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PREPARATION OF OIL AND GAS EMISSIONS INVENTORIES FOR USE IN PHOTOCHEMICAL GRID MODELING

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1. INTRODUCTION

In recent years, elevated 8-hr ozone concentrations have been observed during late winter and early spring in the Upper Green River Basin (UGRB) in southwest Wyoming, where significant oil and gas development activities are occurring. To support air quality management in the region, AECOM and Sonoma Technology, Inc., are conducting photochemical grid modeling with the Community Multiscale Air Quality (CMAQ) model and the Comprehensive Air Quality Model with extensions (CAMx) to determine which model best replicates winter ozone formation processes in the UGRB.

To support this effort, the project team is converting detailed oil and gas emissions inventories for winter 2008 to air quality model-ready formats. These inventories were developed by the Air Quality Division of the Wyoming Department of Environmental Quality (WDEQ) and contain detailed emissions data for all permitted wells. The inventory covers a variety of sources, including drill rigs, tanks and pressurized vessels, dehydration units, pneumatic pumps, and process heaters, and also includes detailed data that is not typically available in oil and gas inventories, such as speciated volatile organic compound (VOC) emissions, stack parameters, location coordinates for individual wells, and temporal information for intermittent sources.

For regional photochemical grid modeling, it is beneficial to develop several nested modeling domains with finer grid spacing around the areas of primary interest (U.S. Environmental Protection Agency, 2007). Four nested domains were developed when conducting the meteorological modeling (ENVIRON International Corporation and Alpine Geophysics, 2011), and model-ready emissions for CMAQ and CAMx were generated for all four modeling grids (see **Figure 1**):

- A 36-km grid covering the continental United States;
- A 12-km grid covering the western United States;
- A high-resolution (4-km) grid covering much of western Wyoming and portions of neighboring states; and
- A very-high-resolution (1.33-km) grid covering Wyoming's ozone nonattainment area and surrounding terrain.

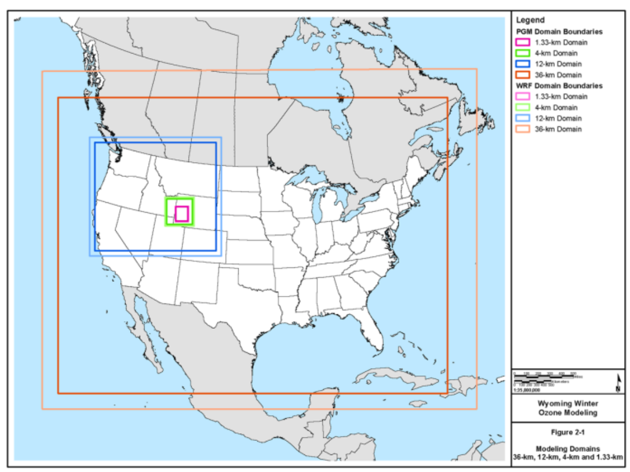

Fig. 1. Boundaries of the 36-km, 12-km, 4-km, and 1.33-km modeling domains.

Historically, emissions modeling efforts for the oil and gas production sector have typically represented emissions as nonpoint sources and have spatially and temporally allocated emissions using default or modified profiles. However, for this project, oil and gas wells are being treated as

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discrete point sources with multiple emissions processes (e.g., engines, tanks, and flares) during modeling with the Sparse Matrix Operator Kernel Emissions (SMOKE) model. This paper describes the methods used to prepare the detailed oil and gas inventories for use in air quality modeling applications.

2. OIL AND GAS EMISSIONS PROCESSING

WDEQ provided two detailed oil and gas emissions inventories for sources in Wyoming: (1) a winter 2008 (February-March) inventory for UGRB (Sublette County) sources, and (2) an annualized 2008 inventory for all oil and gas sources in the state. The data for both inventories are well-specific and include the American Petroleum Institute (API) number, oil and gas production levels, and location coordinates for each well. **Figure 2** shows the locations of all wells in the winter inventory for Sublette County, and **Figure 3** shows well locations for the annualized statewide inventory.

