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CHARACTERIZATION AND INTERNATIONAL TRANSPORT OF OZONE PRECURSOR EMISSIONS IN THE EL PASO, TEXAS REGION

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Developing a clear understanding into the highly variable ozone production, transport, and distribution characteristics within any regions of interest is critically important for City, County, and State managers, just as it is important for policymakers and regulators. It does understandably become even more important when a metropolitan City (El Paso) is adjacent to a major international City (Juarez, Mexico). Understanding nternational transport of ozone and its precursors is important to the El Paso Metropolitan Planning Organization (EPMPO).

Successful ozone modeling efforts require: (i) emissions measurements with spatial and temporal adequacy, (ii) high-resolution and robust meteorological information, and (iii) various model components that have undergone extensive testing for robustness.

This portion of the overall study conducted at Regional Earth System Predictability Research (RESPR) has addressed two of the above ingredients to a large extent, while model testing has received lesser focus due to time constraints.

RESPR has completed three coupled met-chemistry episode simulations from three different years (2011, 2012, and 2013). RESPR has simulated meteorological information for 5 consecutive days for each of the three episodes by using a nested grid, with the finest resolution (1-km) in the innermost grid (grid 3).

In addition to the robust meteorology produced for the three episodes, RESPR has produced 15 months of simulations or five summer months, from May through September, for the three years of 2011, 20012, and 2013.

As part of the input preparation effort, RESPR has also completed emissions modeling with added improvements in mobile and biogenic emissions.

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From the three coupled met-chemistry simulations conducted for this study, RESPR is able to provide some conclusions that the EPMPO can rely on for defining the direction of its future endeavors. One of the important conclusions is that international transport of ozone and its precursors is highly likely, depending on the prevailing meteorological conditions. Also, depending on certain meteorological conditions, international transport may likely take place in the opposite direction, i.e., from the U.S. to Mexico. Other conclusions are provided elsewhere in this report.

While the conclusions offered in this study should only be considered qualitative in nature, RESPR recommends further model evaluation against ozone observations before such conclusions can be considered fully quantitative.

RESPR also highlights that upon further model evalution, the comprehensive modeling approach adopted for this study can yield both short-term and long-term ozone forecasting capablities for the EPMPO for the health management/mitigation purposes, as well as for the purposes of long-range planning, respectively.

Finally, this robust modeling capability will allow the EPMPO to devise and implement ozone mitigation strategies such as effective traffic volume control measures and route planning.

1.0 Introduction

The El Paso Metropolitan Planning Organization (EPMPO) has sponsored this study to Investigate how ozone and its precursors (Nitrogen Oxides, NOx, and volatile organic compounds, VOCs) vary during the peak ozone months of May through September. With a major international metropolitan City, Juarez, Mexico, as a neighbor to the south of City of El Paso, the EPMPO has reasons to understand its own emissions sources, but that of its neighbor's as well. Ozone can be produced at locations, as well as

transported from other locations to or from those locations. Similarly, ozone precursors can be transported from their original locations of release, such as power plants as an example, leading to international transport of ozone and its precursors. Studies of this nature shed light on emissions sources and help characterize ozone behavior within the planning area. The EPMPO is particularly interested in the City and its suburban areas, but has expressed the desire to understand the County-wide distribution of ozone and the international transport from Juarez. The EPMPO knows that international transport can occur in either direction, i.e., net transport to or out of Juarez, from or into the surrounding areas, including City of El Paso and El Paso County is likely depending on the prevailing conditions.

In order to accomplish a meaningful investigation into such a characterization effort, quality measurements of ozone and its precursors, good meteorology data sets, and robust models employed by people with cutting-edge expertise and a long track record of using computational fluid dynamics (CDF) models are required.

The EPMPO has tasked the New Mexico State University (NMSU), Department of Geography, and a New Mexico small business, Regional Earth System Predictability Research (RESPR) for this study. RESPR has over a decade of meteorological modeling experience based on innovative approaches to producing high-quality weather data for various applications. The original developer of this technology at RESPR, Dr. James Stalker, has taken on the task of coupling meteorological modeling approach, as part of the overall RESPR responsibilities on the project. He has also undertaken the emissions modeling effort for preparing detailed emissions.

Ozone found in the upper layers of the atmosphere (i.e., within the upper troposphere and stratosphere) has known benefits such as its ability to block ultraviolet (UV) radiation reaching the ground. Near surface ozone levels tend to be much smaller compared to those at the higher alttidues, but surface ozone has negative effects on, for example, health, such as causes of respitory, eye, and skin irritation. There are known emissions sources of precursors of ozone near the surface and at elevated heights (e.g., near smoke stacks) to ozone production/depletion in various locales in the U.S. and around the world.

Such precursor emissions sources can be grouped into two broad categories. The first group of emissions is the anthropogenic type, which includes emissions released from human activity from vehicles, power plants, oil and gas operations, agriculture, etc., to mention a few. The second group of emissions is the biogenic type which includes gases released from various kinds of vegetation. Through land use changes made, for example, via agricultural activity, some biogenic emissions can arguably be counted as part of the anthropogenic emissions group. In general, these two emissions groups are classified as mutually exclusive, which is the definition adhered to in this study.

The relative importance of the two emissions groups mentioned above, along with the conducive meteorological conditions, such as hot, dry, and low-wind conditions, can lead to the high ozone levels observed and the highly variable intra- and inter-seasonal and annual variability of surface ozone due to emissions variability and meteorology in all parts of the world.

To add to the above-stated complexity posed by the two groups of emissions, the dynamically-active atmosphere can lead to non-linear variability of ozone of its own through both horizontal and vertical transport and mixing. For example, those ozone

concentations mentioned to be found aloft can be transported down to the surface in certain favorable meteorological conditions, in addition to the transport and mixing of precursors and ozone with neighbring locales.

In the face of such problem complexity and the policy and compliance requirements set forth by the U.S. Envrionmental Protection Agency (EPA), metropolitan cities such as El Paso are wise to make the investment to get studies of the kind presented in report done.

Although this study can not address all the issues noted above, one of the main objectives for this research team from the beginning has been about addressing deficiencies and shortcomings in the current approaches. In this regard, three notable areas for improvement have been identified: 1) the meteorology, 2) the emissions, and 3) the models. The improvements sought in this study have been in the same order as above in that meteorology has received the highest focus for improvement, while emissions received the second most focus. Models have received relatively lesser focus in this study and more focus should be given to several of the models used here in any continuation studies contemplated in the future.

3.0 Coupled Air-Chemistry Modeling

3.1 Overview

A coupled air-chemistry modeling effort involves various CFD and other models to produce model output in multiple intermediate steps, and to ultimately achieve the model output of the sought-after air pollutants. The main pollutant studied in this effort is ozone. This suite of models and our team's expertise can readily investigate characteristics of many other air pollutants of interest to metropolitan cities such as El

Paso City, including particulate matter (PM) for assessing visibility and its detrimental effects on health.

Various sources of input, such as emissions and meteorological information, are required in this type of effort to investigate and characterize air pollutants.

There are essentially three main components to the development of ozone simulations that have to deal with the emissions modeling (SMOKE—defined below), meteorology (RESPR approach using RAMS (defined below), hereafter referred to as the RESPR-RAMS meteorology model), and a coupled air-chemistry model (CAMx—defined below).

All the components are listed below:

<u>Models</u>

RESPR-RAMS meteorology model

[Regional Atmospheric Modeling System (version 4.3) (see Cotton et al. 2003 and Stalker and Knupp 2003 for further details.)]

