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SIMULATION OF WINTERTIME HIGH OZONE CONCENTRATIONS IN SOUTHWESTERN WYOMING

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1. INTRODUCTION

Oil and gas production in the western states has increased as demand for domestic sources of energy has risen. Under the National Environmental Policy Act (NEPA), the development of an oil and gas production project on federal land usually involves the preparation of an Environmental Impact Statement (EIS) or Environmental Assessment (EA) that discloses the potential environment effects of the project. Such environmental effects include the potential impacts of emissions from oil and gas production on air quality (AQ) and air quality-related values (AQRVs), which include visibility and acid deposition. High wintertime ozone concentrations have recently been observed in otherwise rural regions of the U.S. where intensive oil and gas production activity is occurring (ENVIRON, 2008a: Schnell et al., 2009). Therefore, recent oil and gas EISs have applied photochemical grid models (PGMs) to address potential ozone impacts as well as AQ and AQRV impacts (BLM, 2006).

The basic modeling strategy used in an EIS that employs a PGM is to first simulate a current year base case without the proposed Project using a comprehensive regional emission inventory of actual emissions from all sources (motor vehicles. power plants, biogenic sources, etc.). The base case simulation is evaluated with respect to ambient air quality measurements. If the base case simulation reproduces concentrations of observed species with reasonable fidelity, then the model can be used in a future year assessment of Project impacts. The future year modeling involves development of a future year Project emission inventory as well as a future year regional emission inventory. Project AQ and AQRV impacts are determined from the future year PGM simulations.

This paper presents the use of the <u>Comprehensive Air Quality Model with Extensions</u> (CAMx) (ENVIRON, 2008b) PGM to simulate winter high ozone events in southwest Wyoming

2. MODEL CONFIGURATION

To assess the AQ and AQRV impacts of the proposed oil and gas development located in southwest Wyoming, CAMx is applied for both base year and future year simulations on a 36/12/4 km nested-grid modeling domain (Figure 1). The 36 km grid covers the continental United States and serves to provide boundary conditions to the finer grids. Boundary conditions for the 36 km continental U.S. modeling domain are based on the output of the GEOS-CHEM global chemistry model simulation.



Fig. 1. 36/12/4 km Nested CAMx Modeling Domain.

The main study area lies within the 12/4 km modeling domain shown in Figure 2. Also shown in Figure 2 is the proposed oil and gas development project area, locations of monitoring sites and several Wilderness Areas within the Wind River Range in southwest Wyoming. Of particular note are the state industrial monitoring sites to the immediate southwest of the Bridger-Fitzpatrick Wilderness Areas where high wintertime ozone concentrations have been observed.

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Fig. 2. CAMx 12/4 km modeling domain.

CAMx was applied for the calendar years of 2005 and 2006 using actual emissions of NOx, SO₂, PM₁₀, PM_{2.5}, VOC and CO from all sources for those years. Detailed emission inventories of oil and gas production sources in the 12/4 km domain have been compiled for these periods, and a comprehensive regional emission inventory for the 36/12/4 km modeling domain has been prepared. CAMx output gas and particle phase model concentrations were compared against observed values for the two modeled base years in a model performance evaluation. In addition to comparison of predicted and observed ozone concentrations, the model performance evaluation also assessed the ability of the model to reproduce the observed particulate matter (PM_{2.5}) mass and individual PM species (e.g., sulfate, nitrate, elemental carbon, organic carbon and crustal) as well as ozone and PM2.5 and ozone precursor and related product species.

3. WINTER OZONE FIELD STUDY

During the winters of 2007, 2008 and 2009, the Wyoming Department of Environment Quality (WDEQ) collected enhanced meteorological and air quality observations to help understand the causes of the winter elevated ozone concentrations. Figure 3 displays the locations of the fixed year-round monitoring sites that include the Pinedale CASTNet site as well as WDEQ Boulder, Jonah and Daniel ozone monitoring sites in Sublette County, Wyoming. The enhanced winter field study collected additional ozone precursor (VOC and NOx) air quality measurements and additional surface and upperair meteorological observations, as well as ultraviolet (UV) radiation measurements.



Fig. 3. Southwest Wyoming study area for the winter field study showing the fixed monitoring sites in Sublette County.

