Moving Towards Improved Basin-level Oil and Gas Inventories and Reconciliation with Measurements

Amnon Bar-Ilan, John Grant, Rajashi Parikh, Ralph Morris ENVIRON International Corporation, 773 San Marin Drive, Suite 2115, Novato, CA 94998

Garvin Heath, Viktor Diakov National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, CO 80401

> Dan Zimmerle Colorado State University, Fort Collins, CO 80523

Lee Gribovicz Airstar Consulting, 3570 East 8th St. Casper, WY 82609

ABSTRACT

The Western Regional Air Partnership (WRAP) Phase III emission inventories for oil and gas have been widely distributed and used for inventory, reporting, and air quality modeling in the Rocky Mountain region. We report on the most recent basin for which a WRAP Phase III-type inventory has been developed – the Williston Basin in Montana/North Dakota including the Bakken oil formation. We discuss several innovations that were implemented in this basin including the use of tribal minor new source review (MNSR) data available through Subpart OOOO, and the estimation of oil-production specific source categories in the Bakken formation. We then discuss the comparison of WRAP Phase III inventories with measured inventories, including a case study of inventory analysis relative to measurement data in the Denver-Julesburg (D-J) Basin in Colorado. Inverse modeling was performed and compared to aircraft measurements of volatile organic compound (VOC) fluxes from Weld County in the D-J Basin and determined that inventories were undercounting several key VOC species. This led to identification of potential sources of additional VOC emissions and modification of the inventory. Finally we discuss the implications of these past efforts on a new project sponsored by the US Department of Energy's National Energy Technology Laboratory and carried out by a large research consortium led by the Colorado School of Mines, the National Renewable Energy Laboratory and the National Oceanic and Atmospheric Administration. The project includes the development of a new emission inventory protocol that enhances and extends prior emission inventories of oil and gas air pollutant emitting sources.

INTRODUCTION

Oil and gas exploration and production activities occur extensively throughout the Rocky Mountain States in the United States – which includes the states of New Mexico, Colorado, Utah, Wyoming, Montana and North Dakota. These activities include a large number of processes and equipment which can generate air pollution emissions. Given the scope of these activities, these emissions can contribute significantly to the overall county-level or state-level emissions inventories of these Rocky Mountain States. Individual states have undertaken efforts to develop emissions inventories of oil and gas activities occurring within each state. The Western Regional Air Partnership (WRAP) has sponsored the development of regional inventories for oil and gas, intended to cover multistate regions in the Western United States. The WRAP inventories were developed in two phases – the Phase I inventory¹ which was the first-ever attempt to develop a comprehensive regional inventory of oil and gas activities, and the Phase II inventory² which included a more detailed analysis of compressor engine and drilling rig emissions. Each of these past projects encountered limitations in the availability of data and the comprehensiveness and accuracy of the inventories they generated. Thus WRAP identified the need for a new, comprehensive inventory of oil and gas activities in the Rocky Mountain States. This led to the development of the Phase III inventories. The Phase III inventory project was begun in 2007, and was a comprehensive inventory of all major oil and gas exploration and production activities, processes and equipment in the Rocky Mountain States. The Phase III project covers criteria pollutants, including nitrogen oxides (NOx), carbon monoxide (CO), volatile organic compounds (VOC), sulfur oxides (SOx) and particulate matter (PM). The inventory considers a base year of 2006, and "midterm" projections to 2012 or 2015. The inventory considers both combustion-generated emissions and those from oil and gas exploration or production processes:

- Combustion-generated emissions includes gas compressor engines, tank and separator heaters, boilers and reboilers in dehydrators and gas sweetening processes, flaring, drilling rig and workover rig engines, and miscellaneous engines (e.g. on-site generators, air compressors, vapor recovery units);
- Process emissions includes flashing and working and breathing losses from condensate and oil tanks, venting emissions from dehydrators and gas sweetening units, fugitive emissions from well site and central facility components, vented emissions from pneumatic devices, vented emissions from pneumatic chemical injection pumps, vented emissions from well completions and recompletions, and vented emissions from well blowdowns.

The Phase III inventory considers all oil and gas exploration and production activities up to the outlet of a natural gas processing facility, or the inlet to a refinery. This scope is generally consistent with the definition of the "upstream" oil and gas sector, as defined separately from oil refining and natural gas transmission and distribution.³ The Phase III inventory scope does not include on-road and off-road mobile sources associated with exploration and production activity, with the exception of drilling and workover rigs. However these mobile sources have been addressed in a new pilot study for the U.S. Environmental Protection Agency (EPA) that focused on the Piceance Basin in Northwestern Colorado.⁴

Since the development of the Phase III inventories, these inventories have been regularly updated through projections and further analysis, to a calendar year of 2008 in the WestJump Air Quality Modeling Study (AQMS)⁵ and to a calendar year of 2011 as part of the Three-State Air Quality Study (3SAQS)⁶. The inventories have also been used extensively in air quality modeling for predicting photochemical ozone formation and PM concentrations, both for research studies and for State Implementation Plan (SIP) modeling under a regulatory framework⁷. The EPA has used the WRAP Phase III inventories or their recent projections in the national modeling platform⁸. Most recently the methodologies developed in the WRAP Phase III inventories have been applied to the development of a comprehensive criteria pollutant inventory for the Williston Basin in Montana and North Dakota with a base year of 2011 under the direction and sponsorship of the Bureau of Land Management (BLM). The methodology and results of this work are presented here, including several key innovations that were applied to the Williston Basin inventory.

In addition, this paper discusses the application of the inventories to regional modeling and comparison of model predictions with recent top-down measurements of VOC flux in an oil and gas basin. A case study is presented of top-down measurements conducted by the National Oceanic and Atmospheric Administration (NOAA) in the Denver-Julesburg (D-J) Basin in North-Central Colorado and its comparison to photochemical ozone modeling conducted for the Denver ozone SIP.