• CAMx

[Comprehensive Air Quality Model with Extensions (version 6.20), available at http://www.camx.com/download/default.aspx.]

• MCIP

[The Meteorology-Chemistry Interface Processor (version 4.2) (see Otte and Pleim 2010 for details.)]

Spatial Allocator

[see https://www.epa.gov/air-research/spatial-allocator-air-quality-modeling for further details.]

SMOKE

[Sparse Matrix Operator Kernel Emissions (version 3.6.5), see https://www.cmascenter.org/smoke/ for details.]

RAMS2CAMx

[RAMS meteorology data conversion tool for CAMx, available from Environ at http://www.camx.com/download/support-software.aspx.]

• TUV photolysis

[Photolysis rate development tool available from Environ at http://www.camx.com/download/support-software.aspx.]

• O3MAP

[An ozone map processing tool that produces output for the TUV photolysis tool, available from Environ at http://www.camx.com/download/support-software.aspx.]

ICBCPREP

[A tool that allows to prepare initial/boundary conditions for CAMx, along with the bndextr tool, available from Environ at http://www.camx.com/download/support-software.aspx.]

CMAQ2CAMx

[A tool that allows Community Multi-Scale Air Quality (CMAQ) Modeling System-ready emissions files to be converted to CAMx-ready emissions files, available from Environ at http://www.camx.com/download/support-software.aspx.]

<u>Input</u>

• Meteorology input to the RESPR-RAMS model

[National Centers for Environmental Prediction (NCEP) North American Model (NAM) 12-km meteorology data are used as model input.]

• Emissions (from EPA and the EPMPO)

[EPA-provided database was used for many of the emissions. The EPMPO's mobile emissions and the NMSU's land use and land cover data were used for emissions as well.]

<u>Output</u>

- RESPR-RAMS meteorology output (1-km, 5-km, and 25-km horizontal resolution)
- SMOKE-ready meteorology data from MCIP

- SMOKE-ready emissions from Spatial Allocator and the EPA 2011eh platform
- Gridded/speciated/temporal data from SMOKE
- RESPR-RAMS meteorology output from RAMS2CAMx for CAMx
- CAMx-ready emissions data for CAMx
- Simulation output of ozone and other pollutants from CAMx

These model components and various input and output are also shown schematically in Figure 1.



Figure 1. Various model components and the input and output flow for ozone modeling.

The orange boxes in Figure 1 indicate new models required specifically for this study unlike for conventional air pollution modeling projects. The yellow boxes show where extensive customization was required because of the novel meteorological modeling approach employed in the current study. Many of the rest of the blue boxes also required customization to a lesser degree. Customization was mainly required at various stages of the modeling effort because of the RESPR-RAMS model type and approach.

Since meteorology and emissions are two of the main ingredients of any photochemical modeling endeavors, the next two subsections focus on detailing the RESPR-RAMS modeling approach and the emissions preparation effort using Spatial Allocator and SMOKE, respectively.

3.2 Description of the RESPR-RAMS modeling approach

RESPR, the small New Mexico business that Dr. Stalker owns, was established in 2002, after a decade-long research effort by him in the area of atmospheric computational fluid dynamics (CFD) research. At RESPR, Dr. Stalker investigated an innovative idea that had the potential to yield an answer to the long-standing question of why atmospheric predictability is severely limited. He recognized during those early days of growing his small business that there was a fundamental limitation in the approaches being used by the atmospheric community. The idea was essentially about recognizing that there are two types of atmospheric variables. The first type of variables are of the state variable kind. These are variables that are commonly measured and extensively used by the community. The examples of this type of variables are wind, temperature, pressure, etc. that help us understand the state of the atmosphere. The other kind of variables are of the physical process variable kind. These latter type of variables are lesser known or unknown to most practicing weather professionals. There are a number of reasons why the latter type of variables do not receive much attention

from the community. One reason may be due to the fact that measurements of this type of variables are few and far in between, other than those collected during expensive field experiments. There are instrumentation-related challenges to obtaining this type of variables also. Another reason might be that there is the conventional belief that we can determine how the atmosphere works based on state variables alone.

The problem that Dr. Stalker realized in the early 2000's is that even though the underlying physical processes tend to constantly shape the state variables that we measure and use, the relations between the process and state variables are poorly represented or ignored to a large extent. In other words, the wind speed or temperature of the same magnitude at different times of the same day, as an example, has been understandably shaped by distinctly different sets of underlying physical processes at those two times. The reason for the distinguishing sets of physical processes in the morning, as opposed to later in the evening, is that the atmosphere is completely different at those two times. Traditional approaches that rely on the state variables tend to produce "similar" results for those two times of the day, without capturing the differences in the underlying physical processes.

Dr. Stalker developed a method to adjust initialized state variables over a period of simulation time by enabling the underlying physical processes to shape the state variables in what he calls an adiabatic mixing method. As a result of this method, final state variables, upon receiving influences of the underlying physical processes as they may occur at different times of the day, are more accurate when compared against actual observations than the state variables obtained using any of the traditional weather modeling approaches.

The RESPR atmospheric simulation platform is based on this methodology and has been used for this study in simulating the 15-months of meteorology for the conceptual

models and the meteorology for the three coupled met-chemistry episode simulations discussed in Section 3.4. Also, over the past decade, meteorological information based on the RESPR atmospheric platform was produced for different types of applications, including renewable energy site assessment and forecasting.

A manuscript based on his methodology is being prepared for publication titled "On Pushing Predictability Envelope by Going Beyond State Variables."

3.3 Preparation of emissions using Spatial Allocator and SMOKE

As mentioned in Section 3.2, RESPR-RAMS uses a rotated polar stereographic coordinate system. This new coordinate system has required us to run Spatial Allocator to create new spatial allocation (surrogate) files. A number of surrogate codes received new spatial allocations. A partial list of the surrogate codes that have been produced for this study are shown in Table 1. There are over a hundred surrogate codes included in the study. Shapefiles from various online sources, including the EPA database, have been used as input to Spatial Allocator to develop the surrogate files for use in emissions modeling.

| Surrogate code | Description |
|----------------|---------------------|
| 10 | Mexico population |
| 100 | Population |
| 105 | Population by State |
| 110 | Housing |
| 12 | Mexico housing |
| 120 | Urban population |
| 130 | Rural population |
| 131 | Urban housing |
| 132 | Suburban housing |
| 133 | Exurban housing |
| 134 | Rural housing |

| 137 | Hosing change |
|-----|--------------------------------|
| 14 | Mexico residential heatingwood |
| 140 | Housing change and population |

Table 1. A partial list of surrogate codes that received new spatial allocation.

While the new spatial allocation exercise was required because of the RESPR-RAMS model projection, our study has taken advantage of finer-resolution emissions data sets to improve such emissions as input to CAMx for ozone simulations. We have particularly improved emissions from mobile sources for the Cities of El Paso and Juarez, Mexico. These data sets have been provided by the EPMPO. Based on a travel demand model, the EPMPO has produced mobile emissions for El Paso (2010) and for Juarez, Mexico (2008).

The EPMPO has used travel demand modeling for a number of years. The EPMPO uses a variety of software within the four step modeling process to obtain travel speeds and link volumes throughout the EPMPO region. The EPMPO uses Transcad, TP+ and Viper, and Excel spreadsheets. The software programs along with demographic data, a detailed travel demand network, and substantial understanding of travel behavior for both the El Paso region and Ciudad Juarez provide the basis for the EPMPO's modeling effort.

