Preparation of Oil and Gas Emissions Inventories for Use in Photochemical Grid Modeling

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ABSTRACT

In recent years, elevated 8-hour ozone concentrations have been observed during "winter" months (February and March) 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 model (CMAQ) and the Comprehensive Air Quality Model with extensions (CAMx) to determine the model that 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 the winter of 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. Emissions are estimated for criteria pollutants, nitrous acid (HONO), and formaldehyde for a variety of sources, such as drill rigs, tanks and pressurized vessels, dehydration units, pneumatic pumps, and process heaters. For select sources, the inventory also contains detailed data that is not typically available, such as speciated volatile organic compound (VOC) emissions, stack parameters, and spatial and temporal information for intermittent sources.

Emissions data for the winter of 2008 are being converted to formats compatible with the Sparse Matrix Operator Kernel Emissions (SMOKE) model, with individual oil and gas equipment modeled at the well head as discrete point sources. This paper will describe the processes used to prepare the detailed oil and gas inventories and the other main source sectors (e.g. mobile, nonpoint, point, fire, and biogenic) for use in air quality modeling applications.

INTRODUCTION

Several episodes of elevated 8-hour ozone concentrations in the Upper Green River Basin (UGRB) have been measured since monitoring began in 2005. These episodes typically occur in the late winter and early spring. In order to better understand the conditions that may lead to formation of winter ozone in southwest Wyoming, field studies (Upper Green Winter Ozone Studies [UGWOS]) were conducted each "winter" (February and March) from 2007 through 2011. The episodes that occurred in February and March 2008 were selected for this modeling analysis because of several

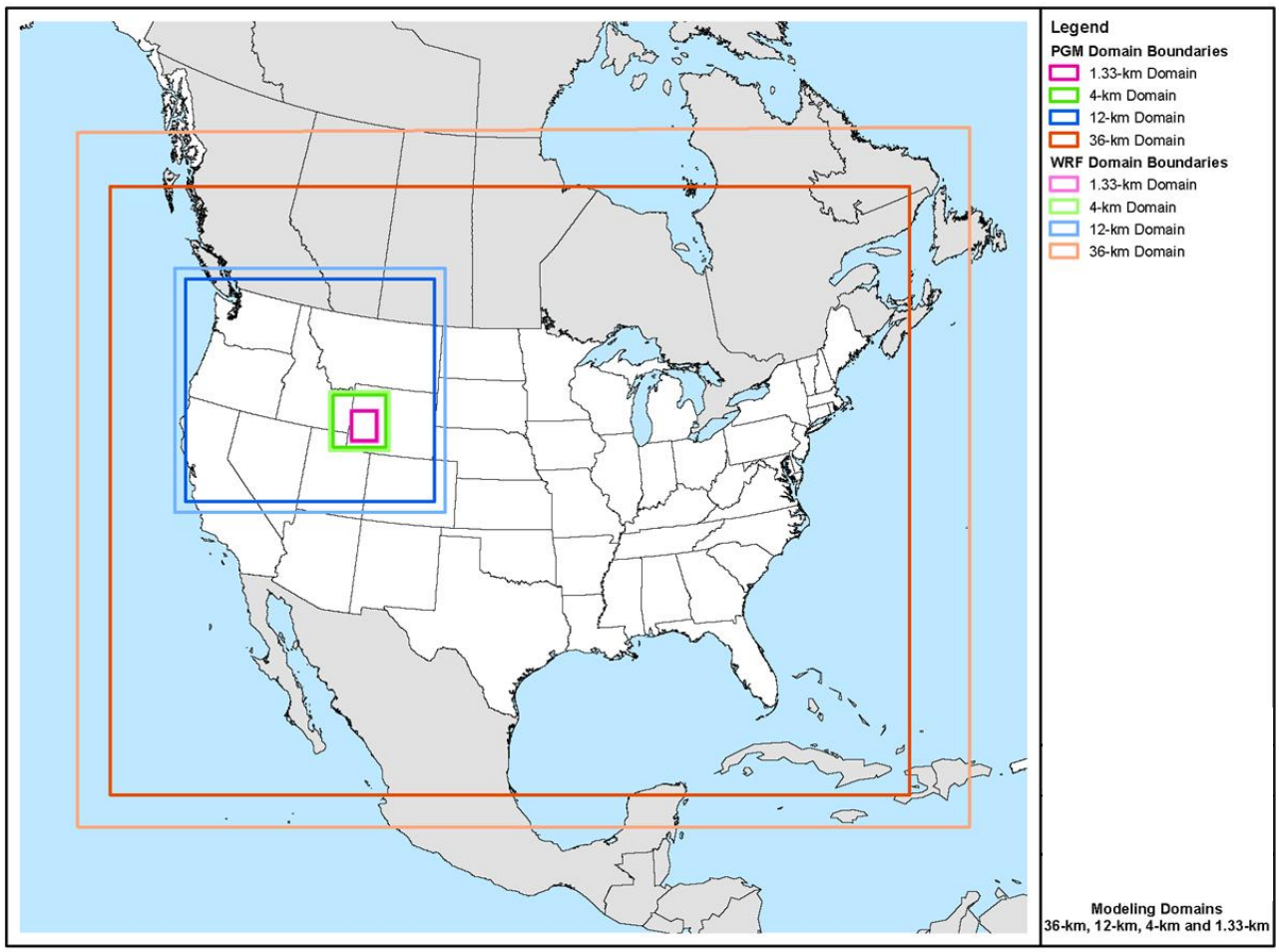
factors, including number of episodes, monitored values of peak ozone concentrations, availability and type of monitoring data during the episodes, and availability of data required for the modeling analysis.

