with the magnitudes, locations and times of differences seen in core model ozone.
- Both CHS and PPM runs took an average of 9 minutes per day (PA) and 10 minutes per day (RTRAC) to complete the 2 day simulation. For both Probing Tools, model runtimes differed to within 1 minute using the two advection schemes.
- We confirmed that the use of the PPM solver properly affects only the vertical advection flux reported by PA; all other fluxes remain the same as the CHS case. PPM resulted in a slight increase in vertical contribution to ozone in the PA test sub-domain during the day and a slight decrease during the night.
- RTRAC simulated reactive plumes of formaldehyde from oil and gas sources across the US. The largest formaldehyde differences arising from PPM vertical advection were negative and occurred at night in complex terrain, where they were relatively on par with negative ozone differences seen at similar hours and in similar terrain.

Recommendations

Based on the results of vertical advection sensitivity analyses, Ramboll recommends the following:

- Use either the PPM vertical advection solver or the original CHS as both yield mostly similar results.
- Continue to use the WRF hybrid vertical layer coordinate, which is the default configuration in current WRF distributions.
- Continue to locate the CAMx model top sufficiently well above features of concern, such as ozone fluxes through the tropopause.

- Consider CAMx tests that utilize every WRF layer without layer collapsing to improve resolution of upper atmospheric dynamics and check results against ozonesonde data over the intermountain west (i.e., Boulder and El Paso).
- Keep track of creatively different advection schemes, such as semi-Lagangian methods, that have the potential to further reduce numerical diffusion.

1.0 INTRODUCTION

The Texas Commission on Environmental Quality (TCEQ) uses the Comprehensive Air quality Model with extensions (CAMx; Ramboll, 2022) for State Implementation Planning (SIP) purposes and continually seeks to improve model fidelity. CAMx has replicated the vertical distribution of observed ozone profiles from the surface to the upper troposphere (10-12 km) but has tended to over predict stratospheric ozone above that altitude with larger vertical gradients than observed. Vertical resolution and inaccuracies in vertical advection are potential causes of excessive numerical diffusion of ozone from top boundary conditions. Overstating vertical transport from top boundary conditions can lead to overestimates of stratospheric ozone intrusion into the troposphere and potentially to ground level.

Ramboll (2020a) investigated the overprediction of upper-tropospheric ozone by testing increased vertical resolution and an alternative vertical advection scheme called the Piecewise Parabolic Method (PPM; Colella and Woodward, 1984). The PPM possesses high-order accuracy and reduces numerical diffusion, thereby improving accuracy in transporting upper tropospheric and lower stratospheric ozone into the mid-troposphere and possibly down to the surface. Ramboll (2020a) recommended implementing PPM into CAMx permanently since it offers several benefits with no downside to the original CAMx hybrid scheme (CHS).

1.1 Project Objectives

This project involved extended testing of the PPM vertical advection solver for the CAMx core model and its Probing Tools: Source Apportionment (SA), Decoupled Direct Method (DDM), Process Analysis (PA), and Reactive Tracers (RTRAC). Ramboll conducted multiple tests of CAMx using the TCEQ’s 2019 modeling platform. We ensured that the Probing Tools perform correctly using PPM and compared model results and performance between model runs using the original CHS and PPM advection solvers.

1.2 Report Organization

This report documents the approach and results from the testing and analyses conducted in this project. Chapter 2 describes the TCEQ 2019 modeling platform and CAMx configuration, presents comparisons of simulated ozone profiles against available ozonesonde datasets, and presents a model performance evaluation for simulated ozone concentrations in the El Paso area using the CHS and PPM vertical advection schemes. Chapter 3 describes Probing Tools tests and summarizes results from each. Chapter 4 presents a summary and recommendations.

2.0 CAMx CORE MODEL TESTING

2.1 Model Configuration

As decided in consultation with TCEQ staff, Ramboll ran CAMx for the month of August 2019 on a two-way nested grid system comprising a North American domain (36 km grid spacing), US domain (12 km grid spacing), and El Paso domain (4 km grid spacing). Figure 2-1 presents the nesting arrangement for these grids, Figure 2-2 shows detail for the El Paso domain, and Figure 2-3 shows the vertical grid structure.

Figure 2-1. Nested grid domains in the TCEQ 2019 modeling platform.

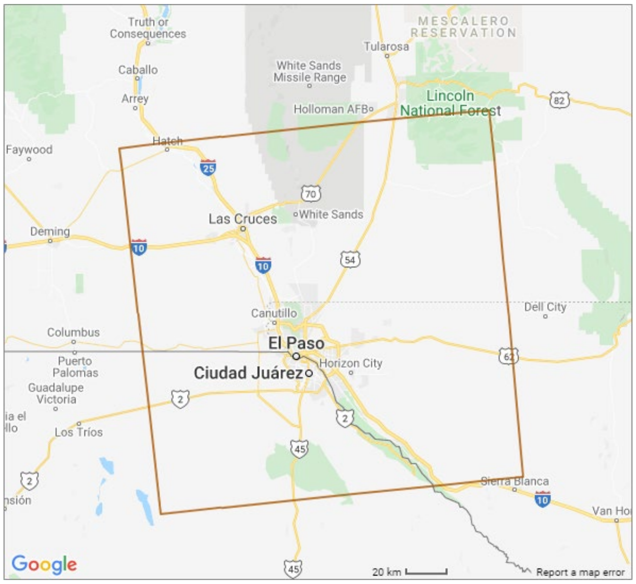
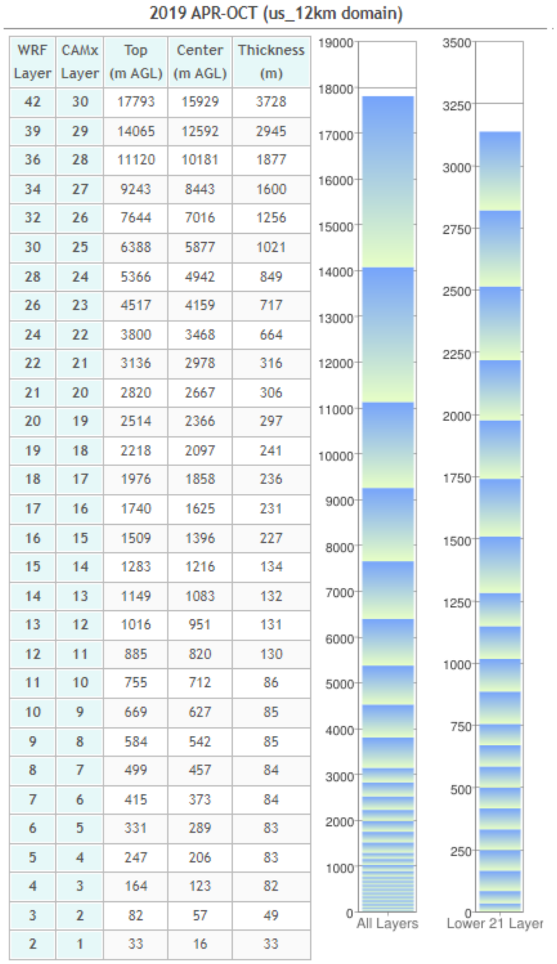


Figure 2-2. Coverage of the El Paso 4 km nested grid in the TCEQ 2019 modeling platform.



2019 APR-OCT (us_12km domain)

WRF Layer	CAMx Layer	Top (m AGL)	Center (m AGL)	Thickness (m)
42	30	17793	15929	3728
39	29	14065	12592	2945
36	28	11120	10181	1877
34	27	9243	8443	1600
32	26	7644	7016	1256
30	25	6388	5877	1021
28	24	5366	4942	849
26	23	4517	4159	717
24	22	3800	3468	664
22	21	3136	2978	316
21	20	2820	2667	306
20	19	2514	2366	297
19	18	2218	2097	241
18	17	1976	1858	236
17	16	1740	1625	231
16	15	1509	1396	227
15	14	1283	1216	134
14	13	1149	1083	132
13	12	1016	951	131
12	11	885	820	130
11	10	755	712	86
10	9	669	627	85
9	8	584	542	85
8	7	499	457	84
7	6	415	373	84
6	5	331	289	83
5	4	247	206	83
4	3	164	123	82
3	2	82	57	49
2	1	33	16	33

Figure 2-3. Vertical grid structure for all CAMx nested grid domains in the TCEQ 2019 modeling platform.

The TCEQ provided the following 2019 modeling platform datasets for this project:

- All CAMx-ready gridded and point anthropogenic, biogenic, and fire emission input files for all grids;
- All CAMx-ready meteorological input files derived using the Weather Research and Forecasting model (WRF; Skamarock et al., 2019) ;
- All CAMx-ready ancillary input files (initial/boundary/top conditions, photolysis rates, ozone column map).

The TCEQ also provided example model configuration files and scripts to facilitate Ramboll's model setup. Table 2-1 lists the CAMx configuration for the tests described in this Section.

Table 2-1. CAMx model configuration for tests using the TCEQ 2019 modeling platform.

Model Options/Settings	CAMx Configuration
Version	v7.20
Date Range	August 1-31, 2019
Time Zone	Central Standard Time (CST)
Map Projection	Lambert Conic Conformal
2-Way Nested Grid System	36/12/4 km (El Paso) horizontal grid resolution, 30 vertical layers up to ~20 km
Horizontal Advection	PPM
Vertical Advection	IMPLICIT and PPM
Gas-Phase Chemistry	CB6r5
Particulate Chemistry	None
Chemistry Solver	EBI
Dry Deposition	WESELY89
Plume-in-Grid	Off
Bi-directional Ammonia	Off
Wet Deposition	On
ACM2 Boundary Layer Diffusion	Off
Surface Chemistry Model	Off
Inline Ix Emissions	On
Super Stepping	On
3-D Output	On (all grids)
Output Species	O_3, NO, NO_2
Parallelization	MPI (8 nodes), OMP (3 threads per node)

We ran CAMx twice: one run employed the original implicit CHS solver (CAMx namelist keyword "IMPLICIT") while the other employed the explicit PPM vertical advection solver (keyword "PPM"). All other inputs and model settings were the same among the two runs.