The results of the travel demand model include volumes on each of the network links, as well as travel speeds. The model output also includes the ridership on El Paso Sun Metro Transit system. Combined with the use of EPA's Motor Vehicle Emissions Software (MOVES), this modeling approach can generate ozone precursor emissions at the national, state, and local levels. MOVES does not provide ozone amounts directly rather it provides nitrous oxides, carbon monoxide, and volatile oxygenated compound amounts by vehicle class for each link in the EPMPO network.

The study notes improvements (as shown in Figs. 2 and 3) in the mobile emissions representation compared with the data available from the EPA modeling platform database, hereafter referred to as the EPADB2011 (ftp://ftp.epa.gov/EmisInventory/2011v6/v2platform/).



Figure 2. Road links contained within the EPADB2011.



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Figure 3. Road linked provided by the EPMPO.

As mentioned before, another aspect of the emissions improvement effort undertaken for this study is about refining the biogenic representation. A brief overview on the data sources and the methodology used to improve the land use/land cover (LULC) representation is given in the following paragraph:

The biogenic precursor emissions were derived from the LULC data sets for the southwest United States and northern Mexico. The LULC map was developed using two different data sources which were then combined and consolidated into one polygon layer.

The two data sources are:

Mexico data- Source- Comisión Nacional para el Conocimiento y Uso de la Biodiversidad (CONABIO) Resolution- 1:250000 Projected coordinate system- Lambert Conformal Conic projection ITRF92 Site- http://www.conabio.gob.mx/ Accessed – February 16, 2016; Acquired - March 1, 2016

United States data-Source – United States Department of the Interior; United States Geological Survey National Land Cover Database 2011 Resolution – 1:250000 Projected coordinate system – Albers Conical Equal Area Site - http://www.mrlc.gov/nlcd11_data.php Accessed – November 24, 2015; Acquired – November 24, 2015.

The NLCD data were originally in raster format. The NLCD raster data geographic extent was clipped using the raster clip tool in the Data Management toolbox in ArcMap. The raster data were converted into a polygon layer using the "raster to polygon" tool in the ArcMap conversion toolbox. The Mexico data were originally in vector format. The Mexican LULC data were left in the vector format so that it could be matched to the NCLD data. The initial number of vegetation and land use categories for the NCLD data were 14 and the Mexican data were 18. The Mexico data and US data were reclassified to match the number of categories and have the same categories on both sides of the international border. The Mexico data were reclassified by comparing the description column against the Biogenic Emissions Landcover Database—version 4 (BELD4) classification. The description in the BELD4 uses NLCD classes thus the grid codes were only renamed to match the NLCD names used in the BELD 4 classification.

Of the 276 BELD4 land use/land cover categories, only 10 categories (within the 25-km domain) and 18 categories (within the 1-km domain) were found to be relevant to the study area. These categories are included in Table 2.

| BELD4 category name (25-km domain) | BELD4 category name (1-km domain) | Description |
|--|---|-----------------------------------|
| MODIS_0 | | Water |
| MODIS_1 | | Evergreen needleleaf forest |
| MODIS_3 | | Deciduous needleleaf forest |
| MODIS_6 | | Closed shrublands |
| MODIS_7 | MODIS_7 | Open shrublands |
| MODIS_8 | | Woody savannas |
| MODIS_10 | | Grasslands |
| MODIS_12 | | Croplands |
| MODIS_13 | | Urban and build-up land |
| MODIS_16 | MODIS_16 | Barren or sparsely vegetated land |
| | MODIS_4 | Deciduous broadleaf forest |
| | NLCD_11 | Open water |
| | NLCD_21 | Developed open space |
| | NLCD_22 | Developed land—low intensity |
| | NLCD_23 | Developed land—medium intensity |
| | NLCD_24 | Developed land—high intensity |
| | NLCD_31 | Barren land |
| | NLCD_41 | Deciduous forest |
| | NLCD_42 | Evergreen forest |
| | NLCD_51 | Dwarf shrub |
| | NLCD_52 | Shrub/scrub |
| | NLCD_71 | Grassland/Herbaceous |
| | NLCD_81 | Pasture/Hay |
| | NLCD_82 | Cultivated crops |
| | NLCD_90 | Woody wetlands |
| | NLCD_95 | Emergent herbaceous wetlands |

Table 2. BELD4 categories identified within 25- and 1-km model domains.

The above-mentioned shapefiles have been used as input to Spatial Allocator to create SMOKE-ready biogenic profile (BGPRO) and BELD4 NetCDF-formatted files.

As a result of the new BELD4 input files, this study notes improvements (as shown in Figs. 4 and 5) in the biogenic emissions representation compared with the EPADB2011. The Department of Geography, at NMSU, has led this effort.



Figure 4. EPA-provided urban development land cover extent (white).



Figure 5. NMSU-provided urban development land cover extent (white).

After the input data have been prepared and/or obtained from the EPADB2011, as the case may be, the SMOKE model has been used to produce output for four broad source category types (area, point, mobile, and biogenic sources). A total of eighteen sub-categories have been considered for this study and all of the sub-categories available for the study regions and individual episode periods have been included (see Table 3 for details). In other words, where input data were not available for certain sub-categories (e.g., c3marine and emissions from other regions (Mexico)), such sub-categories were omitted from the total merged emissions files.

| | , | | | |
|---|--|-----------------------------|------------------------|--|
| Sub-category | Description | General source category | SMOKE output file name | |
| Egu | Electrical generating units | Point (P) | PGTS_identifiers | |
| Dust | Fugitive dust | Area (A) | AGTS_identifiers | |
| Ag | Agriculture | Area (A) | AGTS_identifiers | |
| Ag fire | Agriculture fire | Area (A) | AGTS_identifiers | |
| C1c2 rail | Railroad emissions | Area (A) | AGTS_identifiers | |
| C3marine | Marine sources (N/A) | Area (A) | AGTS_identifiers | |
| Canada-Mexico dust | Fugitive dust (N/A) | Area (A) | AGTS_identifiers | |
| Canada-Mexico area | Other area sources | Area (A) | AGTS_identifiers | |
| Canada-Mexico mobile | Other mobile sources (Mexican emissions combined) | Mobile (M) MGTS_identifiers | | |
| Canada-Mexico point | Other point sources | Point (P) | PGTS_identifiers | |
| Mobile—rate per distance | Mobile sources from on- road emissions | Mobile (M) | MGTS_identifiers | |
| Mobile—rate per hour | Mobile—rate per hour Mobile sources from on- road emissions/hotelling | | MGTS_identifiers | |
| Mobile—rate per vehicle | Mobile sources from off- network emissions | Mobile (M) | MGTS_identifiers | |
| Mobile—rate per profiles Mobile sources from off- network emissions/parked/after trip vehicles | | Mobile (M) | MGTS_identifiers | |
| Negu Unidentified (independent) electrical generating units | | Point (P) | PGTS_identifiers | |
| Nonpt | U.S. nonpoint emissions | Area (A) | AGTS_identifiers | |
| Nonroad | U.S. nonroad emissions | Area (A) | AGTS_identifiers | |
| Nonpoint (oil &gas) | From unspecified oil & gas operations | Area (A) | AGTS_identifiers | |
| Point (oil &gas) | From location specific oil & gas operations | Point (P) | PGTS_identifiers | |
| RWC | Residential wood combustion | Area (A) | AGTS_identifiers | |
| Biogenics | BELD4 | Biogenics (B) | BGTS_identifiers | |
| Total | Merged emissions | N/A | EGTS_identifiers | |

Table 3. Emissions source sub-categories modeled using SMOKE.