Two state-of-the-science photochemical grid models (PGM), the Community Multiscale Air Quality model (CMAQ) and the Comprehensive Air Quality Model with extensions (CAMx), will be run and evaluated to determine which model best replicates the specific conditions and processes that lead to ozone formation in the UGRB. Once a model is selected, it will be used for air quality management purposes such as the assessment of control strategies and future compliance with the ozone National Ambient Air Quality Standards (NAAQS).

For regional photochemical grid modeling, it is beneficial to develop several nested modeling domains with finer grid spacing around the areas of primary interest.[1] Four nested domains were developed when conducting the meteorological modeling,[2] 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.

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



To develop a winter ozone model suitable for air quality management decisions, the best available data for the UGRB must be used to prepare air quality model-ready emission inputs. For 2008, these data sets include the detailed 2008 emissions data for oil and gas production sources assembled by WDEQ and the EPA's 2008 National Emissions Inventory (NEI), version 2. These inventories were supplemented with other data sources for development of mobile, biogenic, and fire emissions.

The emissions inputs were prepared for air quality modeling with the newest release of the SMOKE modeling system, version 3.0. The SMOKE model converts "raw" emissions inventory data (i.e., annualized or average-day criteria pollutant emissions at the county or facility level) to the resolution required by the air quality model (i.e., hourly emissions of model species assigned to modeling domain grid cells and vertical layers). SMOKE processes the emissions inventory data using a collection of interrelated programs that carry out the core functions of emissions modeling, including spatial allocation, temporal allocation, and chemical speciation.

OIL AND GAS EMISSIONS SOURCES

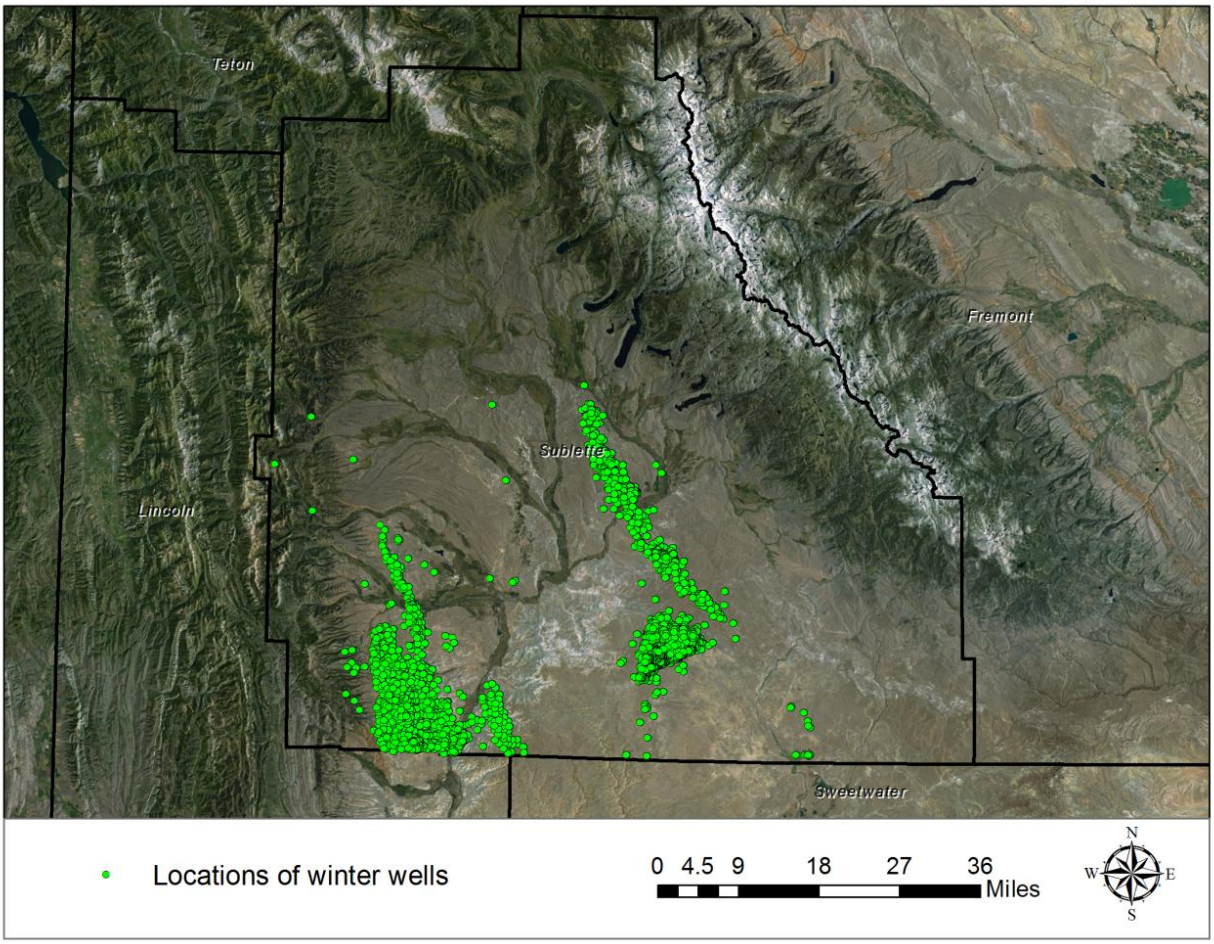
The method used to process the oil and gas emissions varied by geographic area in order to retain highly detailed information where available. WDEQ has two different oil and gas emissions inventories: one for winter activities in UGRB, and second for annual emissions occurring in the whole state.