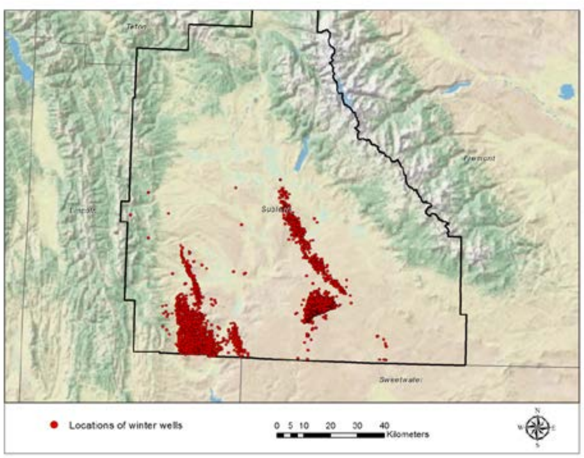

Fig. 2. Locations of oil and gas wells in Sublette County in February-March 2008.

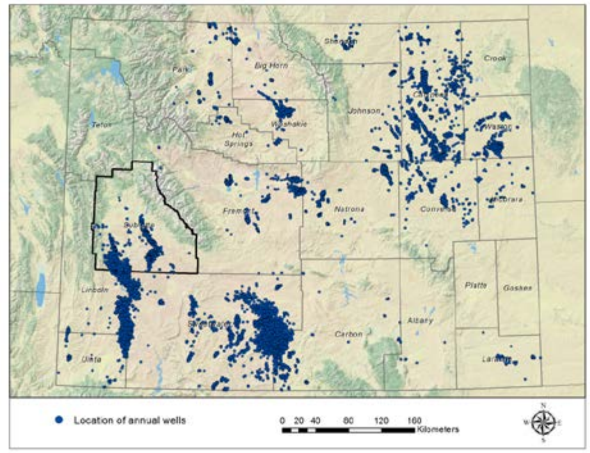

Fig. 3. Locations of oil and gas wells in the statewide, annualized 2008 emissions inventory.

WDEQ developed the winter 2008 inventory by surveying all oil and gas operators in Sublette County. Operators were asked to provide emission and control information for the sources listed in **Table 1**, as well as temporal information (e.g., start and end times for drilling and venting/blowdown events) where applicable. In addition, WDEQ developed speciated VOC emissions for a subset of sources (identified in Table 1) using field-specific gas and liquid analyses submitted by oil and gas operators as part of the New Source Review permit application process, which is required by WDEQ for all new or modified production sites in Wyoming. For modeling purposes, WDEQ also added stack parameter information (e.g., stack height, gas exit temperature) for each source, based on data listed in permit applications and professional judgment.

Table 1. Oil and gas emissions (tons) by source category for Sublette County, February-March 2008.

Source Category	NO_x	CO	HONO	Formaldehyde	PM	SO_2	Total VOC	Speciated VOC
Drill rigs	578.2	315.9	17.3	0.3	12.1	7.8	17.4	
Process heaters	86.8	57.2	2.6	0.0			3.2	
Tanks and pressurized vessels	80.2	18.6	2.4				754.4	✓
Glycol dehydration units	136.2	48.2	4.1				689.0	✓
Pneumatic pumps	14.3	3.5	0.4				565.6	✓
Fugitives							394.9	✓
Truck loading							143.4	✓
Compressor engines	236.8	188.8	7.1	24.1	1.5	0.1	143.2	
Workover engines	36.4	33.9	1.1		1.5	0.5	3.3	
Well vent and blowdown events							30.9	✓
Well completions	1.4	0.3	0.0				5.5	✓
Total	**1,170.3**	**666.4**	**35.0**	**24.4**	**15.1**	**8.4**	**2,679.1**	

2.1 Prepare SMOKE-Ready Files

The oil and gas emissions data provided by WDEQ were subjected to several quality assurance (QA) checks, which are described in more detail in the *Results and Quality Assurance* section below. In addition, API numbers in both the winter and annualized data were converted into a common format to facilitate the matching of wells between the two inventories. The data were then converted to SMOKE-ready format by treating each well as a discrete point source with multiple emissions-producing processes (e.g., engines or flares) that have distinct stack parameters. Specifically, the winter 2008 inventory for Sublette County was converted to SMOKE's PTHOUR format to preserve the temporal detail in that data, while the annualized statewide inventory was converted to SMOKE's PTINV format. Perl scripts were written to perform the file conversions. The process is shown in **Figure 4**.