These speciated, gridded, and diurnal emissions files have been created in hourly format to match the 25-hour meteorology files produced from the RESPR-RAMS model (additional details provided in Section 3.4). In fact, these meteorology data sets were used as input while running the SMOKE model for the three general source category types, i.e., mobile sources, point sources, and biogenic sources.

The total (merged) emissions files, named with the 'EGTS_identifiers' in Table 3, do contain emissions from all sub-categories except the PTEGU sources. These latter emissions are the point sources from electric generating units (EGUs). Emissions from the EGUs require special attention within CAMx as they have additional features, such as stack heights, stack diameters, etc. This type of points sources have been handled as the inline point source input to the CAMx runs, where such sources may be dispersed to multiple model layers as the case may be, depending on the meteorological conditions that may have existed during the three episodes.

A couple of others notes regarding the emissions preparation are: (1) emissions from fugitive dust were not included in the merged files as the current effort does not focus on particulate matter and (2) agriculture sub-category source emissions were not available for the 2011 episode runs.

In summary (see Table 4), the emissions modeling effort requires multiple steps in which the information of various emissions to start with is critically important, as it is used in all the subsequent steps. With the overall objective for the EPMPO to address international transport from Mexico quantitatively, the emissions sources for various categories become crucially important, but are usually unavailable for Mexico. With this limitation in mind, international transport is attempted to be addressed rather qualitatively in this study.

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| Step 1 | Step 2 | Step 3 | Step 4 | Step 5 |
|--------------------|--------------------|------------|----------|------------------|
| Emissions database | Spatial allocation | Speciation | Gridding | Diurnal profiles |

Table 4. The five-step emissions modeling process.

In addition to the 5-step process outlined in Table 4, the RESPR-RAMS produced meteorology gets used in some of the steps via the SMOKE model.

It is also worth noting that other input files (e.g., emission factor tables, temporal profile files, etc.), available from the EPADB2011, have been utilized to the fullest extent possible for this study.

3.4 Simulation results of ozone episodes

Simulations of three high-ozone episodes have been completed, one episode from each of the three years (2011-2013), to showcase the impact of the high-resolution (1-km) meteorology and improved emissions from mobile sources for El Paso and Juarez and biogenics. The simulation strategy used for all three episodes is the same, in which a nested grid, with 25-km, 5-km, and 1-km model domains, has been used to produce meteorological conditions for 5 consecutive days. In addition to the improved meteorology and emissions referred to above, an expanded innermost (1-km) domain (175 x 175) has been utilized, at the request of the EPMPO, to simulate County-wide ozone variability and potential sources of ozone via international transport (i.e., from Juarez, Mexico).

Meteorological conditions for the first three days of each simulation period are simulated in the coarsest, outer grid only. Meteorological conditions for the last two days of each high-ozone episode period are simulated using all three grids. The same vertical grid structure, with 35 model levels, is used for all three grids, for all three episodes (see

Table 5). Since the RESPR-RAMS uses the sigma-z vertical coordinate system, layer thickness compression adjustments are accounted for within CAMx. Both RAMS2CAMx and MCIP assign staggered cell face heights, using the mid-layer heights shown in Table 5, appropriately for certain meteorology variables (e.g., wind components). Only 35 of the 45 meteorology model levels are used for the coupled met-chemistry simulations discussed in the next several subsections.

| Layer # | Mid-layer height (m), above ground level |
|---------|--|
| 1 | 10 |
| 2 | 30 |
| 3 | 70 |
| 4 | 130 |
| 5 | 210 |
| 6 | 310 |
| 7 | 430 |
| 8 | 580 |
| 9 | 750 |
| 10 | 950 |
| 11 | 1200 |
| 12 | 1400 |
| 13 | 1580 |
| 14 | 1740 |
| 15 | 1890 |
| 16 | 1990 |
| 17 | 2090 |
| 18 | 2240 |
| 19 | 2440 |
| 20 | 2740 |
| 21 | 3240 |
| 22 | 4040 |
| 23 | 4940 |
| 24 | 5860 |

| 25 | 6780 |
|----|-------|
| 26 | 7680 |
| 27 | 8220 |
| 28 | 8780 |
| 29 | 9180 |
| 30 | 9530 |
| 31 | 10080 |
| 32 | 10330 |
| 33 | 10630 |
| 34 | 11030 |
| 35 | 12430 |

Table 5. Mid-layer heights of 35 coupled met-chemistry model levels used in CAMx.

The three simulation episode periods are summarized in Table 6.

| Episode | Day 1 | Day 2 | Day 3 | Day 4 | Day 5 |
|---------------|------------|-----------|-------------|-----------------------|-----------------------|
| 1 | 06/29/13 | 06/30/13 | 07/01/13 | <mark>07/02/13</mark> | <mark>07/03/13</mark> |
| (Day of week) | (Saturday) | (Sunday) | (Monday) | (Tuesday) | (Wednesday) |
| 2 | 06/25/12 | 06/26/12 | 06/27/12 | <mark>06/28/12</mark> | <mark>06/29/12</mark> |
| (Day of week) | (Monday) | (Tuesday) | (Wednesday) | (Thursday) | (Friday) |
| 3 | 06/18/11 | 06/19/11 | 06/20/11 | <mark>06/21/11</mark> | <mark>06/22/11</mark> |
| (Day of week) | (Saturday) | (Sunday) | (Monday) | (Tuesday) | (Wednesday) |

Table 6. The list of five consecutive meteorology days used for each of the three high-
ozone episodes.

All daylong (25 hours) meteorology simulation output files, prepared in hourly format, have the same time stamps shown in Table 7.

| Hour | Time (UTC) | Local Time (El Paso, TX) | Ozone output available? |
|------|-------------|-----------------------------|-------------------------------|
| 1 | 12:30:00 AM | 06:30:00 PM (*) | No |

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| | 25 | 12:30:00 AM (+) | 06:30:00 PM | Yes |

Table 7. Time stamps of the hourly meteorology and photochemistry output used for all three episodes ('+' indicates next day & "*" indicates previous day within their respective time zones).

As noted in the previous section, the individual sub-category and the total emissions files are also prepared for daylong emissions (25 hours), in hourly format, to match the time stamps of the meteorology (shown in Table 7).

In the next three subsections, simulation results of the three episodes are presented. Some background information is provided here that is common to all three episodes. First, the emissions modeling required extensive time and effort in gathering input (e.g., mobile sources for Cities of El Paso and Juarez), spatial allocation, and the SMOKE modeling effort than what was anticipated in early stages of the study. Because of this additional effort, we have had to resort to a "one-way" nesting approach for coupled met-chemistry modeling effort than the fully-coupled (two-way nesting) simulations originally contemplated using CAMx. The one-way nesting we refer to here is the procedure in which boundary/initial conditions for day 4 are provided from the day 3 coarse-resolution (25-km) runs. On day 5, the restart option, available in CAMx, is used from the previous day (day 4) conditions. This type of one-way nesting approach was required because of the prolonged time line for the emissions modeling mentioned above.

The negative influences (if any) of the one-way nesting used for these simulations should be evaluated against actual observations of ozone, just as those results that are usually produced using a fully-coupled met-chemistry modeling approach. Since observations of ozone are not available at many locations for validation within this large domain, one of the recommendations the current study makes is about investing in ozone monitoring. We also recommend that a two-way nesting approach is used within CAMx and evaluated in future investigations.

3.4.1 Episode 1 (June 29-July 3, 2013)

The ozone output near the surface (level 1) from the 25-km run for day 1 (June 29, 2013) is shown in Figure 6. Figure 6 shows that the combined ozone plume from the two metropolitan Cities (hereafter refer to as the COP) is slightly pushed to the northwest in response to the southeasterly flow.