WDEQ developed a detailed emissions inventory for the UGRB for winter 2008 (February-March) by surveying all oil and gas operators in Sublette County. Operators were asked to provide emissions and control information for the following emissions sources:

- Drill rig engines;
- Process heaters (including separators, line heaters, tank heaters, and dehydration unit reboilers);
- Tanks and pressurized vessels (flashing emissions);
- Glycol dehydration units;
- Pneumatic pumps;
- Fugitives;
- Truck loading;
- Well head and workover engines;
- Venting and blowdown events;
- Well completions (including flares); and
- Compressor stations.

WDEQ provided a complete list of oil and gas wells in Sublette County with well location (see **Figure 2**), well type, oil and gas production levels, temporal information for intermittent sources (e.g., start and end times for drilling and venting/blowdown events), and well-specific emissions by source type. Emissions data were provided for 20 pollutants, including oxides of nitrogen (NO_x) and speciated volatile organic compounds (VOCs).

Figure 2. Locations of active oil and gas wells in Sublette County for February-March 2008.



The speciated VOC emissions were developed from gas and liquid analyses submitted by oil and gas operators as part of the New Source Review (NSR) permit application process required by WDEQ for all new or modified production sites in Wyoming. Field-wide average gas analyses were used to determine speciated hydrocarbon emissions from a variety of sources, including venting/blowdowns, fugitives, pneumatic pumps, and dehydration units. **Table 1** summarizes WDEQ's winter 2008 inventory,[3] which provides a listing of total emissions by source category for February-March 2008 and identifies source categories for which speciated VOC emissions are available. For modeling purposes, stack parameter information was added by the State of Wyoming for the emissions sources on the basis of stack test reports, engineering estimates listed in permit applications, and professional judgment.

The emissions data provided by WDEQ were 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, a Perl script was written to convert the original Excel-based emissions data to SMOKE-ready "PTDAY" emissions files. These day-specific PTDAY files were generated to preserve the temporal and spatial variability of the raw emissions data.

Table 1. Total oil and gas emissions (tons) for 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	