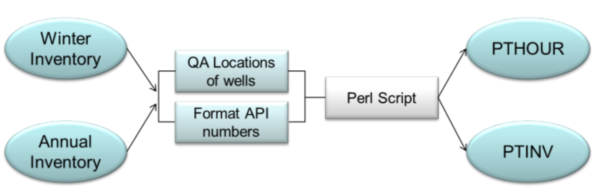

Fig. 4. Flow diagram of the steps followed to process the WDEQ oil and gas inventories for 2008.

2.2 Chemical Speciation

To retain the chemical resolution of the speciated VOC emissions data in the WDEQ oil and gas inventories, new SMOKE-ready speciation profiles were developed. In SMOKE, speciation profiles are used to translate VOC emissions into reactivity groups used in the photochemical mechanism chosen for air quality modeling (in this case, the Carbon Bond V (CB05) mechanism). Field- and process-specific speciated VOC emissions data were converted to CB05 speciation profiles using a spreadsheet tool derived from Dr. William Carter's database, which maps individual hydrocarbon species to air quality model-ready species groups. In addition, WDEQ calculated HONO emissions by assuming that 3% of reported NO_x emissions from combustion sources are emitted as HONO. Therefore, NO_x speciation profiles were adjusted to reflect the appropriate proportion of HONO emissions.

2.3 Non-Wyoming Oil and Gas Sources

For oil and gas sources outside Wyoming, 2008 emissions were derived from 2006 and 2012 data developed during the Western Regional Air Partnership (WRAP) Phase II and Phase III emissions inventory projects. These inventories covered oil and gas production basins in Colorado, New Mexico, Utah, and other western states. For non-WRAP states, we used oil and gas emissions from version 2 of the 2008 National Emissions

Inventory (NEI) (we removed oil and gas emissions for WRAP states from the 2008 NEI data to avoid double-counting).

2.4 Other Emissions Sources

For emissions sources not related to oil and gas production, we relied on a variety of data sources, including

- Version 2 of EPA's 2008 NEI;
- Day-specific fire emissions data for 2008 from the BlueSky Framework;
- Biogenic emissions from Version 2.1 of the Model of Emissions of Gases and Aerosols from Nature (MEGAN) model; and
- Outputs from EPA's Motor Vehicle Emission Simulator (MOVES) on-road mobile source emissions model.

These emissions data were processed through SMOKE and merged with oil and gas production emissions data.

3. RESULTS AND QUALITY ASSURANCE

This section provides descriptions and results of quality assurance checks that were performed on the emissions data, as well as summaries and plots of SMOKE emissions outputs. Quality assurance checks were performed both prior to and after emissions modeling with SMOKE. The emissions spreadsheets provided by WDEQ included summaries of emissions by source, county, and pollutant for the annualized 2008 data, and summaries of emissions by field and pollutant for the winter 2008 data. We added summary tables of emissions by source and pollutant to the winter 2008 data for Sublette County and used this information to track emission totals across further processing steps.

3.1 Location Coordinates

To ensure that reported location coordinates for each well in the WDEQ inventories were reasonable (i.e., within proper state and county bounds, and in known oil and gas production areas), we plotted well locations for both the annualized and winter inventories. We also applied range changes to reported latitude and longitude values to ensure that they fell within expected ranges. These checks identified issues with approximately 25% of the location coordinates reported in the annualized inventory (5,000 records out of 20,000 total). The issues identified included

- Missing data;
- Transposed latitude and longitude coordinates;
- Latitude and longitude coordinates reported as degrees/minutes/seconds rather than decimal degrees;
- Longitude coordinates with a missing negative sign (locations to the west of the prime meridian should be reported as negative); and
- Latitude or longitude coordinates with a misplaced decimal point (e.g., 4.4183 instead of 44.183).

These records were flagged and corrected prior to conversion of the emissions data to SMOKE-ready format. We filled missing latitude and longitude coordinate fields by using API numbers to obtain locations from a well database on the Wyoming Oil and Gas Conservation Commission website (http://wogcc.state.wy.us/) or by assigning the well a location coordinate that would place it in the proper field and county.