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Figure 6. The COP is oriented in the northwest direction at the end of day 1.

On day 2 (June 30, 2013), the COP is slightly pushed to the north from where it was the previous day (on day 1), in response to the southerly flow on day 2 (shown in Figure 7).



Figure 7. The COP is oriented in the north direction at the end of day 2.

On day 3 (July 1, 2013), the COP gets moved to the west in response to a faster easterly flow as shown in Figure 8. Figure 8 also shows that the plume actually gets dispersed and diffused indicating more horizontal mixing in addition to transport.

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Figure 8. The coherent structure of the COP is absent at the end of day 3, with relatively higher ozone concentrations to the west, northwest, southwest, and south of the metropolitan Cities.

On day 4, the high-resolution (1-km) simulation is performed using the initial and boundary conditions from day 3. Figure 9 shows that the ozone levels are in the 40 to

55 PPB range in the western part of El Paso County with the highest values found further downstream in southern New Mexico.



Figure 9. Relatively higher ozone concentrations are found to the west of El Paso City, with higher concentrations found within El Paso County along the El Paso County-New Mexico border.

The high-resolution simulation continued on day 5 as a restart run from the previous day (day 4). The El Paso County ozone distribution changes further from the previous day (day 4) on day 5 in that the relatively higher ozone concentrations to the west are now pushed further to the west (into New Mexico), while those higher ozone concentrations to the north of El Paso City get transported southward into El Paso County (as shown in Figure 10).



Figure 10. Higher ozone concentrations from the previous day (day 4) are transported south (found to the east of El Paso City).

From these 5-day ozone simulations, it can be qualitatively inferred that the COP gets transported to the west first and gets broken up through horizontal mixing before some of it gets transported back into El Paso County, depending on the prevailing meteorological conditions. The fate of the original COP may take on highly variable ozone distributions within El Paso City and County, in response to the emissions and meteorology. Based on this episode, it can be deduced that international transport seems to be present, although the ultimate ozone concentrations found in El Paso County seem to result from multiple interactions and pathways than direct transport from Mexico.

Time series data of ozone concentrations for the two high-resolution simulation days (days 4 and 5) are shown in Figure 11 at the University of Texas, El Paso monitor location (hereafter referred to as UTEPM). The UTEPM is also the center point of the nested model domains used for the RESPR-RAMS simulations. Figure 11 shows that on both days, the ozone behavior during the evening to early morning hours indicate relatively stronger transport from adjacent areas, while the afternoon ozone concentrations indicate loss of ozone due to transport to the adjacent areas and due to possible surface deposition. Peak ozone values are simulated at 4:30PM and 2:30PM on days 4 and 5, respectively (see Figure 11).

These simulated values of ozone at the UTEPM are compared with ozone observations over the same two days to shed light on the performance of the coupled met-chemistry modeling effort conducted for this study.

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Figure 11. Time series of simulated ozone at the UTEPM during days 4 and 5 (episode 1).

3.4.2 Episode 2 (June 25-June 29, 2012)

The ozone output near the surface (level 1) from the 25-km run for day 1 (June 25, 2012) is shown in Figure 12. Figure 12 shows that the COP from the two cities is prominently pushed to the northwest in response to the relatively stronger southeasterly flow.

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Figure 12. The COP is oriented in the northwest direction at the end of day 1.

On day 2 (June 26, 2012), the COP is pushed to the north from where it was the previous day (on day 1), in response to the southerly flow on day 2 (shown in Figure 13).



Figure 13. The COP is oriented in the north direction at the end of day 2.

On day 3 (June 27, 2012), the COP gets moved to the north in response to a weak southerly flow as shown in Figure 14. Figure 14 shows that the plume does not get dispersed or diffused, as was the case on day 3 of episode 1, indicating relatively weaker horizontal transport and mixing.



Figure 14. The COP structure is intact at the end of day 3.

On day 4, the high-resolution (1-km) simulation is performed using the initial and boundary conditions from day 3. Figure 15 shows that the ozone levels are in the 60 to 90 PPB range in the western part of El Paso County with the highest values found near

the El Paso County-Dona Ana County (New Mexico) border. Also, the entire El Paso County shows ozone concentrations in excess of 60 PPB (see Figure 15).



Figure 15. Higher ozone concentrations are found west of El Paso City, with relatively higher concentrations found within El Paso County along the El Paso County-New Mexico border.

The high-resolution simulation continued on day 5 as a restart run from the previous day (day 4). The El Paso County ozone distribution changes further from the previous day

(day 4) on day 5 in that the higher ozone concentrations to the west of El Paso City are now pushed further to northeast (into northwest of El Paso County and New Mexico), while relatively higher ozone concentrations to the north of El Paso City get transported southward into El Paso County over a wider area (as shown in Figure 16).



Figure 16. Relatively higher ozone concentrations from the previous day (day 4) are transported south (found to the east of El Paso City over a wider region of El Paso County).

From these 5-day ozone simulations, it can be qualitatively inferred that the COP gets transported to the northwest first and the coherent structure of the COP is maintained through day 3. The high-resolution simulation days (days 4 and 5) show that high ozone concentrations are transported to a wider region of El Paso County. Based on this episode, it can be deduced that international transport seems to be present. It also appears that ozone concentrations found in El Paso County seem to result from international transport without going through multiple stages and pathways as during episode 1. The area affected is also much wider within El Paso County during episode 2. It is noteworthy, however, that the collective effect of the COP is what can be deduced here, not specifically from international transport alone.

Time series data of ozone concentrations for the two high-resolution simulation days (days 4 and 5) are shown in Figure 17 at UTEPM. Figure 17 shows that on both days, the ozone behavior during the evening to early morning hours seems to follow usual pattern of slowing ozone production, while the afternoon ozone concentrations indicate no significant loss due to transport to the adjacent areas on day 4. Day 5 shows relatively smaller ozone concentrations in the after indicating loss due to transport to adjacent areas. Peak ozone values are simulated at 12:30PM and 4:30PM on days 4 and 5, respectively (see Figure 17).

Also, these simulated values of ozone at the UTEPM are compared with ozone observations over the same two days, as for episode 1, to shed light on the performance of the coupled met-chemistry modeling effort conducted for this study.

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Figure 17. Time series of simulated ozone at the UTEPM during days 4 and 5 (episode

2).

3.4.3 Episode 3 (June 18-June 22, 2011)

The ozone output near the surface (level 1) from the 25-km run for day 1 (June 18, 2011) is shown in Figure 18. Figure 18 shows that the COP from the two cities is prominently pushed to the east in response to the relatively stronger westerly flow.



Figure 18. The COP is oriented in the east direction at the end of day 1.

On day 2 (June 19, 2011), the COP is pushed to the northeast from where it was the previous day (on day 1), in response to the southwesterly flow on day 2 (shown in Figure 19).



Figure 19. The COP is oriented in the northeast direction at the end of day 2.

On day 3 (June 20, 2011), the COP gets moved further to the east in response to a stronger westerly flow as shown in Figure 20. Figure 20 shows that the plume does not get dispersed or diffused, as was the case on day 3 of episode 1, even though relatively stronger horizontal transport is present.



Figure 20. The COP structure is intact at the end of day 3 (episode 3).

On day 4, the high-resolution (1-km) simulation is performed using the initial and boundary conditions from day 3. Figure 21 shows that the ozone levels are in the 55 to 60 PPB range in the western part of El Paso County. The rest of El Paso County shows ozone concentrations below 60 PPB (see Figure 21). The highest ozone concentrations are found well to the south of the Metropolitan Cities in Mexico.