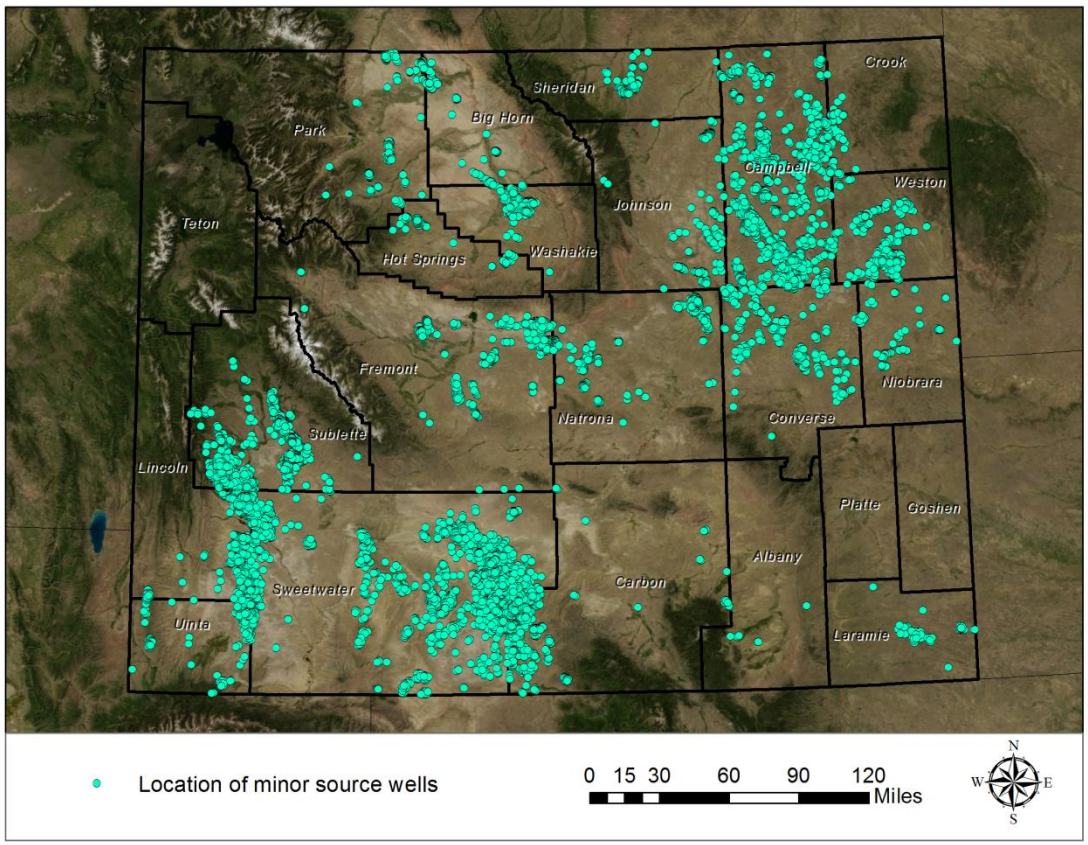
To capture the distribution of species in the speciated VOC emissions data, new SMOKE-ready speciation profiles were developed. In SMOKE speciated VOC emissions cannot be treated explicitly; rather, VOC emissions are processed using speciation profiles that translate VOC emissions into reactivity groups used in the photochemical mechanism (in this case, the Carbon Bond V [CB05] mechanism). The conversion was performed using a spreadsheet tool derived from Dr. William Carter that maps individual hydrocarbon species to air quality model-ready species groups (see http://www.engr.ucr.edu/~carter/emitdb/). **Table 2** lists the hydrocarbon species included in the emissions inventory and the corresponding CB05 species. 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.

Table 2. Species mapping used to convert speciated VOC emissions to SMOKE-ready speciation profiles.

Inventory Compound	Moles of CB05 species per mole of inventory compound					
	Paraffins	Toluene	Xylene	Methane	Ethane	Unreactive
methane	-	-	-	1.00	-	-
ethane	-	-	-	-	1.00	-
propane	1.50	-	-	-	-	1.50
2-methylpropane; isobutane	4.00	-	-	-	-	-
n-butane	4.00	-	-	-	-	-
isomers of pentane	5.00	-	-	-	-	-
n-pentane	5.00	-	-	-	-	-
isomers of hexane	5.83	-	-	-	-	0.17
benzene	1.00	-	-	-	-	5.00
toluene	-	1.00	-	-	-	-
ethylbenzene	1.00	1.00	-	-	-	-
m-xylene and p-xylene	-	-	1.00	-	-	-
isomers of heptane	6.81	-	-	-	-	0.19
isomers of octane (c8 paraffin)	7.75	-	-	-	-	0.25
isomers of nonane (c9 paraffin)	8.88	-	-	-	-	0.13
2,2,4-trimethylpentane	7.00	-	-	-	-	1.00
isomers of decane (c10 paraffin)	9.88	-	-	-	-	0.13

For Wyoming oil and gas sources outside Sublette County, emissions were obtained from WDEQ's annual statewide minor source inventory for 2008. Similar to the detailed winter emissions inventory, WDEQ prepared an annualized 2008 inventory for the entire state by surveying all oil and gas operators in the state. WDEQ provided a complete list of oil and gas wells in Wyoming with well location (see **Figure 3**), well type, annual oil and gas production levels, and well-specific emissions by source type. Emissions (tons per year) were provided for PM_{10}, NO_x, VOC, formaldehyde, CO and SO_2. The well-specific emissions sources listed above are represented in both the 2008 winter inventory for Sublette County and also the 2008 annual statewide minor source inventory. To address this issue, well-specific records in the winter inventory were matched to corresponding records in the annual inventory using the well's American Petroleum Institute (API) number. For records with missing API numbers, the well name or location coordinates were used to match records.