We compiled the model using the Portland Fortran90 compiler, version 13.4. Both cases were run on a 24-core Intel Xeon X5675 3 GHz server using a combination of Message Passing Interface (MPI) parallelization across 8 cores (1 master and 7 compute nodes) with 3 Open Multi-Processing (OMP) parallelization threads per core. Both runs took an average of 1.6 hours per day to complete the 31-day simulation. Model runtimes differed by only 1% using the two advection schemes.

2.2 Graphical Comparisons for Ozone

Figures 2-4 and 2-5 present spatial plots of average, largest positive, and largest negative differences in 1-hour surface ozone between the CHS and PPM runs over the entire August 2019 modeling period. Results on the US 12 km modeling grid are shown in Figure 2-4 and results on the El Paso 4 km modeling grid are shown in Figure 2-5.

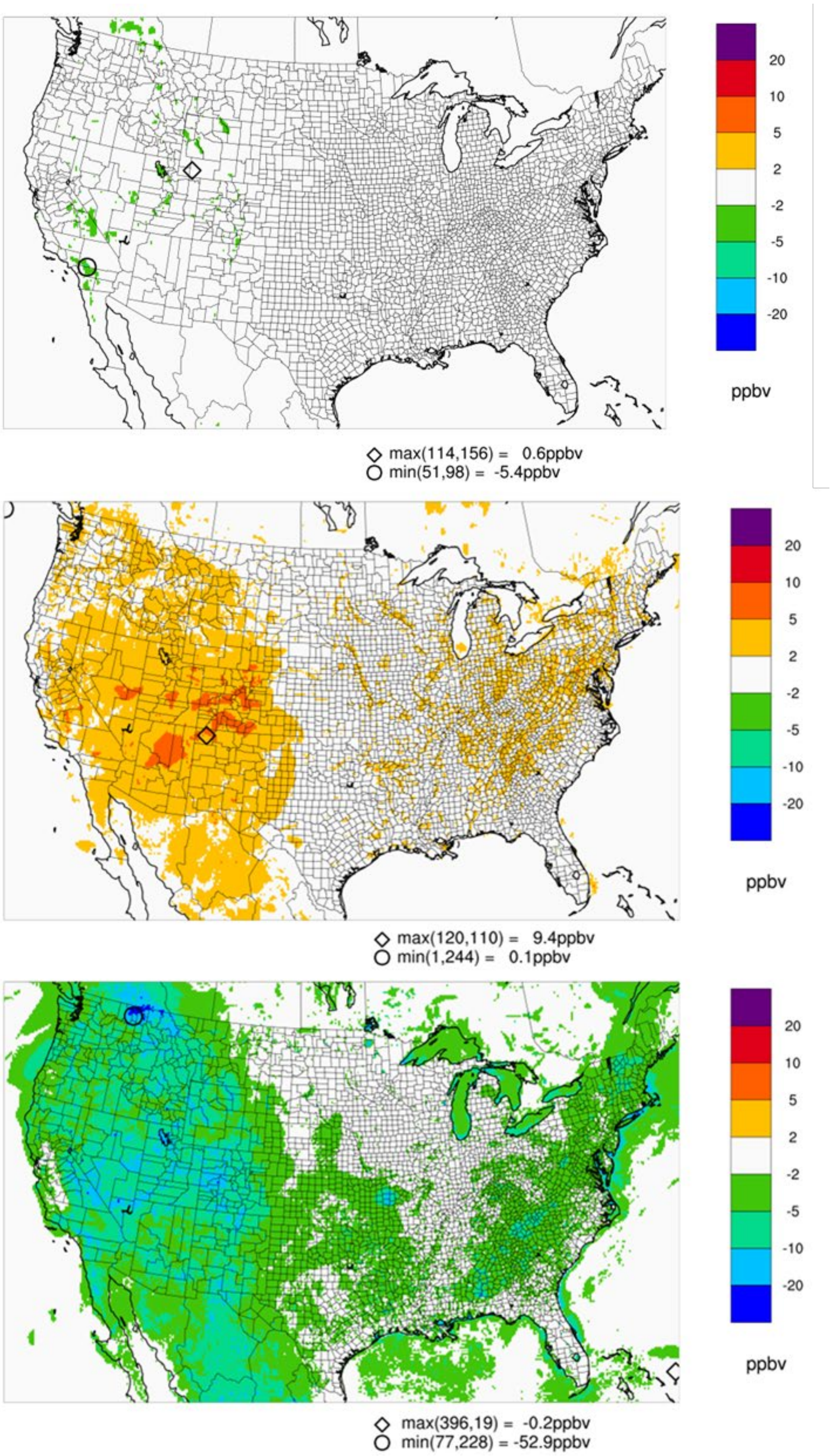


Figure 2-4. **Average (top), minimum (center), and maximum (bottom) 1-hour surface ozone differences between CAMx runs using different vertical advection solvers (PPM minus CHS) over August 2019 across the US 12 km domain.**

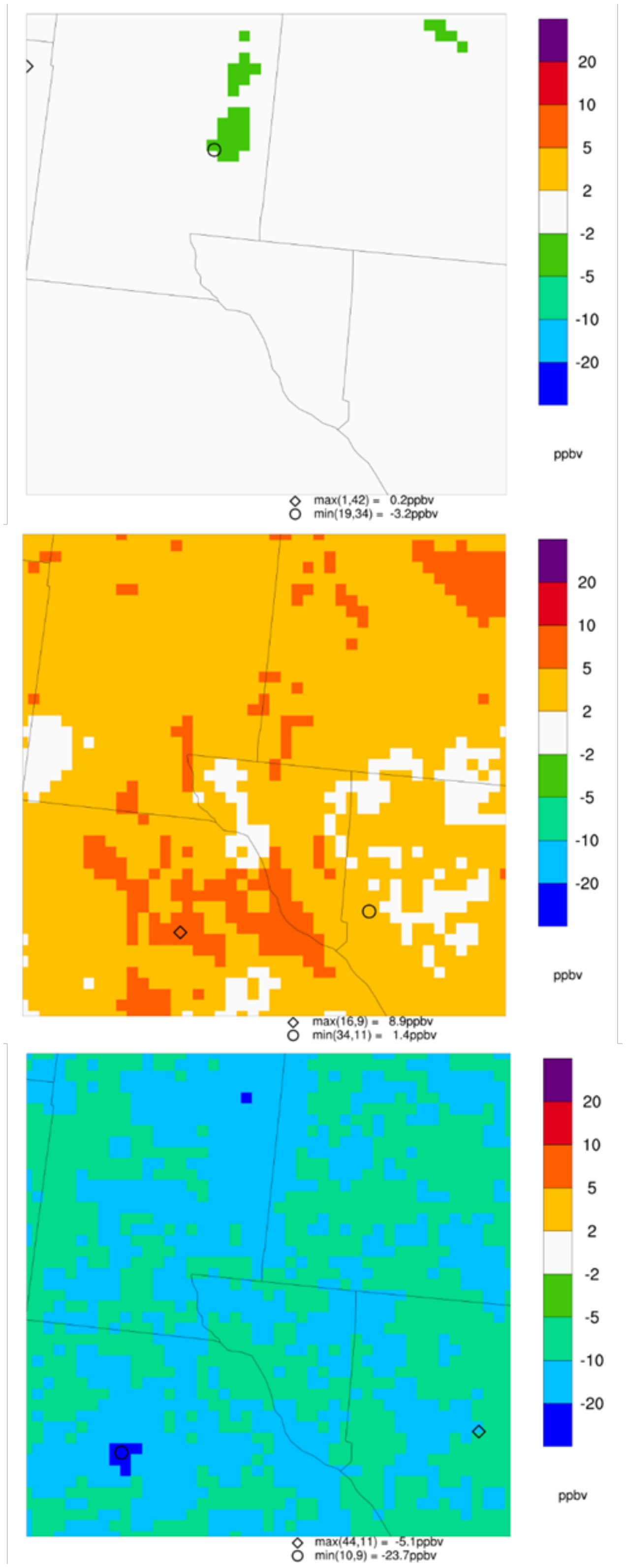


Figure 2-5. Average (top), minimum (center), and maximum (bottom) 1-hour surface ozone differences between CAMx runs using different vertical advection solvers (PPM minus CHS) over August 2019 across the El Paso 4 km domain.

The monthly average 1-hour ozone differences were small, ranging within ±5 ppb on both domains, with the largest average differences occurring in the complex terrain of the western US. However, the range of differences at individual hours was rather substantial (-50 ppb to +10 ppb) and again the largest differences were anchored to complex terrain. The largest negative values consistently exceeded the largest positive values. Animations of surface ozone differences revealed that negative differences tend to occur at night while positive differences occur during the day, while both are related to convective activity (see examples in Figure 2-6). The smaller positive differences are likely moderated by daytime boundary layer mixing, whereas larger negative differences are likely maintained by minimal nighttime mixing. Differences just above the surface layer (not shown) were smaller and more balanced between positive and negative, suggesting an influence from how the two solvers treat the surface boundary condition. PPM has higher-order accuracy than CHS in all layers except at the bottom and top boundaries, where PPM employs a first-order solution (more numerically diffusive) while the CHS employs a second-order solution (less numerically diffusive).