Figure 21. Relatively lower ozone concentrations are found to the west of El Paso City, with relatively higher concentrations found within El Paso County in the south central part of the County.

The high-resolution simulation continued on day 5 as a restart run from the previous day (day 4). The El Paso County ozone distribution changes further from the previous day (day 4) on day 5 in that higher ozone concentrations, up to 80 PPB, are now found to the west of El Paso City. Also, relatively higher ozone concentrations, up to 60 PPB, are found within a broader central part of El Paso County (as shown in Figure 22). Highest ozone concentrations are found in Mexico.



Figure 22. Relatively higher ozone concentrations from the previous day (day 4) are transported to the northeast (found to the west of El Paso City). A wider central part of El Paso County have relatively higher ozone concentrations compared with the previous day (day4).

From these 5-day ozone simulations, it can be qualitatively inferred that the COP gets transported to the east first and the coherent structure of the COP is maintained through day 3. The high-resolution simulation days (days 4 and 5) show that high ozone concentrations are transported to the south into Mexico. Based on this episode, it can be deduced that international transport seems to be present, except it is in the opposite direction into Mexico. It also appears that ozone concentrations found in El Paso County seem to result from transport toward the northwest on day 5. The area affected is also much wider within El Paso County during episode 3, similar to episode 2.

Time series data of ozone concentrations for the two high-resolution simulation days (days 4 and 5) are shown in Figure 23 at UTEPM. Figure 23 shows that on both days, the ozone behavior during the evening to early morning hours seems to follow usual pattern of slowing ozone production, while the afternoon ozone concentrations indicate no significant loss due to transport to the adjacent areas on day 5. Day 4 shows relatively smaller ozone concentrations in the afternoon indicating loss due to transport to adjacent areas. Peak ozone values are simulated at 4:30PM and 5:30PM on days 4 and 5, respectively (see Figure 23).

Also, these simulated values of ozone at the UTEPM are compared with ozone observations over the same two days, as for episodes 1 and 2, to shed light on the performance of the coupled met-chemistry modeling effort conducted for this study.

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Figure 23. Time series of simulated ozone at the UTEPM during days 4 and 5 (episode 3).

3.4.4 Comparison against observations for assessing model performance

Simulation results from the three episodes, presented in Subsection 3.4.3, show how ozone concentrations vary in and around El Paso and within El Paso County. Local production of ozone and ozone gain and loss due to transport can vary significantly due to the emissions of precursors and meteorological conditions. Even though the overall

approach employed for this study should be further improved from all the standpoints of emissions, spatial allocation, SMOKE modeling, meteorology, and coupled metchemistry modeling, some results of comparison against observations of ozone at the UTEPM are provided in Tables 8 (episode 1), 9 (episode 2), and 10 (episode 3).

| Episode ==>hour | Simulated Ozone-Day 4 (PPB) | Observed Ozone-Day 4 (PPB) | Simulated- Observed (PPB) | Simulated Ozone-Day 5 (PPB) | Observed Ozone-Day 5 (PPB) | Simulated- Observed (PPB) |
|--------------------|-----------------------------------|----------------------------------|---------------------------------|-----------------------------------|----------------------------------|---------------------------------|
| 1==>1 | 44.3 | 50.2 | -5.9 | 49.9 | 54.9 | -5 |
| 1==>2 | 41.4 | 48.6 | -7.2 | 50.9 | 54.5 | -3.6 |
| 1==>3 | 39.9 | 46 | -6.1 | 50.1 | 55.4 | -5.3 |
| 1==>4 | 36.8 | 43 | -6.2 | 47.1 | 54.7 | -7.6 |
| 1==>5 | 35.9 | 40.3 | -4.4 | 44 | 51.5 | -7.5 |
| 1==>6 | 36.2 | 37.2 | -1 | 41.2 | 51.3 | -10.1 |
| 1==>7 | 36.7 | 42.4 | -5.7 | 40.1 | 44.5 | -4.4 |
| 1==>8 | 37 | 45.9 | -8.9 | 37.2 | 49.4 | -12.2 |
| 1==>9 | 37 | 46.1 | -9.1 | 38.5 | 53.2 | -14.7 |
| 1==>10 | 37.2 | 44.2 | -7 | 43.2 | 52.3 | -9.1 |
| 1==>11 | 36.7 | 44.5 | -7.8 | 43.5 | 48.5 | -5 |
| 1==>12 | 36 | 41.7 | -5.7 | 43 | 48.3 | -5.3 |
| 1==>13 | 35.2 | 40.4 | -5.2 | 41.1 | 48.4 | -7.3 |
| 1==>14 | 29.5 | 41.8 | -12.3 | 41 | 52.1 | -11.1 |
| 1==>15 | 25.6 | 50.3 | -24.7 | 33.2 | 51.6 | -18.4 |
| 1==>16 | 26.9 | 55.7 | -28.8 | 32 | 57.6 | -25.6 |
| 1==>17 | 30 | 62 | -32 | 34.5 | 69.3 | -34.8 |
| 1==>18 | 33.8 | 64.5 | -30.7 | 39 | 76 | -37 |
| 1==>19 | 39 | 65.5 | -26.5 | 45.3 | 83.9 | -38.6 |
| 1==>20 | 46.5 | 67.8 | -21.3 | 53.7 | 86.7 | -33 |
| 1==>21 | 49.8 | 66.3 | -16.5 | 53.1 | 93.7 | -40.6 |
| 1==>22 | 50.4 | 66.2 | -15.8 | 51.1 | 90 | -38.9 |
| 1==>23 | 49.7 | 63.5 | -13.8 | 52.8 | 86 | -33.2 |
| 1==>24 | 48.8 | 58.7 | -9.9 | 53.5 | 79.5 | -26 |

Table 8. Comparison of simulated ozone against observed ozone at the UEPM (episode

1).

| Episode ==>hour | Simulated Ozone-Day 4 (PPB) | Observed Ozone-Day 4 (PPB) | Simulated- Observed (PPB) | Simulated Ozone-Day 5 (PPB) | Observed Ozone-Day 5 (PPB) | Simulated- Observed (PPB) |
|--------------------|-----------------------------------|----------------------------------|---------------------------------|-----------------------------------|----------------------------------|---------------------------------|
| 2==>1 | 42.3 | 29.7 | 12.6 | 45.5 | 47.5 | -2 |
| 2==>2 | 42.1 | 7.6 | 34.5 | 41.1 | 16 | 25.1 |
| 2==>3 | 42.3 | 13.8 | 28.5 | 40.9 | 23 | 17.9 |
| 2==>4 | 43.5 | 34.4 | 9.1 | 42.8 | 34.2 | 8 |
| 2==>5 | 40.6 | 36.4 | 4.2 | 38.3 | 34.6 | 3.7 |
| 2==>6 | 32.5 | 39.1 | -6.6 | 37.5 | 33.6 | 3.9 |
| 2==>7 | 28 | 38.2 | -10.2 | 37.3 | 35.8 | 1.5 |
| 2==>8 | 39.8 | 33.4 | 6.4 | 38.6 | 32.5 | 6.1 |
| 2==>9 | 38.5 | 30.5 | 8 | 41 | 27 | 14 |
| 2==>10 | 32.5 | 27.5 | 5 | 40.9 | 29.3 | 11.6 |
| 2==>11 | 30.4 | 26.5 | 3.9 | 40.6 | 22 | 18.6 |
| 2==>12 | 29.8 | 16.9 | 12.9 | 37.3 | 25.4 | 11.9 |
| 2==>13 | 31.8 | 21.4 | 10.4 | 33.8 | 24.3 | 9.5 |
| 2==>14 | 38 | 31.5 | 6.5 | 35.9 | 35.6 | 0.3 |
| 2==>15 | 43.6 | 44 | -0.4 | 38.3 | 49.4 | -11.1 |
| 2==>16 | 55.5 | 64.6 | -9.1 | 41.2 | 58.3 | -17.1 |
| 2==>17 | 67.1 | 78 | -10.9 | 43.9 | 70.7 | -26.8 |
| 2==>18 | 71.3 | 73.5 | -2.2 | 43.2 | 71.5 | -28.3 |
| 2==>19 | 69.9 | 73.5 | -3.6 | 44.5 | 80.9 | -36.4 |
| 2==>20 | 62.2 | 73 | -10.8 | 47.6 | 95.3 | -47.7 |
| 2==>21 | 55.9 | 73.7 | -17.8 | 55.1 | 73.6 | -18.5 |
| 2==>22 | 52.3 | 76.4 | -24.1 | 57.3 | 65.8 | -8.5 |
| 2==>23 | 40 | 73.5 | -33.5 | 51.5 | 57.5 | -6 |
| 2==>24 | 42 | 65.5 | -23.5 | 51.2 | 49.5 | 1.7 |