Finally, the limitations of the inventories are discussed in the context of comparison to top-down measurements, the source category limitations of the inventories, data availability and other issues. This has prompted the Department of Energy's National Energy Technology Laboratory (NETL) to sponsor an ongoing study to improve reconciliation between top-down and bottom-up inventories of oil and gas emissions. The ongoing work is discussed and presented in terms of planned improvements to the inventories and the scope and scale of the NETL study.

METHODS

The general methodology for developing the Williston Basin inventory follows that of the Phase III inventories. More detailed presentation of the specific emissions estimation methodologies by source category are presented in the technical report for the study which is available through the WRAP⁹.

The Williston Basin baseline inventory is developed from a combination of (1) production statistics from a commercially available database; (2) survey data from oil and gas companies; (3) permit data from states and the EPA for larger point-source facilities; and (4) minor source registrations for sources on tribal land from EPA. These four data sources are then compiled to generate the complete baseline inventory for each basin. The tribal minor source data represent a key innovation advanced in this study.

Oil and Gas Production Statistics

Oil and gas related activity data across the entire Williston Basin were obtained from the IHS Enerdeq database queried via online interface. The IHS database uses data from each state's Oil and Gas Conservation Commission (OGCC or equivalent) as sources of information for oil and gas activity. This data is also available directly through database querying tools maintained by the respective agencies, however it was determined that the IHS database is more accurate and complete than these state databases and therefore was chosen as the basis for production statistics for this analysis. Two types of data were queried from the Enerdeq database: production data and well data. Production data includes information relevant to producing wells in the basin while well data includes information relevant to drilling activity ("spuds") and completions in the basin.

Production data were obtained for all counties in the Williston Basin in the form of IHS "298" format data files. The "298" well data contain information regarding historical oil and gas production. The "298" well data were processed with a PERL script to arrive at a database of by- American Petroleum Institute (API)-number, well type, annual gas production, oil production, and water production with latitude and longitude information.

The API number in the IHS database consists of 14 digits as follows: Digits 1 to 2: state identifier; Digits 3 to 5: county identifier; Digits 6 to 10: borehole identifier; Digits 11 to 12: sidetracks; Digits 13 to 14: event sequence code (recompletions).

Based on the expectation that the first 10 digits, which include geographic and borehole identifiers, would predict unique sets of well head equipment, the unique wells were identified by the first 10 digits of the API number.

Well data were also obtained from the IHS Enerdeq database for the counties that make up the Williston Basin in the form of "297" well data. The "297" well data contain information regarding spuds and completions. The "297" well data were processed with a PERL script to arrive at a database of by-API-number, spud and completion dates with latitude and longitude information. Drilling events in 2011 were identified by indication that the spud occurred within 2011. If the well API number indicated the well was a recompletion, it was not counted as a drilling event, though if the API number indicated the well was a sidetrack, it was counted as a drilling event.

Tables 1 and 2 below show the 2011 baseline production statistics and baseline well count statistics, respectively, for the Williston Basin.

Table 1. 2011 production by production type and by county for the Williston Basin (counties without oil and gas production are not shown).

	Liquid Hydrocarbon Production		Gas Pr		
County	Condensate (bbl)	Oil (bbl)	Primary Gas (mcf)	Associated Gas (mcf)	Produced Water (bbl)
Carter, MT	0	27,436	49,295	0	139,164
Custer, MT	0	0	60,449	0	0
Daniels, MT	0	3,230	0	0	12,488

	Liquid Hydrocarbon Production		Gas Pr		
	Condensate	Oil	Primary Gas	Associated Gas	Produced
County	(bbl)	(bbl)	(mcf)	(mcf)	Water (bbl)
Dawson, MT	0	595,113	0	53,615	2,700,813
Fallon, MT	15,418	4,822,211	14,055,984	3,549,143	46,058,213
Garfield, MT	0	13,159	0	1,969	74,713
McCone, MT	0	4,200	0	0	90,419
Prairie, MT	0	63,325	430	0	1,880,916
Richland, MT	31,260	11,962,438	21,204	13,428,072	5,983,761
Roosevelt, MT	0	1,779,002	0	999,229	13,167,825
Sheridan, MT	6,435	1,276,436	1,948	439,261	12,952,771
Valley, MT	0	100,412	1,539,084	8,221	1,002,778
Wibaux, MT	0	741,512	221,939	229,797	12,295,410
Billings, ND	7,054	3,830,377	25,874	4,102,338	22,306,981
Bottineau, ND	36,240	1,750,108	2,952	77,376	37,632,266
Bowman, ND	1,866,510	8,018,738	4,570,444	7,945,295	33,665,670
Burke, ND	16,780	2,235,526	40,185	3,196,199	7,074,419
Divide, ND	38,855	5,186,853	52,420	6,021,999	5,948,983
Dunn, ND	154,372	22,268,833	126,213	15,258,523	12,260,749
Golden Valley, ND	0	652,781	0	498,881	2,417,409
McHenry, ND	0	25,849	0	0	513,965
McKenzie, ND	843,889	29,044,894	2,897,188	41,054,821	21,427,508
McLean, ND	0	747,001	0	316,753	355,773
Mercer, ND	0	2,111	0	0	10,598
Mountrail, ND	123,231	50,959,389	71,989	34,121,971	18,254,096
Renville, ND	44,189	810,957	0	100,171	9,950,411
Slope, ND	254,656	307,887	82,364	518,533	1,213,648
Stark, ND	0	2,344,297	0	1,757,258	10,005,696
Ward, ND	0	38,845	0	11,132	570,370
Williams, ND	606,902	20,076,648	3,607,091	29,101,957	26,750,917
Harding, SD	28,053	1,586,475	1,295,351	11,155,586	3,979,830
Total	4,073,844	171,276,043	28,722,404	173,948,100	310,698,560

Table 2.	. 2011 active v	well counts and	d spuds coun	its by cou	nty for the	e Williston	Basin ((counties	without
oil and g	as production	are not shown).						