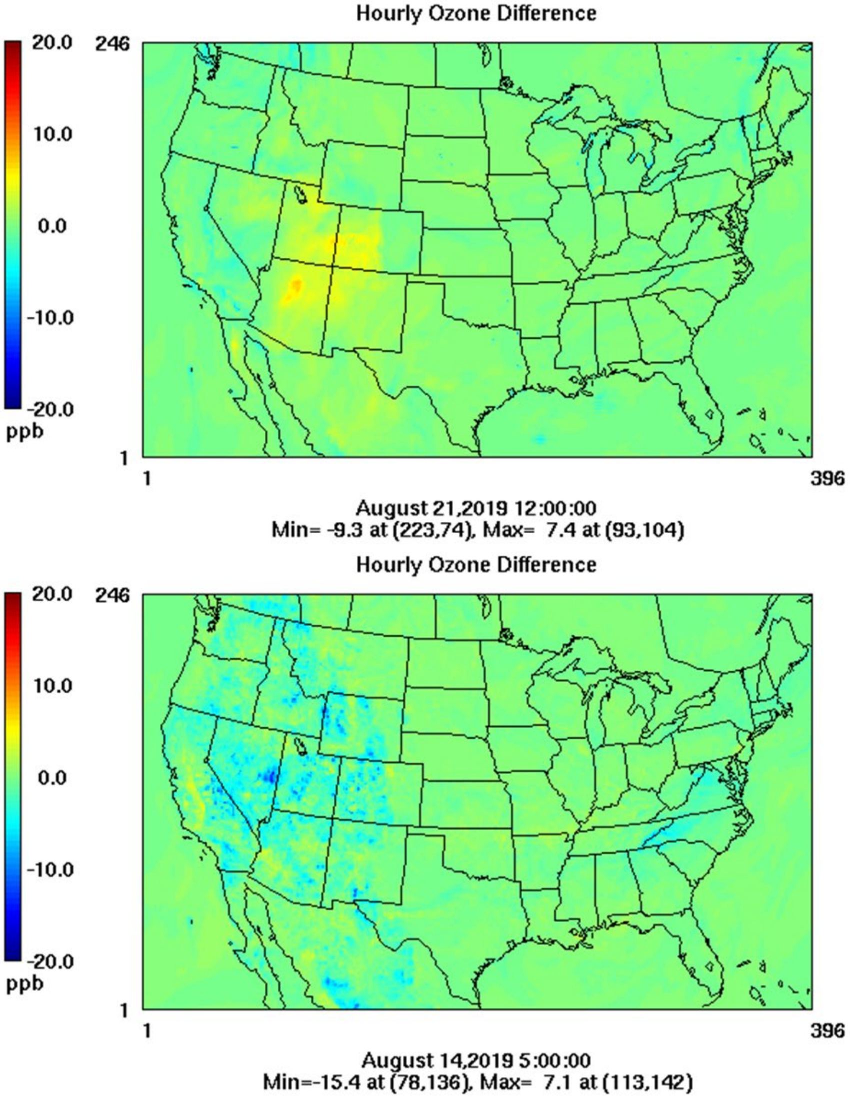


Figure 2-6. Differences in 1-hour surface ozone between CAMx runs (PPM minus CHS) across the US 12 km domain. (Top) Daytime positive differences on August 21 at 12 PM CST; (bottom) nighttime differences on August 14 at 5 AM CST.

2.3 Ozonesonde Analysis

The TCEQ provided data files containing balloon-borne ozonesonde profiles logged during 2019 from two launch sites in Texas: El Paso and San Antonio. The El Paso dataset comprised ozonesonde ascents on 13 days of August, while the San Antonio dataset comprised only 2 ascents on one day and therefore was not used for this analysis.

Ramboll downloaded additional routine ozonesonde data compiled by the National Oceanic and Atmospheric Administration (NOAA; 2022) from sites at Trinidad Head, California and Boulder, Colorado. The Trinidad Head dataset comprised ozonesonde ascents on 4 days of August and the Boulder dataset comprised ascents on 5 days. NOAA ozonesonde data from the only other continental US site at Huntsville, Alabama were not available during August 2019.

We extracted simulated ozone profiles from the CHS and PPM CAMx simulations for the grid columns containing the locations of the El Paso, Trinidad Head and Boulder launch sites, and for the specific ascent days and hours recorded in each file. All profile measurement data were recorded as meters above sea level. The NOAA data had been processed to consistent 100 m levels. The Texas data were reported at variable altitudes and so Ramboll averaged these data to 100 m levels for consistency. We paired the CAMx vertical ozone data points with model layer midpoint altitudes and converted from height above ground to above sea level using the launch site elevations. We time-averaged both measured and simulated ozone profile data over all available ascent days per site during August 2019 to yield composite ozone profiles for comparison.

2.3.1 Trinidad Head, California

Figure 2-7 compares measured and simulated ozone profiles averaged over the 4 ascent days of August when NOAA ozonesondes were recorded. The plot also shows the minimum and maximum range for both measured and modeled profiles over those days. The model replicated the entire August-average ozone profile rather well, and the minimum-maximum ranges were generally consistent through the troposphere. However, measurements exhibited more variability in the stratosphere (above ~10 km). The model was not sensitive to the choice of CHS or PPM vertical advection.

Given that Trinidad Head is located on the northern California coast, these simulated profiles mostly represent western boundary conditions derived from TCEQ’s GEOS-Chem global modeling. This suggests that the ozone boundary conditions during August 2019 properly characterize the vertical atmosphere over the eastern Pacific Ocean.

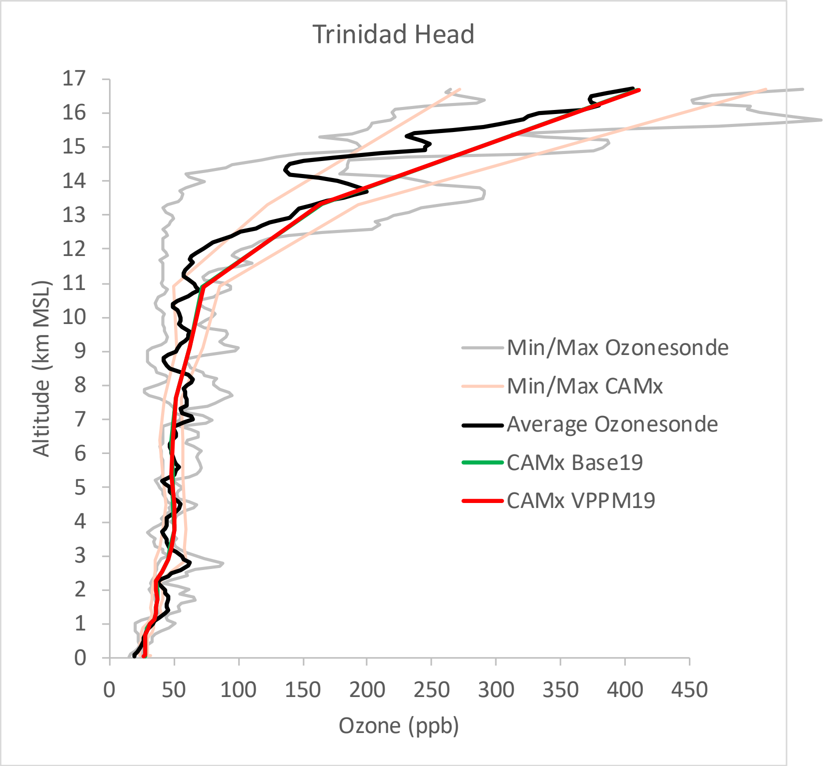


Figure 2-7. **Comparison of measured ozone profiles (black/grey lines) and CAMx-simulated ozone profiles (red/green/orange lines) from the CHS and PPM runs during August 2019 at the Trinidad Head, California ozonesonde site. The average profiles are constructed from measurements and 1-hour model estimates over 4 ascent days.**

2.3.2 Boulder, Colorado

Figure 2-8 compares measured and simulated ozone profiles averaged over the 5 ascent days of August. The model did not replicate the August-average ozone profile as well as at Trinidad Head, with an under prediction tendency through the lower half of the troposphere (up to ~5 km) and a marked over prediction tendency in the stratosphere. Again, the model was not sensitive to the choice of CHS or PPM vertical advection.

The tropospheric underpredictions can be attributed to numerous potential factors, including the fidelity of the meteorological simulation over the complex terrain of Colorado, and uncertainties in natural and anthropogenic emission across the western US. The stratospheric overpredictions are not related to the choice of advection solver. Rather, excessive numerical diffusion from upper model layers and the top boundary conditions likely persists as a result of simulated flow over the Rocky Mountains in conjunction with thick CAMx layers above ~6 km that are 1 to 4 km deep. The reasoning is based on viewing animations of ozone in the upper CAMx layers that show the influence of elevated topography in generating “standing waves” of increased ozone concentration (presumably from higher layers or top boundary conditions) along the mountain crestlines. The use of the hybrid vertical coordinate in WRF (upon which the CAMx layer structure is based) likely alleviates a large proportion of excessive vertical motion in these layers.

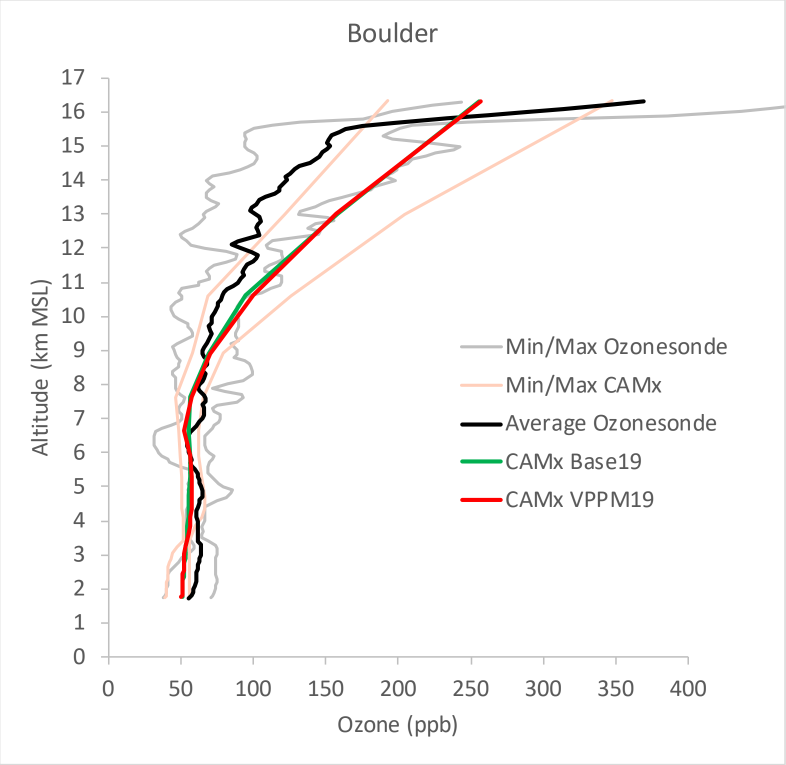


Figure 2-8. **Comparison of measured ozone profiles (black/grey lines) and CAMx-simulated ozone profiles (red/green/orange lines) from the CHS and PPM runs during August 2019 at the Boulder, Colorado ozonesonde site. The average profiles are constructed from measurements and 1-hour model estimates over 5 ascent days.**

CAMx tests using a WRF simulation with the original eta coordinate and the same layer structure could confirm CAMx sensitivity to choice of vertical coordinate (as similarly reported by Ramboll, 2020b). However, gains from the hybrid coordinate are probably mitigated using much deeper WRF layers in the stratosphere compounded by layer aggregation from WRF to CAMx.