Table 9. Comparison of simulated ozone against observed ozone at the UEPM (episode

2).

| Episode | Simulated | Observed | Simulated- | Simulated | Observed | Simulated- |
|---------|-------------|-------------|------------|-------------|-------------|------------|
| ==>hour | Ozone-Day 4 | Ozone-Day 4 | Observed | Ozone-Day 5 | Ozone-Day 5 | Observed |
| | (PPB) | (PPB) | (PPB) | (PPB) | (PPB) | (PPB) |

| 3==>1 | 47.3 | 59.4 | -12.1 | 37.3 | 51.3 | -14 |
|--------|------|------|-------|------|------|-------|
| 3==>2 | 48.3 | 46.7 | 1.6 | 28.6 | 16.9 | 11.7 |
| 3==>3 | 46.5 | 46.6 | -0.1 | 29.7 | 18.2 | 11.5 |
| 3==>4 | 38.7 | 50.3 | -11.6 | 34.1 | 8.4 | 25.7 |
| 3==>5 | 32.8 | 51.7 | -18.9 | 36.5 | 3.3 | 33.2 |
| 3==>6 | 29.7 | 44.2 | -14.5 | 40.7 | 4.7 | 36 |
| 3==>7 | 27.3 | 42.5 | -15.2 | 38.7 | 4.6 | 34.1 |
| 3==>8 | 25.5 | 37.6 | -12.1 | 28.6 | 14 | 14.6 |
| 3==>9 | 23.9 | 24 | -0.1 | 29.8 | 21.3 | 8.5 |
| 3==>10 | 22.7 | 14.4 | 8.3 | 26.9 | 21.2 | 5.7 |
| 3==>11 | 22.2 | 24.7 | -2.5 | 24.3 | 8.7 | 15.6 |
| 3==>12 | 22.4 | 35.2 | -12.8 | 22 | 11.2 | 10.8 |
| 3==>13 | 34.3 | 42.9 | -8.6 | 26 | 38.2 | -12.2 |
| 3==>14 | 37.6 | 42.8 | -5.2 | 30.6 | 43.2 | -12.6 |
| 3==>15 | 33.2 | 47.7 | -14.5 | 30.7 | 50 | -19.3 |
| 3==>16 | 34.4 | 51.1 | -16.7 | 33.9 | 63.4 | -29.5 |
| 3==>17 | 38.2 | 54.6 | -17.4 | 41 | 75.8 | -34.8 |
| 3==>18 | 39.4 | 59 | -19.6 | 43.2 | 78.6 | -35.4 |
| 3==>19 | 39.3 | 61.8 | -22.5 | 44.9 | 78.2 | -33.3 |
| 3==>20 | 39.5 | 63.1 | -23.6 | 50.1 | 77.5 | -27.4 |
| 3==>21 | 39.3 | 62.3 | -23 | 54.1 | 78.7 | -24.6 |
| 3==>22 | 39.9 | 58.8 | -18.9 | 53.6 | 82.7 | -29.1 |
| 3==>23 | 39 | 58 | -19 | 55.6 | 78.1 | -22.5 |
| 3==>24 | 39.2 | 57.8 | -18.6 | 51.9 | 78.4 | -26.5 |

Characterization and International Transport of Ozone Precursor Emissions in the El Paso, Texas Region

Table 10. Comparison of simulated ozone against observed ozone at the UEPM (episode 3).

Model performance based on the single location comparison shown in Tables 8 through 10 indicates the coupled met-chemistry simulations have mostly under estimated ozone at that one location. This issue needs to be addressed in future studies by investigating model coupling issues, validity of vertical diffusion values and the derived planetary boundary layer (PBL) heights, as well as emissions allocation and modeling.

Characterization and International Transport of Ozone Precursor Emissions in the El Paso, Texas Region 4.0 Supporting Understanding for Conceptual Models

Conceptual models are those that lead to qualitative to, in some cases, quantitative understanding of how a set of variables (e.g., meteorology) affects a pollutant's behavior of interest (e.g., ozone). As an example, if a reliable conceptual model can be developed that allows the user to ascertain that certain meteorological conditions, such as low-wind conditions, low humidity, and high temperatures, are conducive to high-ozone occurrence within a region of interest, such a conceptual model is highly desirable to have. However, of high-utility conceptual models about the ozone behavior within a region, such as the El Paso City area, can only be developed based on robust meteorological information, high-quality ozone measurements, coupled met-chemistry modeling efforts, etc.

In this section, robust meteorology data sets produced using the RESPR-RAMS approach are analyzed for the month of May (2011, 2012, and 2013) and how those meteorological variables are related to the observed ozone values are discussed. The analysis examples presented here will allow the EPMPO to further develop other conceptual models based on these data sets.

In the above context, the EPMPO will have access to the simulations of fifteen months (May through September of 2011, 2012, and 2013) that RESPR has completed using three nested grids with 25-km, 5-km, and 1-km model domains. Note that the innermost grid (1-km) for the 15-month meteorology simulations has fewer number of grid cells (60x51), compared with the 1-km finer grid (175x175) employed for the episode simulations. The vertical grid structure has been fine-tuned for the episode simulations too, to take advantage of vertical model levels used by another ozone modeling group, with years of air quality modeling experience.

The example analyses shown in this section give rise to supporting understanding for several conceptual models. For example, the May 2011 simulations show that maximum horizontal wind speed values of up to 9 m/s are typically found over the high-terrain areas of the Franklin Mountains to the north of El Paso City and relatively larger wind speed values over the Sierra de Juarez to the southwest (Figure 24). Figure 24 also shows that the wind speed values in the valley are in the range of 2.5 to 3.5 m/s. The horizontal wind speed gradient between the valley and the Franklin Mountains can be one of the diagnostic parameters that can yield a useful conceptual model for diagnosing if a particular day has the potential for high ozone production. In the analysis presented here, larger is this gradient, less likely is the high-ozone production. As summarized in Table 11, high ozone days were more prevalent in May 2013 (with the smallest horizontal wind speed gradient), compared to May 2011 (with the largest horizontal wind speed gradient).

Similarly, analysis of wind direction for the three months shows that the relative wind direction from the west to northwest and east to southeast into the valley can lead to complex flow interactions. Because of the potential for such complex flow interactions, wind direction alone does not seem to yield a good diagnostic parameter for a conceptual model (see Figure 25).