	Well		
County	Gas Wells	Oil Wells	Spud Count
Carter, MT	17	1	0
Custer, MT	3	0	0
Daniels, MT	0	2	0
Dawson, MT	0	62	2
Fallon, MT	982	495	2
Garfield, MT	0	12	1
McCone, MT	0	7	0
Prairie, MT	1	12	0
Richland, MT	4	995	34
Roosevelt, MT	0	206	29
Sheridan, MT	1	209	9
Valley, MT	149	41	3
Wibaux, MT	32	81	0
Billings, ND	3	460	31
Bottineau, ND	5	533	12
Bowman, ND	212	329	4
Burke, ND	5	433	47
Divide, ND	5	275	95
Dunn, ND	10	701	220
Golden Valley, ND	0	69	7
McHenry, ND	0	17	0

	Well Co		
County	Gas Wells	Oil Wells	Spud Count
McKenzie, ND	46	1,231	353
McLean, ND	0	29	14
Mercer, ND	0	1	0
Mountrail, ND	4	1,124	336
Renville, ND	6	284	5
Slope, ND	5	13	1
Stark, ND	0	102	35
Ward, ND	0	16	0
Williams, ND	38	800	306
Harding, SD	99	136	10
Total	1,627	8,676	1,556

The Williston Basin, unlike all other Rocky Mountain region basins, is characterized by high levels of crude oil production primarily from the Bakken Shale formation. In 2013, the state of North Dakota was ranked the second highest crude oil producer in the fifty United States due almost entirely to the production in the Bakken¹⁰. The Williston Basin is not a large producer of either condensate or natural gas relative to other Rocky Mountain basins and has far fewer primary gas wells than oil wells (by a factor of approximately 5.3 to 1). The vast majority of gas produced in the basin is in the form of associated gas (or casinghead gas) produced as a byproduct from primary oil wells. The majority of this gas is captured and processed for sale, but a significant fraction is not captured due to lack of infrastructure and must instead be flared. This issue is discussed in greater detail below.

Temporal and Geographic Scope

This inventory considers a base year of 2011 for purposes of estimating emissions. All base year well count and production data for the basin obtained from the IHS database were for the calendar year 2011 and data gathered from a number of sources on emissions and equipment were also for calendar year 2011. Emissions from all source categories are assumed to be uniformly distributed throughout the year except for heaters and pneumatic pumps, which are assigned seasonality fractions as they are typically used primarily in winter.

The geographic scope of this inventory is the Williston Basin in Northeastern Montana, North Dakota, and including a small portion of Northwestern South Dakota. For the purposes of this study, the boundaries for the Williston Basin were modified from those of the US Geological Survey (USGS)¹¹ to wholly include Carter, Custer, Daniels, Dawson, Fallon, Garfield, McCone, Prairie, Richland, Roosevelt, Sheridan, Valley, and Wibaux Counties in Montana; Butte and Harding Counties in South Dakota; and all counties in North Dakota. For purposes of this report, only those counties in North Dakota with some oil and gas activity or midstream sources were included, consisting of Barnes, Billings, Bottineau, Bowman, Burke, Burleigh, Divide, Dunn, Golden Valley, McHenry, McIntosh, McKenzie, McLean, Mercer, Morton, Mountrail, Renville, Slope, Stark, Stutsman, Ward and Williams Counties in North Dakota. The geographic scope of the analysis also considers activities by mineral estate ownership: BLM, United States Forest Service (USFS), Bureau of Indian Affairs (BIA) and state or private fee land.

Figure 1 and Figure 2 show the boundaries of the Williston Basin, with the 2011 well locations extracted from the IHS database overlaid. Figure 1 presents wells by type and Figure 2 presents wells by mineral designation. A key innovation in this study was the determination of mineral ownership and assigning of production and well surrogates to mineral ownership designations. This allowed for the emission inventory to be apportioned by mineral ownership designations, which provides regulatory agencies critical data on the fractions of emissions associated with each agency's jurisdiction. Mineral ownership was determined by working closely with BLM and other federal agencies to tag wells by API number for which the mineral ownership designation was BLM, USFS and BIA. All other wells were

assumed to be state/private/fee land. Production associated with those wells was then obtained through the IHS database analysis described in more detail below.

Figure 1. 2011 oil and gas well locations by well type within the Williston Basin.



Williston Basin - 2011 Wells



Williston Basin Wells

2011 Midstream Sources

Permitted midstream sources in the Williston Basin analysis refer to three types of sources for which data was gathered: (1) Title V or major sources in use in midstream, gas gathering applications from permit data from the Montana Department of Environmental Quality (MTDEQ); (2) Title V or major sources in use in midstream applications from NDDOH (North Dakota Department of Health); and (3) Part 71 major sources on tribal land from US EPA Region 8. The three source types are described below. In general, these permitted sources were used to supplement the emissions associated with well-site sources which were derived from survey data and tribal minor source registrations. Most permitted emissions used in this inventory were for midstream facilities which were not included in the exploration and production (E&P) sector surveys described in the next section. Although the MTDEQ and NDDOH register production-site equipment, this study used the detailed survey of operators to estimate emissions from these sources available for processing this data.

Permit Data for Midstream Facilities from State Agencies

Similar to the WRAP Phase III emissions inventories, midstream companies were generally not participants in the survey process conducted in the Williston Basin, with the exception of some gas and oil producers who may also own and operate midstream facilities. Because NDDOH and MTDEQ permit large midstream sources on non-tribal land in each state respectively, it was determined that these permit databases would be the most comprehensive source of data on midstream facilities such as gas plants, compressor stations and associated equipment. Requests were made to the MTDEQ and NDDOH to query their database of permitted facilities to identify midstream oil and gas sources in the Williston Basin using a combination of NAICS (SIC) and SCC codes corresponding to onshore oil and gas

sources. This query was focused on facilities and to the extent possible excluded production sites. It is noted that both NDDOH and MTDEQ require registration of production sites including registration of equipment at the sites, but discussions with both agencies indicated that this information was not considered readily available for use in the inventory.