2.3.3 El Paso, Texas

Figure 2-9 compares measured and simulated ozone profiles averaged over the 13 ascent days of August. Results were similar to Boulder, with large under predictions through the lowest 6 to 7 km of the troposphere and over predictions in the stratosphere that exceed the maximum measured values for the period. The model exhibited more sensitivity to the choice of CHS or PPM vertical advection, with PPM resulting in slightly higher ozone between 7 and 10 km. The tropospheric underpredictions could be attributed to the same issues suggested for Boulder, with perhaps larger contributions from uncertainties in anthropogenic emissions estimates for Mexico. The stratospheric overpredictions are likely caused by the same layer structure issue suggested for Boulder.

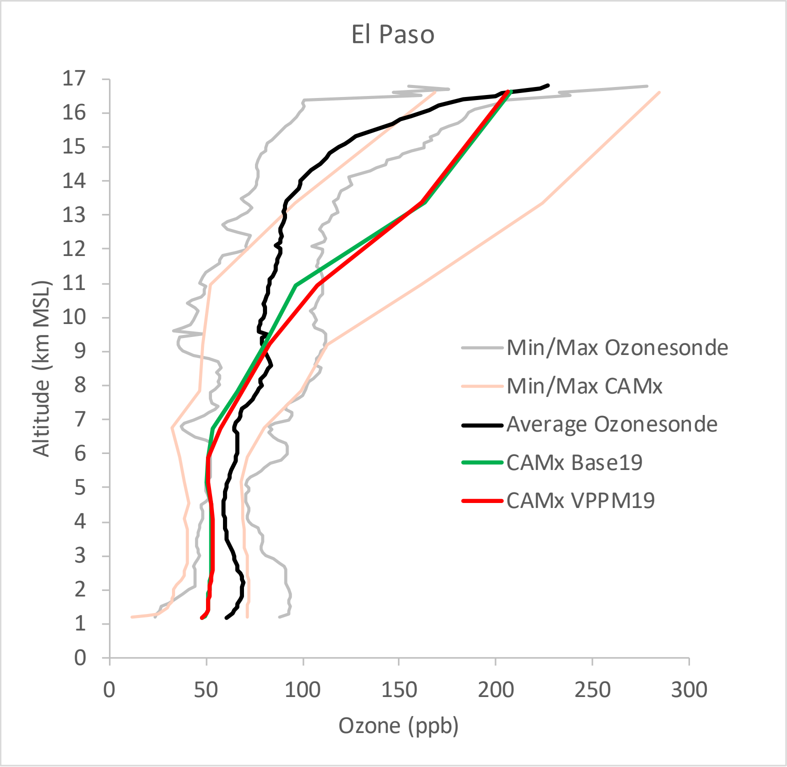


Figure 2-9. Comparison of measured ozone profiles (black/grey lines) and CAMx-simulated ozone profiles (red/green/orange lines) from the CHS and PPM runs during August 2019 at the El Paso, Texas ozonesonde site. The average profiles are constructed from measurements and 1-hour model estimates over 13 ascent days.

2.4 Model Performance Evaluation for Surface Ozone

Ramboll used EPA's Atmospheric Model Evaluation Tool (AMET; EPA, 2022a) to develop statistical model performance metrics for maximum daily 8-hour (MDA8) ozone at Air Quality System (AQS; EPA, 2022b) monitoring sites within the CAMx El Paso 4 km modeling grid. Figure 2-10 shows the locations of the AQS sites in El Paso and Dona Ana Counties used in this analysis.

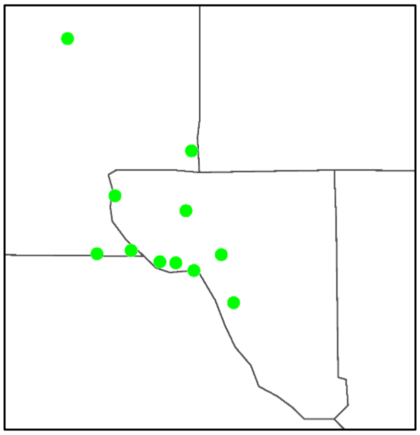


Figure 2-10. Locations of AQS ozone monitoring sites within the El Paso 4-km modeling grid used for the statistical model performance evaluation.

Table 2-2 summarizes pertinent statistical performance across all AQS sites and all days of the August modeling period. The values are compared to model performance benchmarks developed by Emery et al. (2016). Overall, the model under predicted ozone by over 20% according to the normalized bias, which constituted almost the entirety of normalized gross (unsigned) error. Bias was outside the benchmark criteria, while error was just within the criteria. Besides systematically under predicting, scatter plots of ozone (Figures 2-11 and 2-12) indicate a substantial unsystematic error as modeled concentrations do not align along the 1:1 perfect fit line and exhibit much scatter over a wide range of concentration. The correlation coefficient was low at 0.5, which is also outside the benchmark criteria. Bias, error, and correlation were not appreciably affected by the choice of vertical advection solver.

Table 2-2. Statistical model performance metrics for MDA8 ozone over all AQS sites within the El Paso 4-km grid and over the entire month of August 2019. Also shown are pertinent criteria benchmarks (Emery et al., 2016).

Statistic	CHS Case	PPM Case	Criteria Benchmark
Normalized Mean Bias	-21.6%	-22.3%	<±15%
Normalized Gross Error	22.4%	22.9%	<25%
Correlation Coefficient	0.5	0.5	>0.5
Mean Observation	59.1 ppb	59.1 ppb	
Mean Prediction	46.3 ppb	45.9 ppb	
Mean Bias	-12.8 ppb	-13.2 ppb	
Mean Error	13.2 ppb	13.5 ppb	

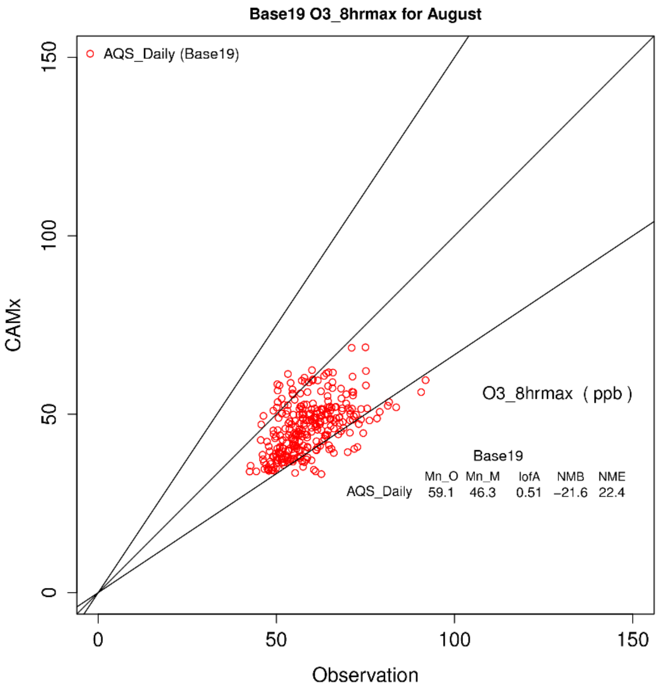


Figure 2-11. Scatter plot of predicted (CHS base case) versus observed MDA8 ozone over all AQS sites within the El Paso 4-km grid and over the entire month of August 2019. Summary statistics are also shown.

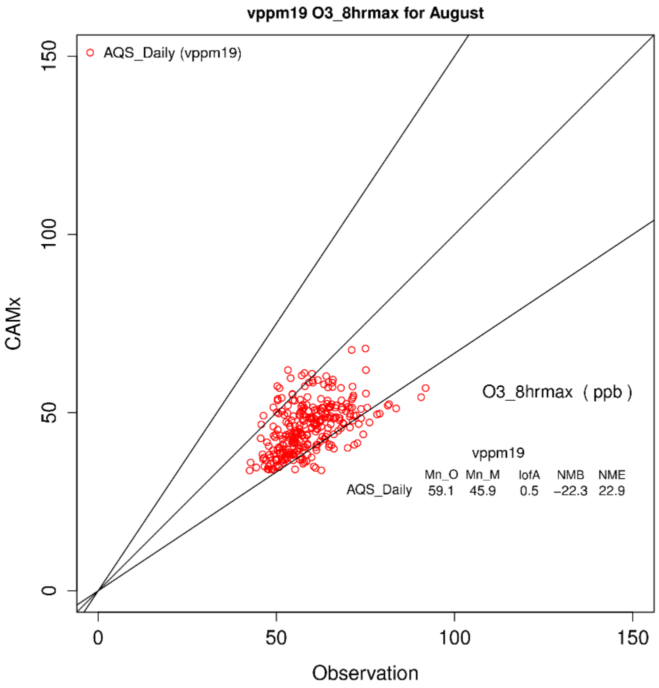


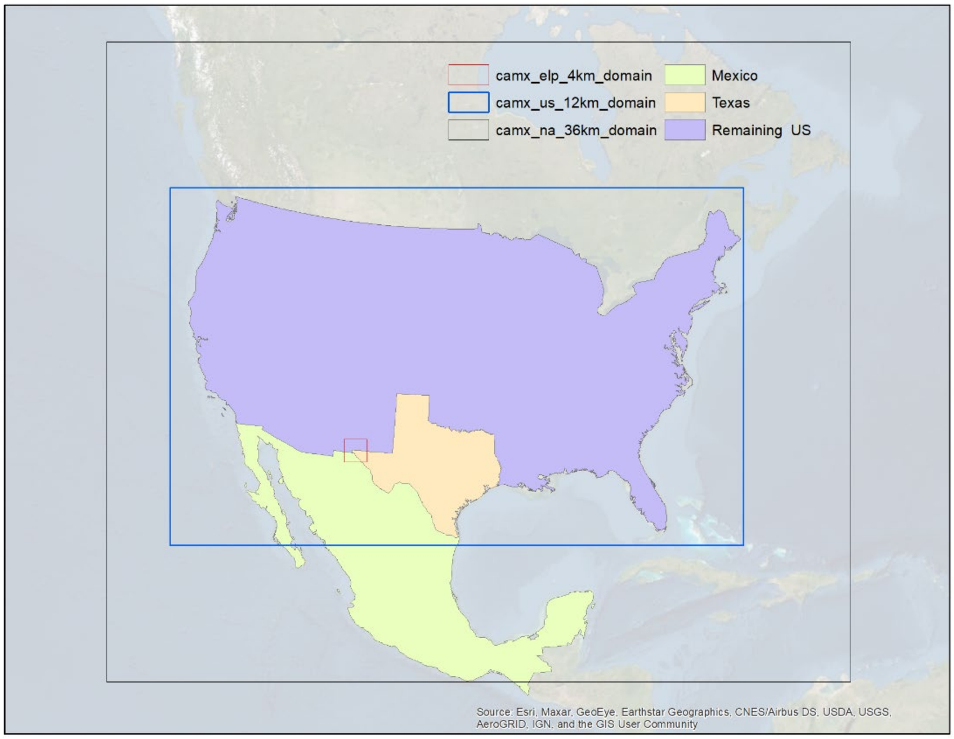
Figure 2-12. Scatter plot of predicted (PPM case) versus observed MDA8 ozone over all AQS sites within the El Paso 4-km grid and over the entire month of August 2019. Summary statistics are also shown.