Relatively higher temperature (shown in Figure 26) and low humidity values (not shown) of 22 degrees (Celsius) and 32% (shown in Table 11), respectively, seem to be conducive to high ozone production. A single diagnostic parameter based on temperature or humidity or a hybrid diagnostic parameter by combining temperature and humidity can be developed to support another conceptual model.

Finally, with respect to wind direction, there is a shift in flow to southerly noted for May 2013, compared with May 2011 or May 2012. Since May 2013 had more number of

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higher ozone days, this southerly flow can be used as a good diagnostic parameter for a conceptual model (see Figure 27 and Table 11). As summarized in Table 11, a host of other atmospheric variables, such as vertical motion, wind shear, planetary boundary layer (PBL) heights can be used as either single diagnostic parameters or as hybrid diagnostic parameters for various conceptual models of interest to the EPMPO.



Figure 24. Maximum wind speed locations found over Franklin Mountains.



Figure 25. Domain-averaged wind direction for the month of May (2012) shows southeasterly wind.



Figure 26. Maximum temperature values (C) are simulated for May 2012.

Wind direction shows a southeasterly shift of 15 degrees compared for May 2013 compared with May 2012 to the south of the Sierra de Juarez mountains (Figure 27).



Figure 4. Southeasterly wind shift of 15 degrees for May (2013) compared to May (2012).

| Variable | May2011 | May2012 | May2013 | Notes/comments |
|------------------------------|---------|---------|---------|---|
| Wind speed (m/s)—max | 9 | 8.5 | 8 | High wind speed values are typically found near mountain tops. |
| Wind speed (m/s)—min | 2.5 | 2.5 | 2.5 | Lowest in wind speed values are found typically in the valley, although May 2013 exhibited relatively stronger wind speed values. |
| Wind direction (deg) —max | 235 | 220 | 230 | Southwesterly wind shift in the valley and southerly wind shift over Sierra de Juarez for May 2013. |
| Wind direction (deg) —min | 180 | 160 | 175 | Southeasterly wind into the valley leads to complex flow interactions as for May 2012. |
| Vertical speed (m/s)—max | 0.6 | 0.3 | 0.5 | Vertical transport in the valley is minimum for May 2012. |
| Vertical speed (m/s)—min | -0.6 | -0.35 | -0.5 | Maximum vertical wind speed values are on the lee side of the mountains. |
| Vertical shear (1/s)—max | >0.039 | >0.032 | >0.032 | Vertical shear differences are not appreciable, but smallest for May 2012. |
| Vertical shear (1/s)—min | >0.015 | >0.014 | >0.014 | |
| Temperature (C)—max | 21.5 | 23.5 | 22.5 | Maximum temperature values are found in the valley. |
| Temperature (C)—min | 16.5 | 19 | 18 | |
| Rel. humidity (%) —max | 29.5 | 36 | 32 | Near maximum relative humidity values are found in the valley. |
| Rel. humidity (%) —min | 23.5 | 29 | 26 | |
| PBL height (m) —max | 1800 | 2100 | 2200 | |
| PBL height (m) —min | 1100 | 1400 | 1400 | |
| Pressure (mb) —max | 890 | 890 | 890 | |
| Pressure | 810 | 820 | 820 | |

| (mb) —min | | | | |
|---|------|------|------|---|
| Total precip (mm) —max | 0 | 0.45 | 0.7 | Precip on mtn tops for May 2012. |
| Total precip (mm) —min | 0 | 0.05 | 0.05 | Trace precip east of valley for May 2013. |
| Solar radiation (kWh/m^2/day) —max | 9.55 | 9.2 | 9.2 | Solar radiation values are near maximum in the valley for months. |
| Solar radiation (kWh/m^2/day) —min | 9.05 | 8.6 | 8.7 | |
| Ozone obs (# of days exceeding 55 PPB at UTEP station) | 15 | 17 | 20 | |

Table 11. Comparative analysis of three months of May (2011, 2012, and 2013).

5.0 Summary, Conclusions, and Recommendations

This study has undertaken a comprehensive approach to performing coupled metchemistry simulations by employing improvements in the mobile and biogenics emissions. It has also made improvements in meteorology by completing finest resolution (1-km) atmospheric simulations, based on the adiabatic mixing methodology that Dr. Stalker developed and perfected over a decade at RESPR. The RESPR-RAMS approach required the development of new surrogate files for spatial allocation of emissions via Spatial Allocator. The study has also chosen the CB6 (carbon bond version 6) chemical mechanism option. The study has completed 1-km resolution coupled met-chemistry simulations using a one-way nesting approach for three specific episodes in 2011 (episode 3), 2012 (episode 2), and 2013 (episode 1). Each episode simulation has been conducted over a 5-day period, with the first three days simulated within the 25-km outer domain for background conditions for the last two days of highresolution (1-km) simulations.

This comprehensive approach was chosen to address many of the deficiencies that tend to exist in the current approaches so the current study did not particularly aim to get the "right" answers for the wrong reasons. Instead it has sought to produce answers for the right reasons.

While the solutions of ozone show some larger deviations from observed ozone (see Tables 8, 9, and 10), this approach provides the basis for future improvements through additional modeling improvements and evaluation studies.

With the recognition of the other unresolved issues that may still exist in the approach undertaken for this study, the study offers the following conclusions:

- The combined ozone plume (COP) from the two metropolitan cities of El Paso and Juarez is wider and more coherent than either single city plume individually.
- Under stagnant meteorological conditions, the COP can maintain its coherent structure for a longer period of time than under meteorological conditions that can transport and diffuse the COP or if the plume was from a single city on either side of the border.
- A high-ozone event in the area is a culmination of emissions, photochemistry, meteorological influences, etc. for several days prior to the actual event. It is critically important to capture all those transformations of ozone and its precursors over that long prior period in order to simulate an ozone event with the highest accuracy.
- Ozone at a location can be viewed as a result of: net local ozone production [A] + net horizontal transport [B] + net vertical transport [C] net loss due to dry and wet deposition [D] +/- other sources/sinks due to various chemical interactions [E]. Factors A, B, C, and D are influenced by the meteorological model as well as the photochemical model, while factor E is directly influenced by the

photochemical mechanisms implemented in the photochemical model and indirectly influenced by the meteorology ingested into the photochemical model.

 The three episodes simulated show that international transport is likely common occurrence, although such transport may not be just confined to the western part of El Paso County. International transport can be seen well into New Mexico and into the central parts El Paso County, as well as into Mexico depending on the prevailing meteorological conditions on the day of a high-ozone event. As noted before, the days prior to a high-ozone event are just as important to identify and quantify international transport.

This study recommends the following as part of future met-chemistry modeling efforts:

- Improve emissions, particularly for Mexico, and emissions modeling via further refinements in spatial allocation and SMOKE modeling.
- Improve horizontal/vertical transport and mixing by implementing a fully-coupled (two-way) nested CAMx simulations.
- Improve CAMx simulations further by ingesting more meteorological information on such atmospheric variables as vertical motion, turbulence, precipitation, solar radiation, etc.
- Collect ozone measurements at strategic locations that can be ascertained readily based on the high-resolution ozone simulations presented in this study.
- Conduct extensive model validation efforts against ozone observations for not only the three episodes completed for this study, but for other episodes (to be selected) with their own unique meteorological conditions.
- Upon successful completion of the above-mentioned improvements and model evaluation efforts, the coupled modeling approach used in this study can yield a tool for the EPMPO for performing useful short-term forecasting for the purposes

of health management/mitigation and for performing long-term forecasting, up to 6+ months, for long-range planning purposes.

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