Permit Data from EPA Region 8

Title V and Part 71 permits were requested from EPA Region 8 covering the Williston Basin, primarily for the Fort Berthold and Fort Peck Indian Reservations. Data provided by EPA indicated only a single source in the Fort Peck Indian Reservation meeting the Title V emission thresholds.

Tribal minor source registration emissions were requested from EPA Region 8 covering the Williston Basin, primarily for the Fort Berthold and Fort Peck Indian Reservations. Data provided by EPA indicated eleven compressor stations that did not meet Title V emission threshold, but were reported under EPA's minor source program.

Well Site Sources

Emissions from well site sources were estimated based primarily on two sources of data. A survey effort was conducted to develop basin-wide representative data for well site emission sources. Additionally, tribal minor source well site registrations were obtained from EPA for the Fort Berthold Indian Reservation which allowed for compilation of representative well site data specific to the Fort Berthold Indian Reservation for select well site emission sources. Tribal minor source well site registrations were not obtained from EPA for the Fort Peck Indian Reservation due to the small number of well site registrations that were available for that reservation.

Detailed inventory methodologies for each of the source categories are presented in Section 4.0. Emission estimates were generally made by extending representative emissions per well or per unit of production developed from the survey and tribal minor source data to the entire basin by scaling by the appropriate oil and gas surrogate. Similarly, emissions by mineral designation were estimated by scaling basin-wide emissions by the oil and gas activity surrogate appropriate to each source category.

Surveyed Sources

A survey spreadsheet was forwarded to participating operators in the Williston Basin. The spreadsheet contained requests for specific data related to one of the following 23 source categories:

- Drill Rigs
- Fracing Engines
- Completion Engines
- Initial Completion Venting
- Oil and Condensate Tanks
- Well Truck Loading
- Artificial Lift Engines
- Casinghead Flaring
- Well-site Fugitive Components
- Heaters
- Pneumatic Devices
- Pneumatic Pumps
- Dehydrators
- Workover Rigs
- Refracing Engines
- Recompletion Venting
- Other Flaring

- Miscellaneous Engines
- Well Blowdown (liquids unloading)
- Wellsite Compressor Engines
- Compressor Start-ups and Shutdown
- Water Tanks
- Water Disposal Pits

The companies participating in the survey process for the Williston Basin represented approximately 46% of well ownership in the basin, 70% of gas production in the basin, and 58% of oil production in the basin. Company participation is significantly higher than in the WRAP Phase III Williston Basin Emission Inventory¹² for which the companies participating in the survey process represented approximately 20% of well ownership in the basin, 30% of gas production in the basin, and 33% of oil production in the basin. The percentage of oil and gas activity that was captured in the survey process allow for good representation of oil and gas operations in the basin.

Insufficient survey data was obtained to estimate emissions for certain source categories. These source categories were therefore excluded from the study and include amine units, CBM pump engines, truck loading at gas and natural gas liquid (NGL) processing plants, water disposal pits, and saltwater disposal engines. Finally, potential fugitive emissions from oil and gas pipelines from well heads to the main compressor stations were not estimated, consistent with the previous WRAP Phase III study¹². Insufficient data was available on the components of pipelines or the complete extent of pipelines to tractably estimate basin-wide pipeline fugitive emissions.

It should be noted that the emission estimates calculated for survey-based sources rely on data that is not as rigorously documented as permitted sources. Much of the data provided for these sources is based upon estimates and extrapolation from the survey responses. However the level of detail of the surveys and the extent of participation in the survey effort allow for emissions estimates of survey-based sources which are a significant improvement over previous emission inventory efforts for the Williston Basin.

For emissions from those source categories that relied on estimates of volume of gas vented or leaked, such as tank flashing, well blowdowns, completions, and fugitive emissions, gas composition analyses were requested from all participating companies for gas produced from oil wells (i.e. casinghead or associated gas), gas produced from gas wells (primary gas), and flash gas associated with oil tanks. These composition analyses were averaged to derive basin-wide gas composition averages for oil wells by associated gas production, for gas wells by primary gas production, and for oil tank flash gas based on oil production. The average composition analyses were used to determine the average basin-wide VOC volume and mass fractions of the vented gas by type (i.e. associated gas, primary gas, and oil tank flash gas). It is noted that due to lack of survey data, condensate tank flash gas compositions were taken from the Phase III study¹².

Survey data was aggregated together at the basin-wide level to maintain the confidentiality of each company's data. Survey data was aggregated across all operators by the weighted average contribution of each company's data using the surrogate as the weighting factor. This methodology allows each company's survey data to impact the emissions from each source category in proportion to the company's ownership of the surrogate assigned to each category.

Tribal Minor Source Registrations

EPA promulgated the Indian Country Minor New Source Review Rule in 2011 and has subsequently made a number of revisions to this rulemaking. The rule requires registration of existing and new minor sources on tribal land. Minor sources are defined in attainment areas as those sources which do not meet major permitting thresholds with the potential to emit more than:

• 10 tons per year of carbon monoxide (CO), nitrogen oxides (NOx), sulfur dioxide (SO2), or particulate matter (PM), or

- Five tons per year of volatile organic compounds (VOCs), or
- Five tons per year of particulate matter less than 10 microns (PM10), or
- Three tons per year of particulate matter less than 2.5 microns (PM2.5), or
- 0.1 tons per year of lead, or
- One ton per year of flourides, or
- Two tons per year of hydrogen sulfide (H2S)