3.2 Speciated VOC Emissions

As a QA step for the SMOKE-ready speciated emissions and speciation profiles, we compared the total reported VOC emissions to the sum of the speciated VOC emissions to check for consistency. The total and speciated VOC emissions matched in all cases except for completion emissions for Ultra Petroleum in the Pinedale Field, where the total VOC emissions reported were about 9% higher than the sum of speciated VOC emissions. Since we relied on the total VOC emissions fields to develop SMOKE inputs, the higher emissions value was carried forward. It should also be noted that VOC emissions from well completions represent only 0.2% of the overall VOC inventory for oil and gas sources in Sublette County, so the impact of this inconsistency on air quality model-ready emissions inputs is negligible.

3.3 Emissions Summaries and Graphics

Emissions density and time-series plots for the oil and gas sector were prepared using SMOKE output files to evaluate the spatial and temporal distribution of emissions, as shown in **Figures 5 through 7**. Note that daily VOC and NO_x

emissions from oil and gas sources in the winter 2008 inventory for Sublette County vary little from day to day, as shown in Figure 7. However, there is a small decrease in NO_x emissions near the end of March, which is primarily due to a reduction in drilling activities during the last several days of that month. Also, emissions from oil and gas sources vary little on a diurnal basis in total, though there are some diurnal differences between vertical layers due to meteorological changes (see **Figures 8 and 9**, which show diurnal emissions for model layers 11 and 12).

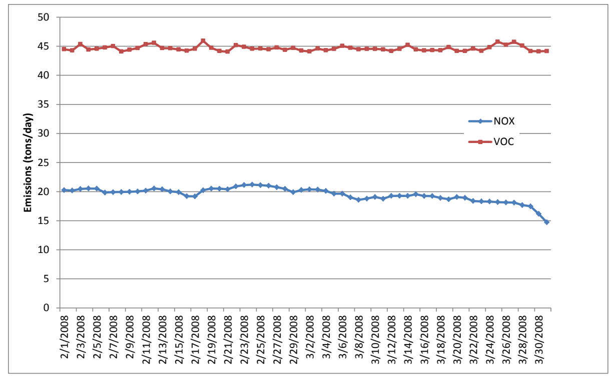

Fig. 7. Daily VOC and NO_x emissions (tons) from oil and gas sources for Sublette County for February-March 2008.

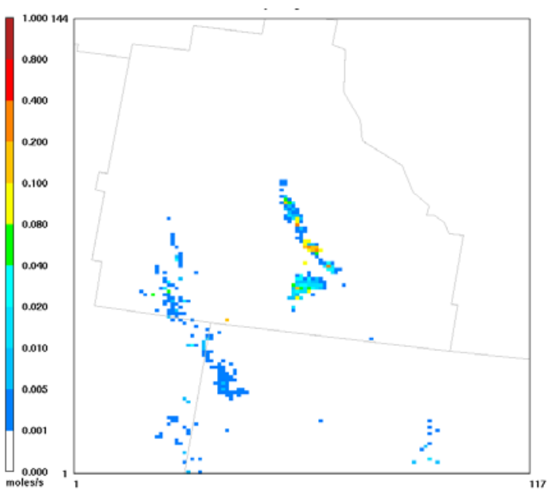

Fig. 5. Sample daily gridded NO_x emissions (moles/s) from oil and gas sources for the 1.33-km domain.

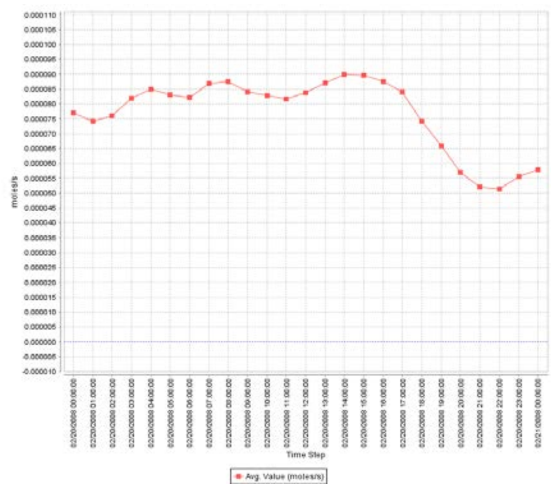

Fig. 8. Diurnal plot of NO emissions (moles/s) from oil and gas sources in the 1.33-km domain for layer 11.