3.0 CAMx PROBING TOOL TESTING

This section presents the evaluation of all four CAMx Probing Tools using the PPM vertical advection scheme. Ramboll applied the Ozone Source Apportionment Tool (OSAT) using TCEQ’s 2019 modeling platform with a simple configuration tracking ozone contributions in El Paso from four source areas and two sectors. We applied the other three Probing Tools using Ramboll’s distributed 2-day test case (June 10-11, 2016).

3.1 Ozone Source Apportionment

Ramboll ran CAMx/OSAT for the month of August 2019 using the TCEQ modeling platform described in Section 2. OSAT tracked ozone and precursor emission contributions from 4 regions: Texas, the remainder of the US, Mexico, and all remaining “other areas” encompassed by the North American 36 km modeling domain (Figure 3-1). OSAT also tracked ozone and precursor contributions from 2 sectors from each region: natural (major fires and biogenic) and anthropogenic. Finally, OSAT tracked contributions from initial conditions (IC) and all 5 boundary conditions (BC) combined (individual contributions from north, south, west, east, and top boundaries were not tracked). This resulted in 100 total tracers for ozone, precursors, and intermediate and recycled NOx products. We ran CAMx twice for the analyses presented here. One run employed the original implicit CHS solver (“IMPLICIT”) while the other employed the explicit PPM vertical advection solver (“PPM”). All other inputs and model settings were the same among the two runs.



Source: Esri, Maxar, GeoEye, Earthstar Geographics, CNES/Airbus DS, USDA, USGS, AeroGRID, IGN, and the GIS User Community

Figure 3-1. OSAT source regions defined for the vertical advection tests. A fourth region not expressly labelled on the map includes all remaining areas outside of Mexico, Texas, and the US within the 36 km modeling domain (Canada, Central America, Caribbean islands, and all oceans labelled “other areas”).

We compiled the model using the Portland Fortran90 compiler, version 13.4. Both cases were run on a 24-core Intel Xeon X5675 3 GHz server using a combination of MPI parallelization across 8 cores (1 master and 7 compute nodes) with 3 OMP parallelization threads per core. To complete the 31 day simulation, the CHS run took an average of 3.7 hours per day, while the PPM run took an average of 3.5 hours per day (almost 6% faster).

Figure 3-2 presents time series of predicted hourly ozone contributions at each hour (local CST) of the August 2019 modeling period for the 4 km grid cell containing the El Paso Chamizal monitoring site. Results are taken from the base CHS run. Source contributions are arranged from global and natural sources at the bottom (IC and BC combined, all natural contributions in the domain combined) to successively more local anthropogenic sources toward the top (other areas, US, Mexico, Texas). The top panel shows the time series as a “landscape” plot, where the colored areas show each of the source categories’ absolute contributions (ppb) that accumulate up to the total simulated hourly ozone. The bottom panel shows the same information but as a relative distribution (%) of the total at each hour. Figure 3-3 shows the period-averaged ozone contributions from each of the six source categories for both the CHS and PPM runs. peaks

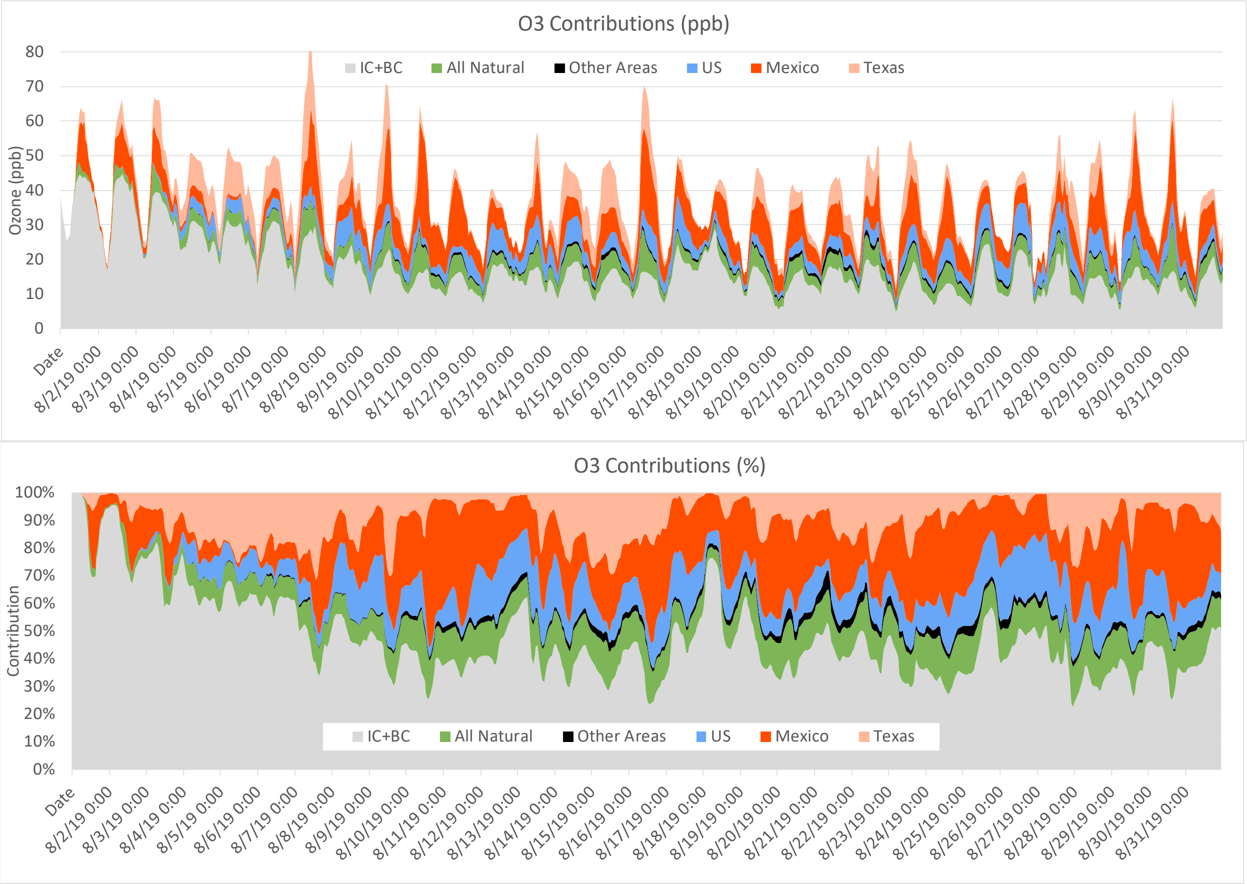


Figure 3-2. Time series of hourly predicted ozone contributions (local CST) at the El Paso Chamizal monitoring site from the base CHS run. The top panel shows each of the source categories’ absolute contributions (ppb) that accumulate up to the total simulated ozone. The bottom panel shows the same information but as a relative distribution (%) of the total.

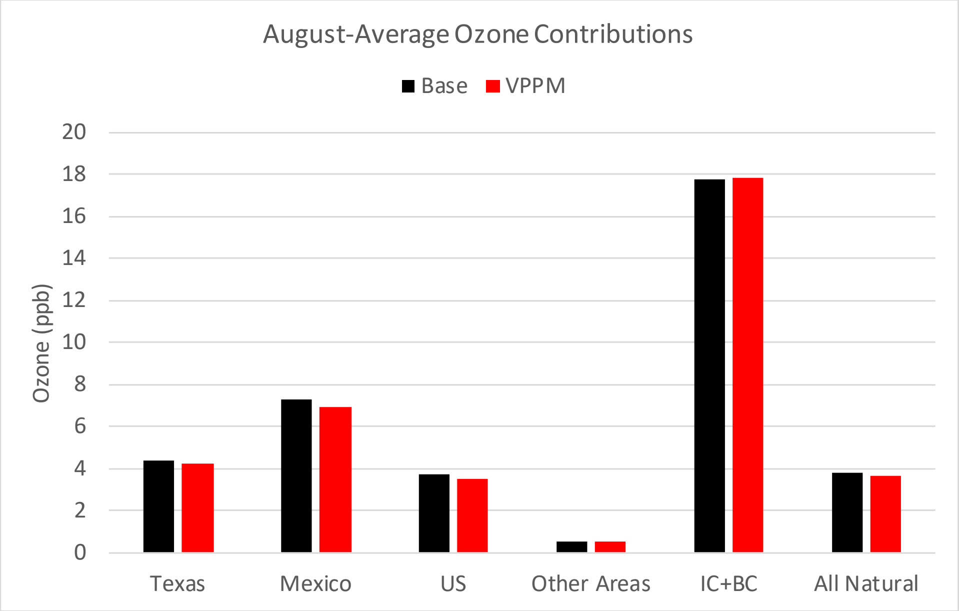


Figure 3-3. Averaged ozone contributions from the CHS and PPM runs over the August 2019 modeling period.