In the development of the Williston Basin emission inventory, minor source permitted emissions summary data, inclusive of both midstream (i.e., compressor station) and well site emissions, were provided by EPA for two tribal reservations within the boundaries of the Williston basin, the FBIR and the Fort Peck Indian Reservation. Midstream permitted source (i.e., compressor station) emissions from the tribal minor source emissions data were incorporated into the draft Williston Basin emission inventory. The tribal minor source emissions summary data also included a significant amount of well site emissions on the FBIR. Subsequent follow-up with EPA and analysis of well site permit registrations indicated the value of analysis of the tribal well site data and the potential for incorporation of this well site data into the Williston Basin emission inventories. Well site emissions from minor source registrations provided by EPA indicated a significant amount of well site emissions for the FBIR, however, well site emissions on the Fort Peck Indian Reservation is not unexpected given that the magnitude of oil production on the Fort Peck Indian Reservation is only 1% of the oil production on the FBIR. The focus of this analysis is the FBIR well site minor source registrations; Fort Peck well site minor source registrations were not analyzed.

Tribal minor source registration data was obtained for seven companies representing 73% of oil production, 74% of gas production, and 69% of active well count on the Fort Berthold Indian Reservation according to the IHS Enerdeq database . This is a large percentage of oil and gas activity on the Fort Berthold Indian Reservation which made it possible to obtain a reasonable representation of oil and gas operations on the Fort Berthold Indian Reservation. Analysis of the well site registrations allowed for estimation of representative emission source inputs for use in developing Fort Berthold area emissions for the following categories:

- Artificial Lift Engines
- Compressor Engines
- Well-Site Fugitive Components
- Heaters
- Miscellaneous Engines
- Oil Tanks
- Truck Loading of Oil
- Water Tanks

For source categories that are not listed above, all Fort Berthold Indian Reservation well site emissions were estimated based on the basin-wide input factors which were developed primarily based on operator surveys. Similarly, all well site emissions outside of the Fort Berthold Indian Reservation were also based on the basin-wide input factors which were developed primarily from operator surveys.

For well site source categories that are available in the tribal minor source registrations (listed in Table 3 below), emission inventory input factors based on the minor source registrations were compiled. The tribal well site input factor data – equipment, process-related data, gas compositions, emission factors, etc. – were compiled for each operator by aggregating across all of each operator's registrations based on the associated oil and gas activity statistic surrogate from each registration to compile operator average input factors.

Table 3. Percent of oil and gas surrogate for each source category for which emissions data was available from Fort Berthold Tribal MNSR data.

Inventory Source Category	Oil and Gas Surrogate	Surrogate Percent Coverage
Artificial Lift Engines	Oil Production	58%
Casinghead Gas	Associated Gas Production	48%
Wellhead Compressor Engines	Active Well Count	59%
Fugitives	Active Well Count	46%
Miscellaneous Engines	Active Well Count	59%
Water Tanks	Water Production	22%
Heaters	Active Well Count	69%
Oil Tank	Oil Production	71%
Truck Loading of Oil	Oil Production	71%
Natural Gas Composition ¹	Gas Production	39%
Flash Gas Composition ¹	Oil Production	24%

Operator average input factors for each source category were aggregated across all operators by the weighted average contribution of each company's well site registration data using the surrogate as the weighting factor. This methodology allows each company's well site registration data to impact the emissions from that source category in proportion to the company's ownership of the surrogate assigned to that category.

The end result of this task is the representative data needed to calculate emissions for each source category representing aggregated tribal well site data. These representative data are shown below in Table 4.

	Fort Berthold EPA Minor Tribal	Williston Basin Survey Producer	
Parameter	Average Data	Data	Unit
Oi	il Tank		
Uncontrolled VOC Emission Factor	5.4	5.6	lb/bbl
Uncontrolled Flashing Emission Factor	66	68	scf/bbl
Fraction of Production Controlled Via Flare	0%	70%	-
Fraction of Production Controlled Via VRUs	0%	13%	-
Fraction of Production Controlled Via Enclosed	100%	6%	-
Combustor			
Casin	ghead Gas		
Fraction of Gas Flared	85%	25%	-
Heating Value	1504	1571	btu/scf
Flaring control efficiency	97%	90%	-
H	eaters		
No. of Heaters per Well	0.98	0.55	count
Heater Rating	0.68	0.61	Mmbtu/hr
Annual Heater Usage	8760	8309	hr
Heater Cycling (fraction of the time the heater is	100%	98%	-
doing work when it is turned on)			
Heating Value	1459	1590	btu/scf
Truc	k Loading		
Fraction of Total Oil Production Sent Directly to	54%	31%	-
Pipeline, Not Subject to Well site Loading			
True vapor pressure of liquid loaded	2.25	2.39	psi
Temperature of Liquid Loaded	529	515	°R
Molecular Weight of Liquid Loaded	46.7	50.0	lb/lb-mole
Mode of Operation	100%	68% - Submerged	-
	submerged loading:	Loading of a Clean	
	dedicated normal	cargo tank	

Table 4	Representative	well site emissio	ns inputs based	on tribal MNSI	R data mining.