Figure 3. Locations of oil and gas wells that were sources of annual 2008 emissions.



For oil and gas sources outside Wyoming, emissions were taken from a WRAP 2008 oil and gas emissions inventory that covers several western states, including Colorado, Montana, New Mexico, and Utah. For non-WRAP states, oil and gas emissions from version 2 of the 2008 NEI were used (oil and gas emissions for WRAP states were removed from the 2008 NEI data to avoid double-counting).

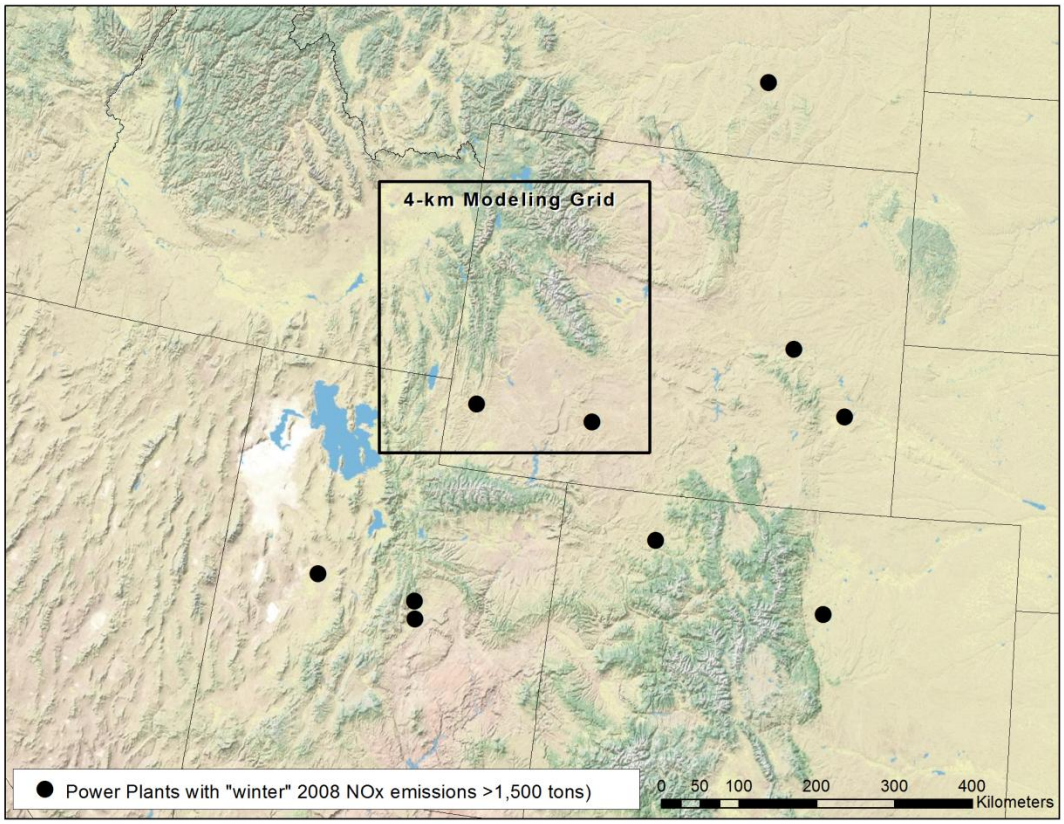
OTHER SOURCES

The following sections briefly describe the other components of the 2008 winter emissions inventory. During the collection and processing of emissions data, special attention was given to the high-resolution 4-km domain and the very-high-resolution 1.33-km domain, since accurate model-ready emissions inputs for those domains will produce the greatest benefits for the air quality modeling simulations. Detailed descriptions of each emission inventory component follow below.

Point Sources

Emissions for point non-oil and gas sources are from the SMOKE-ready version of EPA's 2008 NEI, version 2. Since these data represent annualized emissions, continuous emission monitoring (CEM) data from EPA's Clean Air Markets Division (CAMD) website (http://ampd.epa.gov/ampd/QueryToolie.html) were acquired; these data include unit-level, hourly sulfur dioxide (SO_2) and NO_x emissions data in SMOKE-ready format for power plants and other major point sources. CEM data for facilities that were within 200 km of the 4-km domain and that had NO_x emissions greater than 1,500 tons in February-March 2008 were used in place of annualized 2008 NEI data to improve the temporal resolution of these point sources (the locations of these sources are shown in **Figure 4**).