Although no high ozone readings were measured during the 2007 winter field study, during 2008 several observed high ozone episodes occurred in southwestern Wyoming with a peak daily maximum 8-hour ozone concentration of 122 ppb. The field study results found that the following six conditions occurred at the same time as the observed high winter ozone concentrations (ENVIRON, 2008a):

- 1. White snow on ground (high albedo)
- 2. Shallow inversion (limited mixing)
- 3. Few or no clouds (no attenuation of UV violet radiation)
- 4. Stagnant and/or recirculating winds (build up of pollutants)
- High morning measured total nonmethane hydrocarbon (TNMHC) concentrations (average value during high ozone days of ~4,000 ppbC)
- High morning measured TNMHC:NOx concentration ratios (average values during high ozone days of ~90:1)

The field study also found that the winter elevated ozone concentrations were generally confined to the Jonah-Pinedale oil and gas development area in Sublette County just southwest of the Bridger-Fitzpatrick Wilderness Areas (see Figures 2 and 3). During some of the high ozone events, the ozone column was also reduced resulting in higher incoming UV radiation.

4. WINTER OZONE MODEL PERFORMNACE EVALUATION

As part of the model performance evaluation of the 2005-2006 base year simulations, the model's

ability to simulate observed winter high ozone events in southwestern Wyoming was assessed. A focused CAMx sensitivity analysis was performed using the 12/4 domain for the February 2006 period during which several high ozone days occurred. CAMx was first exercised for a base case using a configuration that is typically used for simulating summer ozone events. Figured 4 displays the predicted and observed hourly ozone concentrations at the Jonah monitor for the CAMx base case simulation. The observed daily maximum hourly ozone concentration exceeds 80 ppb on February 25-27, 2009 (Julian Days 56-58) when the modeled ozone peak is over 20 ppb lower at ~60 ppb. The CAMx base case simulation failed to produce wintertime high ozone concentrations. CAMx sensitivity tests were then conducted guided by field study data collected by the WDEQ. The first sensitivity test introduced the six factors that were observed during the wintertime high ozone events during the field study into the CAMx modeling inputs. Then, each of the factors was evaluated to assess their importance in producing wintertime high ozone events in southwestern Wyoming.



Fig. 4. Predicted and observed hourly ozone concentrations at the Jonah monitoring site for February 2006 and the CAMx base case simulation.

4.1 CAMx Six Factor Sensitivity Test

A CAMx sensitivity test was conducted that modified the CAMx inputs to include the six factors that were observed during the wintertime high ozone events during the 2007 and 2008 field study:

<u>Snow Cover</u>: The CAMx model includes an option for a snow cover input file that changes the default albedo, surface roughness and

surface resistance that are normally defined from the land use input file. Day-specific snow cover information was used to define the spatially varying CAMx snow cover input file for the February 2006 modeling period. The default albedo for snow in CAMx is 0.5. However, the WDEQ field study up/down UV radiometer measured albedo values of 0.8 when fresh white snow was present and completely covered the ground. Based on the WDEQ webcam photographs the February episode days included white snow on ground. Thus, the CAMx snow cover albedo was increased to 0.75.

Shallow Inversion: For the February 25-27, 2006 high observed ozone days, the mixing height in the CAMx model was capped at ~100 m AGL on the high observed ozone days (e.g., February 25-27, 2009). This was done by setting the vertical diffusion coefficient to low values above 100 m AGL within an area in Sublette County that included the state industrial monitoring sites.

<u>Few Clouds</u>: Cloud cover (if any) over Sublette County were removed from the CAMx inputs files.

Stagnant and/or Recirculating Winds: The MM5 wind fields were examined and found to have slow wind speeds. No modifications were made to the MM5 winds for the Six Factor Sensitivity Test since such modifications could result in the CAMx input meteorological fields being no longer dynamic balanced that could introduce spurious effects (e.g., excessive vertical velocities). Thus, the MM5 wind fields remained unchanged in the CAMx Six Factor Sensitivity Test.