		Fort Berthold EPA Minor Tribal	Williston Basin Survey Producer	
Parameter		Average Data	Data	Unit
		service	32% - submerged	
			loading: dedicated	
			vapor balance	
			service	
Saturation Factor for submerged loading	g: dedicated	0.66	0.73	-
normal service				
	Fu	gitives		
GAS DEVICES	1			
Valves	Gas	34	28	count
pump seals	Gas	0	0	count
others (please provide description)	Gas	1	0	count
Connectors	Gas	188	95	count
Flanges	Gas	19	23	count
open-ended lines	Gas	0	3	count
non-GAS DEVICES	•			
Valves	Heavy Oil	0	0	count
Valves	Light Oil	29	19	count
Valves	Water/Oil	7	3	count
pump seals	Heavy Oil	0	0	count
pump seals	Light Oil	0	1	count
pump seals	Water/Oil	1	0	count
others (please provide description)	Heavy Oil	0	0	count
others (please provide description)	Light Oil	0	0	count
others (please provide description)	Water/Oil	1	0	count
Connectors	Heavy Oil	0	0	count
Connectors	Light Oil	97	35	count
Connectors	Water/Oil	43	3	count
Flanges	Heavy Oil	0	0	count
Flanges	Light Oil	33	37	count
Flanges	Water/Oil	2	1	count
open-ended lines	Heavy Oil	0	0	count
open-ended lines	Light Oil	1	0	count
open-ended lines	Water/Oil	0	0	count
	Wellhead Co	mpressor Engines		
Fuel Type		Natural Gas	Natural Gas	-
Engine Rated Power		244	408	HP
No. of Engines per Well		0.26	0.001	count
Hours of operation		8760	8760	hours/year
NOx		1.24	2.00	g/hp-hr
VOC		0.63	1.00	g/hp-hr
СО		2.36	4.00	g/hp-hr
SO ₂		0.00	0.00	g/hp-hr
PM		0.09	0.04	g/hp-hr
	Misc. En	gines – Pump		
Fuel Type		Gasoline	Gasoline	-
Engine Rated Power		8	8	Нр
No. of Engines per Well		0.34	0.06	Count
Hours of operation		1820	683	hours/year
NOx		5.00	3.60	g/hp-hr
VOC		7.01	6.12	g/hp-hr
СО		3.16	284.57	g/hp-hr
SO ₂		0.27	0.03	g/hp-hr
PM		0.32	0.12	g/hp-hr

	Fort Berthold EPA Minor Tribal	Williston Basin Survey Producer	
Parameter	Average Data	Data	Unit
Misc. Engi	ne –Generator		
Fuel Type	Diesel	Diesel	-
Engine Rated Power	181	211	HP
No.of Engines per Well	0.12	0.17	Count
Hours of operation	8021	5735	hours/year
NOx	3.77	2.98	g/hp-hr
VOC	0.68	0.21	g/hp-hr
CO	2.43	2.89	g/hp-hr
SO ₂	0.93	0.00	g/hp-hr
PM	0.21	0.21	g/hp-hr
Misc. Engi	ne - Other – NG	Natural Car	
Fuel Type	Natural Gas	Natural Gas	-
Engine Rated Power	250	400	HP Count
Hours of operation	0.07	0.001	hours/wear
	<u> 8/00</u> 1.70	<u>8/00</u>	nours/year
VOC	0.40	2.00	g/lip-lil g/hp_hr
	1.41	0.50	g/hp-hr
SO.	0.00	0.00	g/hp-hr
PM	0.00	0.00	g/hp-hr
Artificial	U.U.J Lift Engines	0.04	g/np-m
Fuel Type	Natural Gas	Natural Gas	-
Engine Rated Power	80	70	НР
No of Engines per Well	0.02	0 22	Count
Hours of operation	8760	8538	hours/year
NOx	25.85	4.46	g/hp-hr
VOC	0.98	1.09	g/hp-hr
СО	3.14	2.29	g/hp-hr
SO ₂	0.00	0.00	g/hp-hr
PM	0.08	0.18	g/hp-hr
Fraction of Engines Electric	unknown	17%	-
Wat	er Tank		
VOC Emission Factor	0.25	0.05	lb/bbl
Fraction of Production Controlled	100%	63.73%	-
Volume of Gas Flared	Not available	0.15	MCF/bbl
Natural Gas Co	omposition Analysis		
Gas MW	28.06	28.52	g/mol
VOC Fraction (molar)	23%	23%	-
VOC/TOC (weight)	46%	45%	-
VOC MW	51.96	53.77	g/mol
VOC Fraction (weight)	46%	43%	-
CH_4 Fraction (weight)	28%	30%	-
U ₂ Fraction (weight)	1%	1%	-
Heating Value	1504	1571	btu/scf
Flash Gas Cor	nposition Analysis	40.22	a/maal
VOC Eraction (malar)	700/	40.23	g/11101
VOC Traction (motal)	/9% 0.20/	33%0 720/	-
VOC MW	92% 76.60	15%	- a/mol
VOC Fraction (weight)	/0.00 0 2 0/	52.50 770/	g/11101
CH. Fraction (weight)	<u>72/0</u> <u>70/</u>	/ ∠ /0 70/_	-
CO ₂ Fraction (weight)	Δ/0 Ω 10/2	10/	-
Heating Value	2367	2092	 btu/scf

Emission Estimation Methodologies

For each survey-based or tribal MNSR-based source category for well-site emissions, a set of methodologies was used to estimate emissions from these sources for the fraction of activity represented by responding companies or by the tribal MNSR data that was used. These methodologies follow the WRAP Phase III methodologies and were described in detail in a technical report for the Williston inventory⁹.

Two categories were considered in detail that were not in previous WRAP inventories: (1) casinghead gas flaring and capture; and (2) oil loading at rail terminals. These two sources are unique to the Bakken formation among the Rocky Mountain basins in being significant source categories. The Bakken is characterized by substantial amounts of casinghead gas production in a region that historically has not had the infrastructure for capturing, processing and selling this gas. Operators in the Bakken have made progress in building such infrastructure, but there remains a fraction of casinghead gas production that cannot be captured and must be flared in pit flares. Similarly, the boom in oil production has not matched the infrastructure for transferring the crude oil to refineries and other end destinations. This has led to an increase in the use of rail terminals in which oil is loaded into tanker cars and moved by rail to the next destinations. These two methodologies are described in more detail below.