IC/BC was the largest contributor to simulated ozone every hour at El Paso Chamizal, followed by Mexico, Texas, the remainder of the US, natural, and finally other areas of the domain. Note that model underpredictions of ~20% in the El Paso area (as presented in Section 2) render the estimated absolute contributions to be inaccurate but the relative contributions are probably more robust. If the largest proportion of model error stems from underestimated emissions in Mexico, then the ozone contribution from Mexico would be higher than shown in these figures.

The sensitivity of these results to the choice of vertical advection solver was small. On average, PPM advection led to slightly lower contributions from Mexico, Texas, remaining US, other areas, and natural by 3-6%, whereas PPM led to slightly higher IC/BC contributions by less than 1%. This agrees with model performance results presented in Section 2, where PPM led to slightly lower MDA8 ozone by about 1%.

Figure 3-4 compares CHS and PPM hourly time series (local CST) of ozone contributions from each source individually to provide more detail in differences arising from the advection solvers. While relatively small and short-lived, the largest advection-driven differences occurred for IC/BC contributions, which makes sense given the larger distances, vertically deeper distribution, and complex terrain features that are traversed between the boundaries and El Paso. Sensitivity for all other sources were much smaller. These sources either contributed very little, or their largest contributions were more localized and thus less influenced by multi-day histories that are affected by compounding differences arising from deep vertical transport.

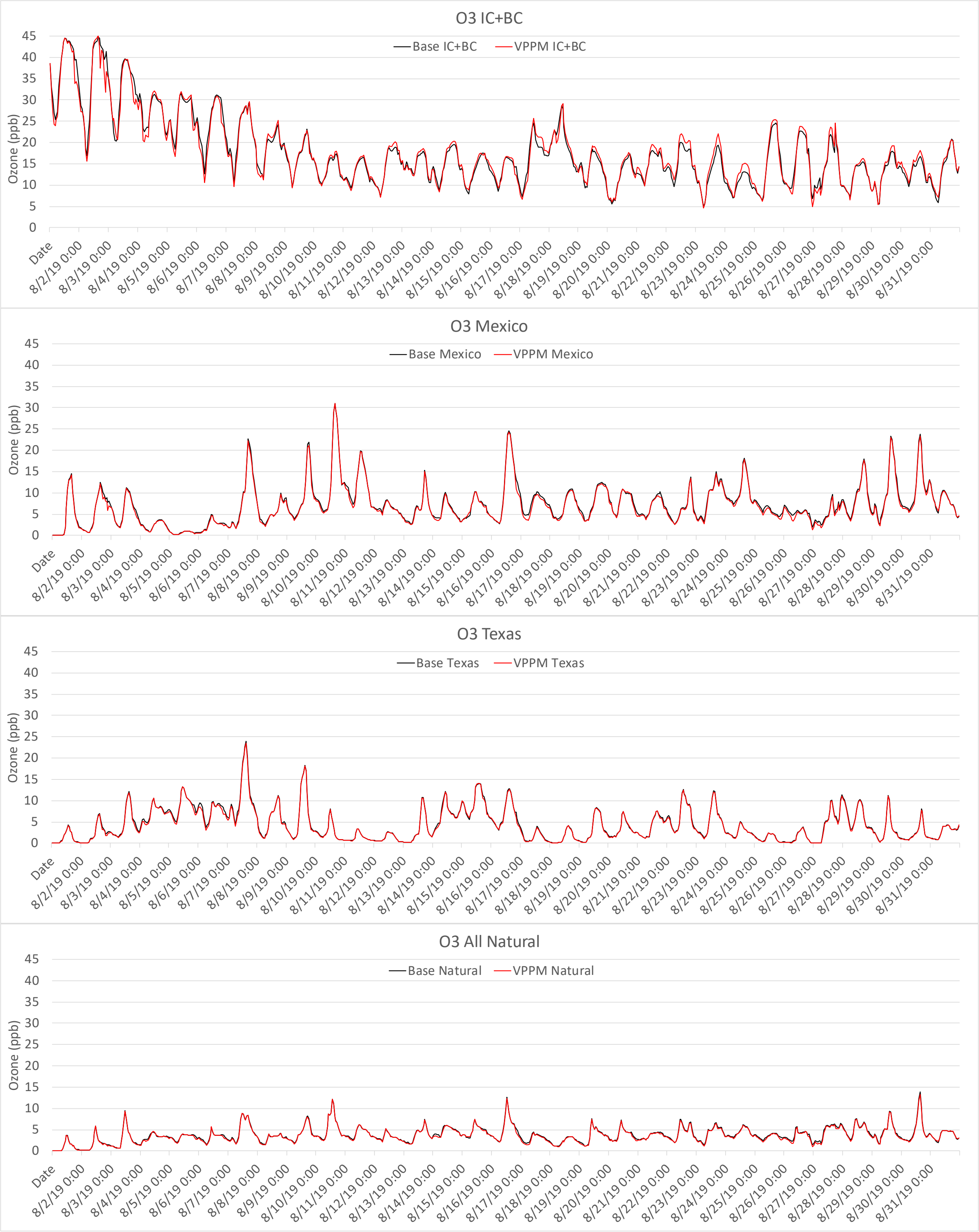


Figure 3-4. **Comparisons of hourly ozone contribution time series from the CHS (base, black) and PPM (VPPM, red) runs for each of the six source categories shown in Figures 3-2 and 3-3. Figures are arranged in order from largest (top) to smallest (bottom) period-averaged ozone contributions. Time is local CST.**

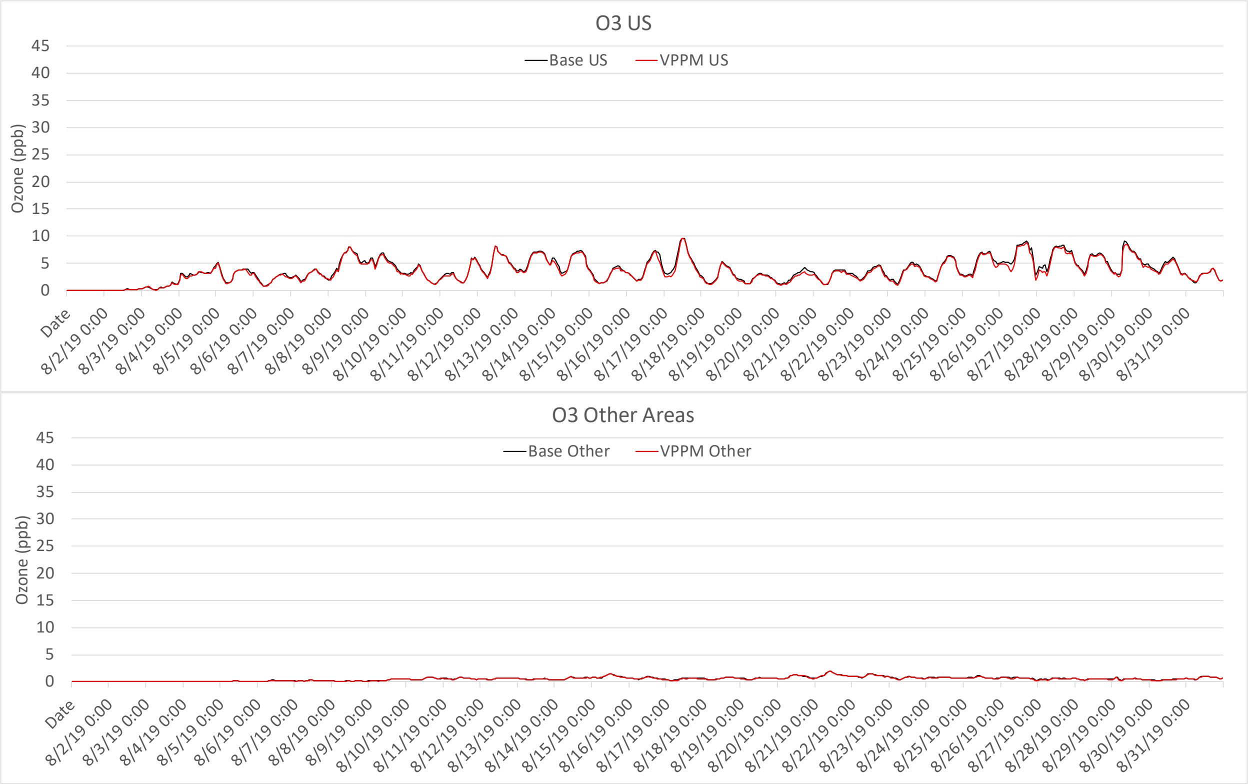


Figure 3-4 (concluded).

3.2 Decoupled Direct Method Configuration

DDM was applied using Ramboll's distributed 2-day test case (June 10-11, 2016). The test case configuration employs a 36 km grid spanning the entire US and a 12 km grid covering the eastern US. For this test application of DDM, only the 36 km grid was used. Following the configuration developed for Ramboll's internal testing of each CAMx distribution, first-order DDM tracked the sensitivity of ozone, NO and NO_2 to biogenic emissions over the entire 36 km grid. This resulted in a total of 6 DDM parameters per modeled species and 678 total sensitivity coefficients. We compared results using the original CHS advection scheme against results using the new PPM scheme.

We compiled the model using the Portland Fortran90 compiler, version 13.4. Both cases were run on a 24-core Intel Xeon X5675 3 GHz server using a combination of MPI parallelization across 8 cores (1 master and 7 compute nodes) with 3 OMP parallelization threads per core. Both runs took an average of 1.0 hours per day to complete the 2 day simulation. Model runtimes differed by less than 1% using the two advection schemes.

Ramboll focused the evaluation on ozone sensitivity to biogenic volatile organic compounds (VOC) on the 36 km grid. The spatial and temporal patterns of ozone sensitivities were similar between the CHS and PPM schemes, with highest positivity sensitivity during the day when biogenic VOC contribute to ozone production, and highest negative sensitivity during the night when biogenic VOC consume ozone as they oxidize. However, sensitivity results using CHS and PPM deviated the most during early morning hours. Figure 3-5 shows the spatial variation of ozone sensitivity using the CHS solver at 1 PM UTC (7 AM CST) on July 11, 2016. This hour exhibited the largest differences in ozone sensitivity between the CHS and PPM solvers, which is consistent with the time when the largest ozone impacts occurred for the core model and OSAT tests described earlier. At this early morning hour, ozone sensitivity was mostly negative with maxima occurring in the biogenic-rich southeast US and through the Rocky Mountains. Additional biogenic VOC would further lower ozone (negative sensitivity) at this hour while less VOC would raise ozone by decreasing the loss rate. Positive ozone sensitivity occurred in the northeastern US, where the sun had just risen at this hour, indicating that the ozone plumes from New York City and Boston would respond positively to increased biogenic VOC in the NOx-rich (VOC-limited) early photochemical environment.