Ambient Concentrations: The emissions inventory in the vicinity of the Jonah and Boulder monitoring sites where the field study VOC and NOx measurements were collected was analyzed to determine whether the emissions in the region could produce the ozone precursor concentrations and TNMHC:NOx ratio conditions observed during the winter field study high ozone days. The emissions inventory TNMHC:NOx ratio was 13:1. This compares to the measure ambient TNMHC:NOx ratio during high wintertime ozone events that averaged 90:1. Thus, the TNMHC emissions inventory in the vicinity of the Jonah/Boulder monitoring sites was adjusted in the Six Factor Sensitivity Test so that the emission inventory TNMHC/NOx ratio matched the average value observed during the winter field study on high ozone days (~90:1). This was done by multiplying the anthropogenic TNMHC emissions in the vicinity of Jonah/Boulder by a factor of 7.

4.2 Six Factor Sensitivity Test Ozone Performance

Figures 5 and 6 displays the predicted and observed hourly ozone concentrations for the CAMx base case and Six Factor sensitivity test at the, respectively, Jonah and Boulder monitoring sites. At the Jonah monitoring site, the Six Factor Sensitivity Test increased the modeled peak ozone concentrations on February 25 and 27 by approximately 10 ppb so that it is closer, albeit still lower than the observed values on these days. On February 26, however, the Six Factor Sensitivity Test increases the predicted peak ozone concentration by 80 ppb so that it is greater than the observed value. At the Boulder monitoring site (Figure 6) the observed ozone reaches 80 ppb on February 26 when the predicted ozone peak for the CAMx base case is ~50 ppb. The addition of the Six Factors increases the predicted ozone peak on February 26 by ~40 ppb. The Six Factor Sensitivity Test modeled peak ozone concentrations agree guite well with the observed ozone peaks during February 25-27, 2006 at the Boulder monitoring site. These results clearly demonstrate that the CAMx model is capable of simulating the winter high ozone events in southwestern Wyoming.



Figure 5. Time series of predicted and observed hourly ozone concentrations at the Jonah monitoring site.



Fig. 6. Time series of predicted and observed hourly ozone concentrations at the Boulder monitoring site.

4.3 Additional Sensitivity Tests

Additional sensitivity tests were performed that removed each of the six factors to determine which ones are most important for simulating the winter high ozone concentrations. The first additional sensitivity test examined the effects of the 7 times TNMHC emissions. Many of the processes in oil and gas production that produce TNMHC emissions are episodic in nature. The southwest Wyoming oil and gas emissions represent an average emissions rate so may underestimate the actual TNMHC emissions during some episodic periods. However, this underestimation is likely not a factor of 7. Thus the first sensitivity test reduced the 7 times TNMHC adjustment to the emissions inventory to 3 times TNMHC. Although not as high ozone peaks were predicted using the 3xTNMHC versus the 7xTNMHC (Six Factor) sensitivity tests, the model still produced winter elevated ozone concentrations. Using the 3xTNMHC starting point a series of sensitivity tests were performed to investigate the effects of each of the Six Factors for producing winter elevated ozone concentrations in southwestern Wyoming:

- The removal of the CAMx snow cover file resulted in large reductions in the predicted peak ozone concentrations. Thus, the albedo effect of white snow appears to be a necessary condition for the winter high ozone concentrations.
- The original MM5 meteorological inputs were used without the capping of the mixing height to ~100 m AGL and removing the cloud cover. The model was still able to produce elevated ozone concentrations with just the adjusted TNMHC emissions inventory (3xTNMHC)

and snow cover input with albedo enhancement (0.7).

5. SUMMARY AND CONCLUSIONS

Wintertime high ozone concentrations have been observed in a rural oil and gas production area in southwest Wyoming. The Wyoming Department of Environmental Quality conducted enhanced field study campaign during the winter of 2007, 2008 and 2009 that found that the elevated ozone concentrations occurred concurrently with Six Factors: (1) white snow on ground; (2) shallow inversion; (3) no or few clouds; (4) stagnant and/or recirculating winds; (5) high morning TNMHC concentrations: and (6) high morning TNMHC:NOx ratio. The CAMx model base case simulation failed to produce winter elevated ozone concentrations in southwest Wyoming. When the Six Factors were added to the CAMx model inputs the model was capable of producing winter high ozone concentrations in southwestern Wyoming. A sensitivity analysis was performed to investigate which of the six factors added to the model were needed to predict the winter high ozone events and we found that the high morning TNMHC concentrations and TNMHC:NOx ratios and enhancement of the UV radiation due to the white snow on the ground were both needed for the model to produce winter high ozone concentrations.

6. ACKNOWLEDGEMENTS

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