Casinghead Gas Capture and Flaring

Casinghead gas venting and flaring emissions were estimated based on survey-based data and data available from the North Dakota Oil and Gas Commission (NDOGC). VOC emissions result from any casinghead gas that is vented to the atmosphere as well as from casinghead gas that is flared. According to operator surveys, less than 0.3% of casinghead gas is vented. NDOGC estimates indicated that in 2011, 63% of produced gas was sold; it was conservatively assumed that any gas not sold was flared, hence 37% of casinghead gas was assumed to be flared. Some casinghead gas is expected to be used at the well site to power gas-fired equipment such as heaters or well site engines, or in other applications such as the generation of electricity or the capture of heavier hydrocarbons. However, data was not available to adequately characterize the percentage of gas that is used in such applications; hence all casinghead gas not sold was conservatively assumed to be flared. Further study to quantify the extent of alternative casinghead gas usage would allow for additional refinement of casinghead gas flaring emissions.

Casinghead gas flaring was assumed to occur only for Bakken Formation Counties, which is consistent with a majority of associated gas production in the Williston Basin occurring in the Bakken Formation Counties. A flare destruction efficiency of 90% was assumed.

VOC emission from casinghead gas were estimated per Equation 1.

(Equation 1)
$$E_{ca sin ghead} = \left[\frac{P \times V_{vented, TOTAL} \times 1000 \times MW_{VOC}}{R \times T} \times Y_{VOC}\right] \times \left[\left(1 - C_{eff}\right) \times F + (1 - F)\right]$$

where:

 $E_{casinghead}$ is the VOC emissions from casinghead gas [lb/year] $V_{vented, TOTAL}$ is the total volume of casinghead gas that is vented [mscf/year] MW_{VOC} is the molecular weight of the VOC [lb/lb-mol] R is the universal gas constant [scf-atm/K-lb-mol] Y_{VOC} is the volume fraction of VOC in the vented gas C_{eff} is the flaring control efficiency F is the fraction of vented volume that is flared 1,000 is the volume units conversion factor [scf/mscf] T is the temperature [K]

P is the pressure in [atm]

The conversion from volume of gas vented to mass of VOC produced was evaluated at standard temperature and pressure.

The total VOC emissions from all casinghead gas venting and flaring as described in Equation 1 represent basin-wide casinghead VOC emissions. County-level emissions from casinghead gas were estimated by allocating the total basin-wide casinghead gas emissions into each county according to the fraction of 2011 associated gas production from oil wells occurring in that county. Emissions by mineral designation were estimated in each county by allocating the county total emissions into each mineral designation according to the fraction of total 2011 associated gas production from oil wells that occurred in each mineral designation in that county.

Rail Loading of Crude Oil

Based on information provided by NDDOH¹³ 29 million barrels of oil was estimated to be loaded onto rail in 2011 in Bakken Formation counties, with 53% of the loading emissions accounted for in the NDDOH provided midstream data; therefore 47% of rail loading emissions were estimated as an area source using the methodology described here. Rail truck loading emissions were estimated based on loading losses per EPA AP-42, Section 5.2 methodology combined with the estimates of volume loaded to rail and controlled by flare. The loading loss rate was estimated based on EPA AP-42, Section 5.2 methodology, following Equation 2 below:

(Equation 2)
$$L = 12.46 \times \left(\frac{S \times V \times M}{T}\right)$$

where:

L is the loading loss rate [lb/1000gal] *S* is the saturation factor taken from AP-42 default values based on operating mode *V* is the true vapor pressure of liquid loaded [psia] *M* is the molecular weight of the vapor [lb/lb-mole] *T* is the temperature of the bulk liquid [$^{\circ}$ R]

Total rail loading emissions were then estimated by combining the calculated loading loss rate with the volume of oil loaded to rail as shown in Equation 3:

(Equation 3)
$$E_{loading} = L \times P \times \frac{42}{1000}$$

where:

 $E_{loading}$ is the rail loading emissions [lb/year] L is the loading loss rate [lb/1000gal] P is the volume of oil loaded to rail not including the volume loaded to rail that is accounted for in midstream source emissions [bbl/yr] 42 is the volume-units conversion factor [gal/bbl] 1,000 is the volume-units conversion factor [gal/1000gal]

The basic emission estimation methodology described in Equations 2 and 3 above accounts for total basin-wide emissions from rail loading losses.

County-level emissions were estimated by allocating the total basin-wide rail loading emissions into each Bakken Formation County according to the fraction of oil production in each county. Rail loading was assumed to be limited to Bakken Formation Counties. Emissions by mineral designation

were estimated in each county by allocating the county total emissions into each mineral designation according to the fraction of total 2011 oil production that occurred in each mineral designation in that county.

General Compilation Methodology

The survey and permit data were compiled in several steps to generate the baseline 2011 inventory. A set of surrogates were applied to each survey-based source category for which survey data was compiled, and similar surrogates were applied to the tribal MNSR input data for those categories in Table 3. The surrogates represented different oil and gas production statistics, such as primary gas production, casinghead gas production, oil production, condensate production, oil or gas well counts and spud (drilling event) counts. For each source category, the total value of the surrogate represented by all responding oil and gas companies whose data contributed to the survey was compared to the total value of the surrogate in the basin (or to the total value of the surrogate in the FBIR for tribal data). A scaling factor was developed, which was the ratio of the total value of the surrogate in the basin to that represented by the combined survey responses. The scaling factor was used to grow the total emissions for survey and tribal MNSR sources for each source category from the survey data to the basin-wide or tribal-wide emissions respectively. This was done because the survey respondents did not represent all activity in the basin.

Following this, the emissions from permitted sources were added to the emissions from the survey-based sources. The permitted sources were treated as point sources, since the exact locations of these sources were known. The resulting emissions inventory represented the total inventory. The surrogates for each source category were then used to scale the inventory down to the county level, such that the final inventories were reported on a county basis. The scaling factors for the county-level emissions estimates were the ratio of a surrogate's value in a single county to that of the entire basin. A similar analysis was conducted for tribal versus non-tribal land. An analysis was conducted to determine the values of surrogates within tribal land in the basin, as opposed to non-tribal land. A similar scaling was then conducted on the total inventory for the basin to determine the tribal portion of the inventory. More details on this methodology are available in the references⁹.