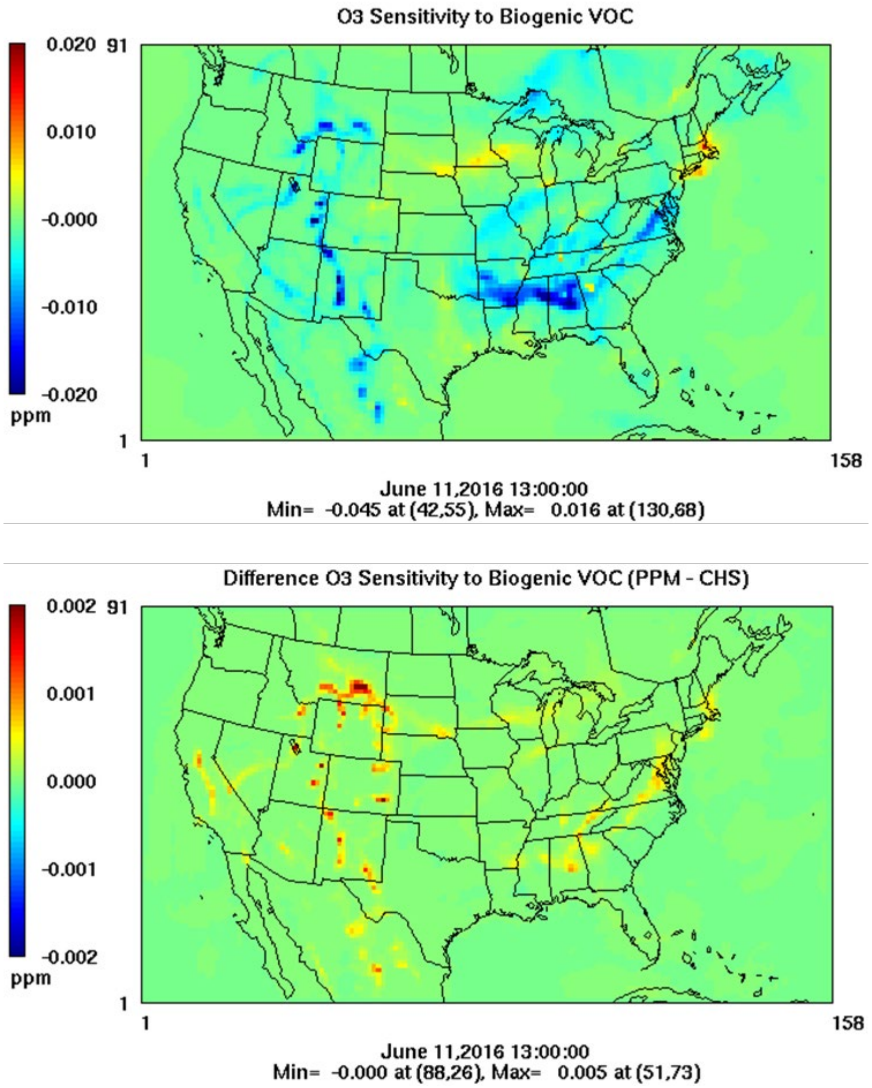


Figure 3-5. (Top) CAMx DDM ozone sensitivity (ppm) to biogenic VOC at 1 PM UTC (7 AM CST) as simulated by the Ramboll CAMx distribution test case using the CHS vertical advection solver. (Bottom) Difference in ozone sensitivity (ppm) between the PPM and CHS solvers at the same date/time.

Ozone sensitivity differences arising from PPM vertical advection were largest in areas of complex terrain, as seen in the earlier tests. Differences at 1 PM UTC on July 11 were entirely positive, meaning less negative sensitivity by a few ppb in areas exhibiting 10+ ppb of negative sensitivity in the CHS case. The positive sensitivity ozone plumes of 10-16 ppb from New York City and Boston also shifted to slightly higher sensitivity by roughly 0.5 ppb. These patterns are consistent with the relative magnitudes, locations and times of differences seen in core model ozone between CHS and PPM solvers.

3.3 Process Analysis Configuration

PA was applied using Ramboll's distributed 2-day test case, invoking all three modules of PA: Integrated Process Rates (IPR), Integrated Reaction Rates (IRR), and the Chemical Process Analysis (CPA). Ramboll focused on results from IPR because it reports fluxes from the advection schemes. For this test application, only the 36 km grid was used, and IPR was configured to report fluxes and other process contributions over a 20x20 grid cell subdomain centered in the middle of the grid from the surface through layer 10 (~750 m). We compared results using the original CHS advection scheme against results using the new PPM scheme.

We compiled the model using the Portland Fortran90 compiler, version 13.4. Both cases were run on a 24-core Intel Xeon X5675 3 GHz server using a combination of MPI parallelization across 8 cores (1 master and 7 compute nodes) with 3 OMP parallelization threads per core. Both runs took an average of 9 minutes per day to complete the 2 day simulation. Model runtimes differed to within 1 minute using the two advection schemes.

Figure 3-6 shows the breakdown of net ozone changes from the tracked processes averaged across the entire 20x20x10 sub-domain volume at each hour of the 2-day simulation. In the CHS case, vertical advection through the top of layer 10 consistently contributed between 0.2 to 2.1 ppb to sub-domain ozone over the entire period, while horizontal advection through all four lateral sides consistently removed between 0.7 to 1.8 ppb. Surface deposition consistently removed between 0.2 to almost 1.5 ppb, with nighttime minimum and daytime maximum rates. Chemistry contributed up to 1.3 ppb during the day and removed up to 0.4 ppb during the night. Net positive contributions led to volumetric ozone increases during daytime hours while net removal led to decreases during nighttime hours, both of which were mostly controlled by chemical production and loss, respectively.

The use of the PPM solver properly affected only the vertical advection flux through the top of layer 10; all other fluxes remained the same as the CHS case. While difficult to determine in the side-by-side comparisons in Figure 3-6, PPM resulted in a slight increase (0.1 ppb maximum) in vertical contribution during the day and a slight decrease (0.2 ppb maximum) during the night.

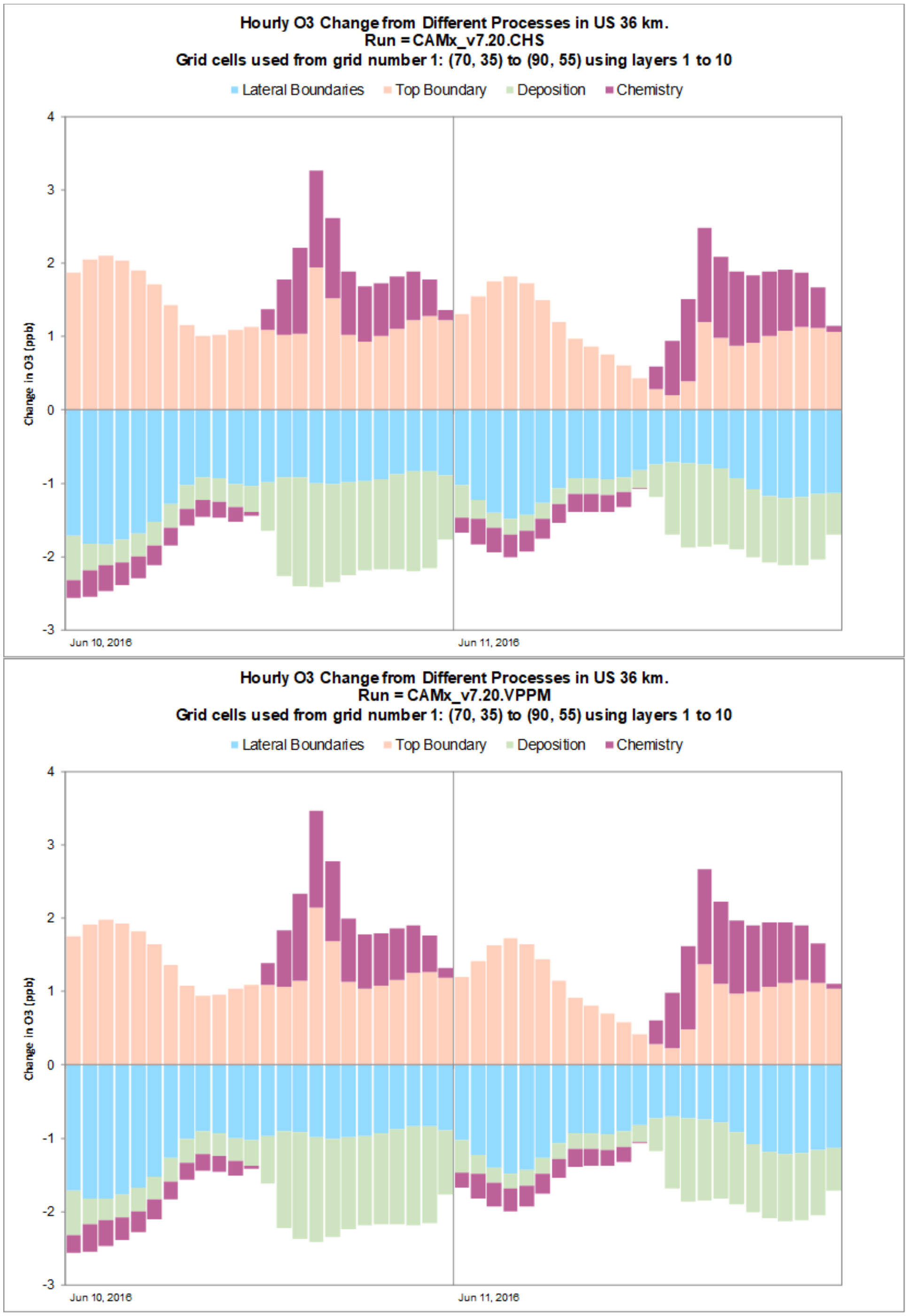


Figure 3-6. Breakdown of net hourly ozone changes by major process tracked by CAMx PA, averaged across the entire IPR 20x20x10 cell sub-domain at each hour of the 2-day Ramboll CAMx distribution test case simulation. (Top) Results using the CHS vertical advection solver. (Bottom) Results using the PPM vertical advection solver. Note that time is in UTC.