Figure 4. Locations of the power plants in the 2008 NEI that were modeled with CEM data.



Nonpoint Sources

For emissions from all nonpoint sources (i.e., stationary sources that are too small, numerous, and/or geographically dispersed to treat as individual point sources), the SMOKE-ready data from the EPA 2008 NEI were used. The nonpoint inventory in the 2008 NEI includes ammonia emissions from livestock husbandry, fertilizer application, and other sources, as well as fugitive dust emissions (e.g., unpaved road dust and agricultural tilling dust).

On-Road Mobile Sources

WDEQ has developed a statewide on-road mobile source inventory for 2008 using emission factors from EPA's MOBILE6 model and vehicle miles traveled (VMT) data derived from Wyoming Department of Transportation (WYDOT) traffic count data. The EPA recently replaced MOBILE6 with the Motor Vehicle Emission Simulator (MOVES) model, which incorporates updated mobile source emission factors and allows for emissions assessments at a variety of spatial scales. Based on these improvements, the on-road inventories for counties in the 4-km modeling domain were updated using the MOVES model.

Running MOVES requires a variety of input data, including vehicle fleet characteristics, vehicle activity data (e.g., VMT), fuel characteristics, emissions control program information, and meteorology. Though MOVES includes a default database that contains this information for each county in the United States, the default data do not necessarily reflect the most accurate or current information at the local level. Therefore, default MOVES data for counties in the 4-km modeling domain were updated with

VMT from WYDOT traffic counts. For counties outside the 4-km modeling domain, the project team relied on SMOKE-ready on-road emission files from the latest version of the 2008 NEI.

Nonroad Mobile Sources

For emissions from all non-road mobile sources, the SMOKE-ready data from the EPA's 2008 NEI were used. These 2008 emissions estimates were primarily prepared with the EPA's NONROAD model, which estimates county-level emissions for a wide variety of non-road equipment types, including agricultural equipment, construction equipment, and recreational vehicles. Emissions from these sources were spatially allocated using SMOKE-ready spatial surrogate data developed by EPA for the 36-km, 12-km, and 4-km grids. For the 1.33-km grid, spatial surrogates were developed using the same spatial data that the EPA uses to develop the SMOKE-ready spatial surrogates for coarser resolution modeling domains.

Biogenic Emissions

The WRAP recently sponsored improvements to the Model of Emissions of Gases and Aerosols from Nature (MEGAN), the biogenic model that has been incorporated into CMAQ.[4] Improvements to MEGAN include a soil model that accounts for NO_x emissions releases associated with fertilizer application and precipitation and incorporates improved land cover data for the Western United States.[5] The project team used this newest version of MEGAN (version 2.1) to develop day-specific biogenic emissions estimates for the period of interest.