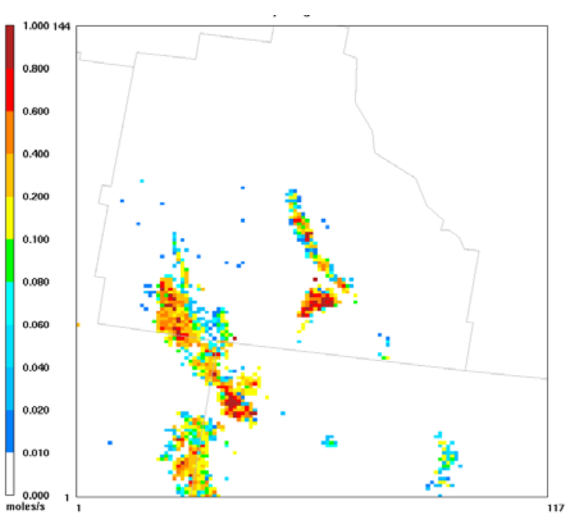

Fig. 6. Sample daily gridded VOC emissions (moles/s) from oil and gas sources for the 1.33-km domain.

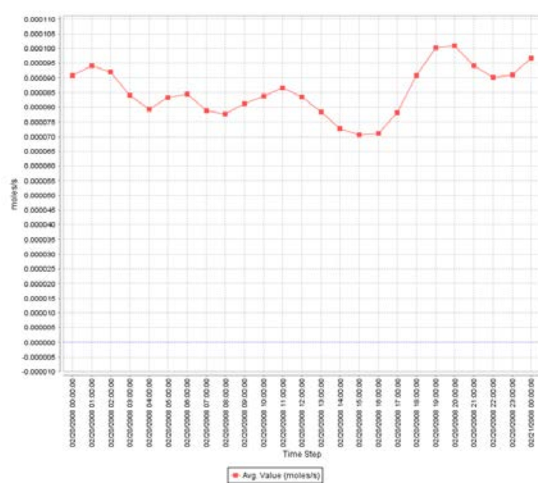

Fig. 9. Diurnal plot of NO emissions (moles/s) from oil and gas sources in the 1.33-km domain for layer 12.

4. CONCLUSIONS

Previous ozone modeling studies have demonstrated the importance of accurately representing the spatial distribution, temporal variations, and chemical speciation of key emissions sources in a region of interest (Steyn et al., 2011; Webster et al., 2007). For Wyoming's UGRB, where oil and gas production sources dominate the emissions inventory, it is critical to characterize these sources as accurately as possible in the emissions inputs used for wintertime ozone modeling efforts.

Historically, air quality modeling efforts for the oil and gas production sector have typically represented emissions from this sector as nonpoint sources, with emissions spatially and temporally allocated using default or modified profiles. Similarly, VOC emissions have generally been chemically speciated using default speciation profiles from EPA's SPECIATE database or other sources. However, the treatment of oil and gas production sources as nonpoint sources does not generally consider potential plume rise. In the UGRB, plume rise may be an important consideration for wintertime ozone episodes, which are typically characterized by a strong surface-based temperature inversion that results in a shallow mixed layer. The injection of emissions plumes into or above this layer is potentially an important issue for ozone formation in the region.

The detailed, well-specific information collected by WDEQ as part of its minor source inventory program allows this project to treat oil and gas wells as discrete point sources, with emissions assigned to actual well location coordinates and emissions from episodic processes such as drilling and blowdown events assigned to the specific days and hours when they occurred. In addition, speciated VOC emissions that were based on field-specific analyses provide local information on the mix of hydrocarbons emitted, thus improving default speciation profiles for the oil and gas production sector. Finally, stack parameters assigned to each oil and gas production source by WDEQ allow plume rise to be characterized more accurately during the emissions modeling process.

These detailed inventories will reduce the uncertainty in the emissions when air quality modeling is conducted for the UGRB (at the time this paper was written, air quality modeling simulations were not complete). In addition, this project provides insight into the methods used to prepare detailed oil and gas emissions inventories for use in air quality modeling simulations.

5. REFERENCES

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