3.4 Reactive Tracer Configuration

RTRAC was applied using Ramboll's distributed 2-day test case. For this test application, only the 36 km grid was used. Following the configuration developed for Ramboll's internal testing of each CAMx distribution, RTRAC was configured to track two reactive gases (formaldehyde and acetaldehyde) and one inert aerosol (primary sulfate) from oil and gas point sources as defined in the EPA's 2016 modeling platform. Both gases were set to decay via photolysis and reactions with OH and NO_3 radicals. We compared results using the original CHS advection scheme against results using the new PPM scheme.

We compiled the model using the Portland Fortran90 compiler, version 13.4. Both cases were run on a 24-core Intel Xeon X5675 3 GHz server using a combination of MPI parallelization across 8 cores (1 master and 7 compute nodes) with 3 OMP parallelization threads per core. Both runs took an average of 10 minutes per day to complete the 2 day simulation. Model runtimes differed to within 1 minute using the two advection schemes.

The evaluation focused on formaldehyde (HCHO) emitted from the oil and gas point sources tracked by RTRAC in the 36 km grid of the 2-day distribution test case. Figure 3-7 shows the spatial variation of HCHO using the CHS solver at 6 AM UTC (12 AM CST) on July 11, 2016. This hour exhibited the largest HCHO differences between the CHS and PPM solvers. RTRAC generated peak HCHO concentrations ranging from 0.025 to over 0.1 ppb centered on the major US oil and gas development basins (Texas, Oklahoma, Gulf Coast, Rocky Mountains, southern California, and Appalachia).

The largest HCHO differences arising from PPM vertical advection occurred in the Rocky Mountains (as seen in earlier ozone tests) as well as Oklahoma and California. PPM reduced concentrations by up to 0.005 ppb at this hour. Peak HCHO differences were relatively on par with negative ozone differences seen at similar hours and in similar terrain.

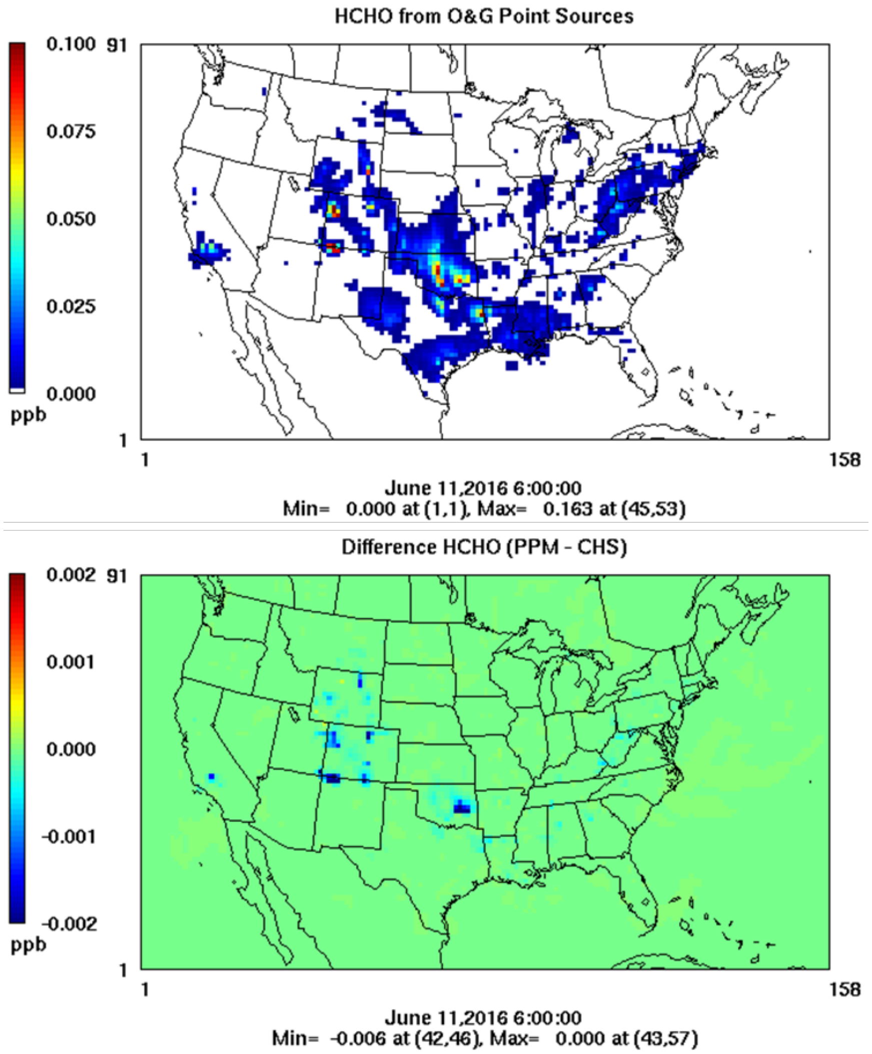


Figure 3-7. (Top) CAMx RTRAC HCHO concentrations (ppb) from US oil and gas point sources at 6 AM UTC (12 AM CST) as simulated by the Ramboll CAMx distribution test case using the CHS vertical advection solver. (Bottom) Difference in HCHO (ppb) between the PPM and CHS solvers at the same date/time.

4.0 CONCLUSIONS AND RECOMMENDATIONS

4.1 CAMx Core Model Results

Ramboll ran CAMx for the month of August using the TCEQ 2019 modeling platform. We compared simulated ozone profiles against available ozonesonde measurements and compared simulated surface ozone patterns against observed concentrations recorded at monitoring sites in the El Paso area. Highlights from core model tests are:

- Model runtimes differed by only 1% using the two advection schemes.
- Simulated vertical ozone profiles were not sensitive to the choice of vertical advection scheme.
- CAMx-predicted vertical ozone profiles on the US west coast were well-replicated, which is most likely reflecting the boundary conditions derived from global modeling.
- CAMx-predicted vertical ozone profiles in Colorado and El Paso exhibited tropospheric under predictions and stratospheric over predictions, the latter of which is likely caused by continued numerical diffusion from the use of thick model layers above ~10 km.
- Use of the WRF hybrid vertical coordinate in the 2019 modeling platform likely mitigated numerical diffusion in the upper layers relative to those previously reported by Ramboll (2020a) using the 2012 platform (although this was not explicitly investigated).
- Surface hourly ozone differences between the two advection schemes were not large on average, but episodically differed as much as -50 to +10 ppb in complex terrain, with the largest negative differences usually occurring at night and the largest positive differences occurring during the day, both apparently associated with convection and the different treatments of surface boundary conditions used in CHS and PPM.
- Simulated surface ozone exhibited an underprediction bias and poorly correlated agreement with measured ozone at monitoring sites in El Paso and Dona Ana Counties, however ozone performance was not appreciably different using the two advection schemes.

4.2 CAMx Probing Tool Results

Ramboll applied OSAT using TCEQ's 2019 modeling platform tracking ozone contributions in El Paso from four source areas by two sectors and IC/BC. The other three Probing Tools were applied using Ramboll's distributed 2016 2-day test case (June 10-11, 2016). Highlights from Probing Tool tests are:

- All Probing Tool results exhibited negligible to minor sensitivity to the choice of vertical advection scheme, with the largest differences occurring mostly during nighttime hours during convective conditions in complex terrain as seen for the core model tests summarized above.
- To complete the 31-day OSAT simulation, the CHS run took an average of 3.7 hours per day, while the PPM run took an average of 3.5 hours per day (almost 6% faster).
- In El Paso, OSAT differences arising from the two advection solvers were relatively small and short-lived. The largest differences were associated with initial/boundary contributions due to their larger ozone contributions, longer transport distances, vertically deeper distribution, and complex terrain features traversed between the boundaries and El Paso.
- Except for IC/BC, Mexico contributed the most to simulated ozone at the El Paso Chamizal monitor, followed by Texas, then other US states and other tracked sources. Model underpredictions render the estimated absolute contributions to be inaccurate but the relative contributions are probably more robust.

- For DDM, both CHS and PPM runs took an average of 1.0 hour per day to complete the 2-day test case simulation. Model runtimes differed by less than 1% using the two advection schemes.
- DDM estimated ozone sensitivity to biogenic emissions. Sensitivity differences arising from PPM vertical advection were largest at night and in areas of complex terrain. These patterns were consistent with the relative magnitudes, locations and times of differences seen in core model ozone.
- Both CHS and PPM runs took an average of 9 minutes per day (PA) and 10 minutes per day (RTRAC) to complete the 2-day simulation. For both Probing Tools, model runtimes differed to within 1 minute using the two advection schemes.
- We confirmed that the use of the PPM solver properly affects only the vertical advection flux reported by PA; all other fluxes remain the same as the CHS case. PPM resulted in a slight increase in vertical contribution to ozone in the PA test sub-domain during the day and a slight decrease during the night.
- RTRAC simulated reactive plumes of formaldehyde from oil and gas sources across the US. The largest formaldehyde differences arising from PPM vertical advection were negative and occurred at night in complex terrain, where they were relatively on par with negative ozone differences seen at similar hours and in similar terrain.

4.3 Recommendations:

Based on the results of vertical advection sensitivity analysis, Ramboll recommends the following:

- Use either the PPM vertical advection solver or the original CHS as both yield mostly similar results.
- Continue to use the WRF hybrid vertical layer coordinate, which is the default configuration in current WRF distributions.
- Continue to locate the CAMx model top sufficiently well above features of concern, such as ozone fluxes through the tropopause.
- Consider CAMx tests that utilize every WRF layer without layer collapsing to improve resolution of upper atmospheric dynamics and check results against ozonesonde data over the intermountain west (i.e., Boulder and El Paso).
- Keep track of creatively different advection schemes, such as semi-Lagangian methods, that have the potential to further reduce numerical diffusion.

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