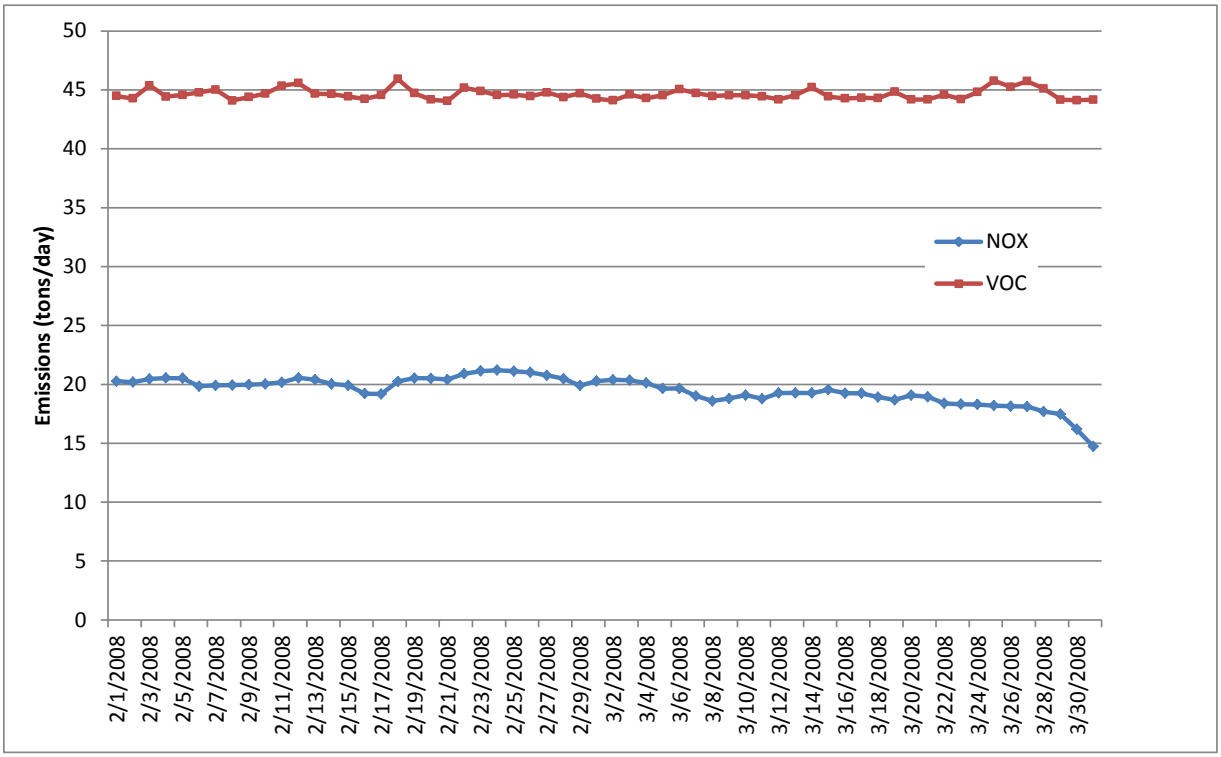
Fires

Day-specific wildland and prescribed fire emissions data for February and March 2008 are from the EPA's 2008 fire emissions inventory.[6] This emissions inventory was developed using the USDA Forest Service's BlueSky Smoke Modeling System to model wildfires as point sources and produce SMOKE-ready emissions files that include plume rise information.[7] This inventory was cross-checked with the WRAP Fire Emissions Tracking System (FETS) to ensure no large fires were missing from the EPA inventory.

RESULTS

Figure 5 shows the total daily emissions for oil and gas sources for Sublette County during February-March 2008. During this period, the VOC and NO_x emissions varied little from day to day, as VOC emissions associated with episodic gas releases due to well venting and blowdown events are relatively small compared to the VOC emissions from more continuous sources such as tanks, pressurized vessels, dehydration units, and pneumatic pumps.

Figure 5. Daily VOC and NO_x emissions (tons) from oil and gas sources for Sublette County for February-March 2008.



Sample gridded (1.33 km domain) daily emissions plots showing the spatial distribution of NO_x and VOC emissions from oil and gas sources are provided in **Figures 6 and 7**, respectively. Since emissions from actual well location coordinates were used as discrete point sources, the gridded output more accurately represents the emission locations.

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

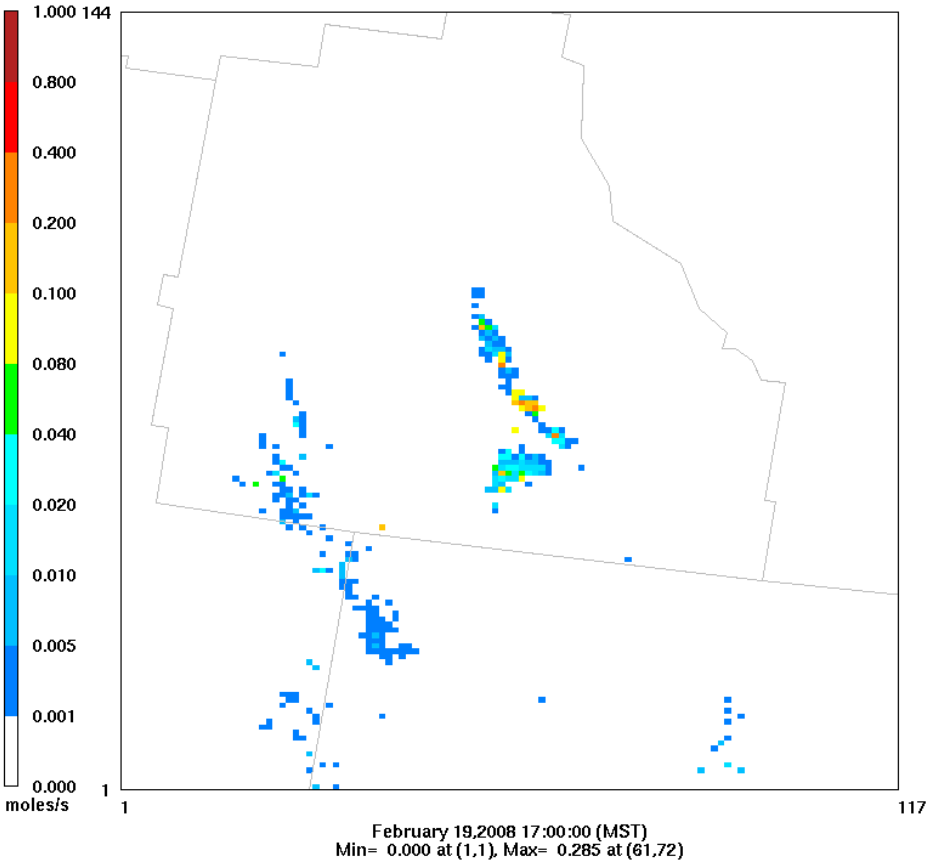


Figure 7. Sample daily gridded VOC emissions (moles/s) from oil and gas sources for the 1.33 km domain.

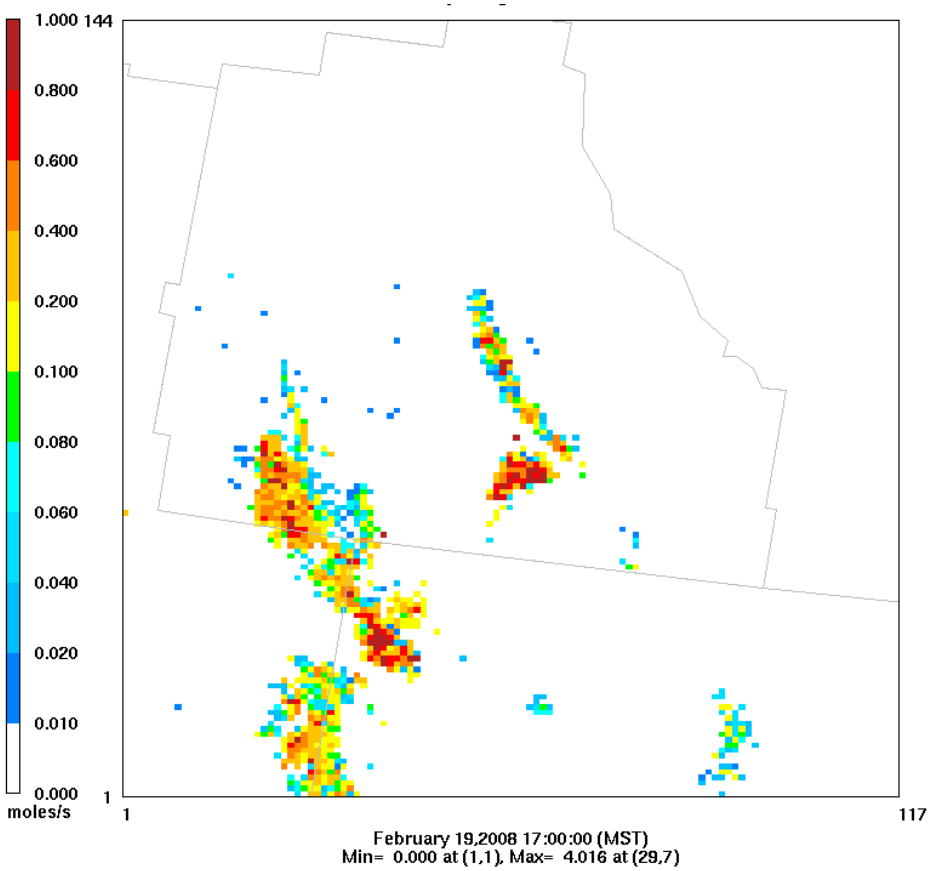


Table 3 summarizes the emissions by source category for Sublette County during February-March 2008. For Sublette County, oil and gas sources represent 72% of the total NO_x emissions and 86% of the total VOC emissions.

Table 3. Emissions (tons) in Sublette County for February-March 2008.

Source	CO	NO_x	VOC	NH_3	SO_2	PM_{10}	$PM_{2.5}$
Point	160.0	215.9	155.0	0.0	0.1	1.0	0.5
Nonpoint	57.0	4.1	40.5	49.0	1.0	1,716.7	183.0
On-road Mobile	1,184.3	184.0	7.9	2.4	4.0	9.8	8.4
Nonroad Mobile	660.5	46.2	237.9	0.1	1.0	9.6	9.0
Fire	13.0	0.0	3.1	0.2	0.2	1.5	1.3
Oil and Gas	664.5	1,170.9	2,677.9	0.0	8.3	15.0	14.9
Total	**2,739.3**	**1,621.2**	**3,122.4**	**51.7**	**14.5**	**1,753.6**	**217.1**

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.[8,9] 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.

For this project, the detailed, well-specific information collected by WDEQ as part of its minor source inventory program allows oil and gas wells to be treated 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. And, 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 inventory 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.

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KEY WORDS

Oil and Gas Emissions
SMOKE
Air Quality Modeling