INVENTORY RESULTS

Results from the combined permitted sources and the combined surveyed sources are presented below for the entire Williston Basin as a series of pie charts and bar graphs including county-level emissions, basin-wide emissions and emissions on tribal and non-tribal land. The quantitative emissions summaries are presented in Table 5. It should be noted that all figures showing county-level emissions only include those counties representing 1% or greater of the total emissions in the basin. A complete list of emissions for all counties is included in the summary emissions spreadsheets that accompany this report.

Figure 3 shows NOx emissions by county and source category in the Williston Basin. Figure 3 shows that NOx emissions are concentrated in McKenzie, Mountrail, Williams, and Dunn Counties in North Dakota, and to a lesser extent in Richland and Fallon Counties in Montana. These counties represent the core Bakken Formation area, with the exception of Fallon County in the Cedar Creek Anticline. Figure 4 shows NOx emissions by mineral designation in the Williston Basin. 77% of NOx emissions are from private/state fee mineral estate with less than 12% of NOx emissions from any other single mineral estate.

Figure 5 shows that VOC emissions are also concentrated in McKenzie, Mountrail, Williams, and Dunn Counties in the core of the Bakken area of North Dakota, and to a lesser extent in Richland and Fallon Counties in Montana. There are also significant VOC emissions in Bowman County in the Cedar Creek Anticline. 78% of VOC emissions are from private/state fee mineral estate with less than 10% of VOC emissions from any other single mineral estate.

Figure 7 shows VOC emissions by mineral designation. Figure 8 shows that VOC emissions from casinghead gas, oil tank flashing, and pneumatic devices are the largest contributors to basin-wide VOC emissions, accounting for approximately 81% of the basin-wide VOC emissions in the Williston Basin in 2011. Condensate tank flashing represents an additional 9% of basin-wide VOC emissions in the Williston Basin in 2011.











Figure 5. 2011 VOC emissions by source category and by county in the Williston Basin.





Figure 7. 2011 Williston Basin NOx emissions proportional contributions by source category.

	NOx	VOC	CO	SOx	PM
County	[tons/yr]	[tons/yr]	[tons/yr]	[tons/yr]	[tons/yr]
Carter, MT	4	120	7	0	0
Custer, MT	0	18	0	0	0
Daniels, MT	2	16	2	0	0
Dawson, MT	82	723	142	4	4
Fallon, MT	1,205	12,080	2,328	140	50
Garfield, MT	12	89	12	0	1
McCone, MT	8	52	10	0	0
Prairie, MT	20	129	59	0	1
Richland, MT	1,703	22,299	3,007	413	82
Roosevelt, MT	539	3,089	819	42	20
Sheridan, MT	285	2,485	581	19	17
Valley, MT	127	1,263	155	3	5
Wibaux, MT	140	1,155	394	5	5
Barnes, ND	119	6	2	3	6
Billings, ND	970	8,578	1,761	407	34
Bottineau, ND	726	5,230	1,442	14	31
Bowman, ND	747	20,548	1,538	51	22
Burke, ND	714	6,798	1,060	137	31
Burleigh, ND	44	0	24	1	0
Divide, ND	685	9,521	1,310	185	29
Dunn, ND	2,905	27,290	4,643	531	99
Golden Valley, ND	92	1,202	190	16	4
Mc Henry, ND	130	136	31	3	7
McIntosh, ND	106	13	97	6	7
McKenzie, ND	6,798	60,939	9,555	1,511	224
McLean, ND	89	510	219	12	3
Mercer, ND	1	8	1	0	0
Morton, ND	219	34	210	12	14
Mountrail, ND	5,576	57,968	8,797	1,195	194
Renville, ND	325	2,864	511	8	16
Slope, ND	20	1,973	52	2	1
Stark, ND	274	3,363	637	58	7
Stutsman, ND	9	0	14	0	0
Ward, ND	18	152	29	1	1
Williams, ND	4,529	43,179	6,391	2,104	134
Butte, SD	0	0	0	0	0
Harding, SD	182	2,657	276	11	9
Totals	29,404	296,488	46,305	6,895	1,060

Table 5. 2011 emissions of all criteria pollutants by county for the Williston Basin.

RECONCILIATION CASE STUDY

Increasingly there has been interest in evaluating the performance of basin-level oil and gas inventories such as the WRAP Phase III or the Williston Basin inventories relative to measurements of methane, VOC or ozone. Some measurement campaigns have focused on estimating a flux of VOC or methane at the basin level and comparing to the inventory data. Other studies have focused on the performance of the inventories through photochemical grid modeling (PGM) of ozone or reactive VOCs relative to measured concentrations. Here we present a case study in which the WRAP Phase III inventory of oil and gas for the D-J Basin is evaluated for performance using the CAMx modeling developed as part of the Denver Metropolitan Area (DMA) ozone SIP.

In November 2007, the Denver Metropolitan Area and North Front Range (DMA/NFR) region was designated as ozone nonattainment area (NAA) based on measured ozone data during 2005-2007 that violated the 1997 0.08 ppm 8-hour ozone NAAQS. This resulted in a requirement to prepare an 8-hour ozone State Implementation Plan (SIP) that demonstrates ozone attainment by 2010. The Denver Regional Air Quality Council (RAQC), in conjunction with the Colorado Department of Health and Environment Air Pollution Control Division (CDPHE/APCD) contracted with ENVIRON International Corporation and Alpine Geophysics, LLC to develop a June-July 2006 photochemical modeling database and conduct ozone attainment demonstration modeling and other analysis that demonstrated that the DMA/NFR NAA would achieve the 1997 8-hour ozone NAAQS by 2010. The documentation of the ozone attainment demonstration modeling and other technical analysis for the 2008 Denver 8-hour ozone SIP is available on the CDPHE/APCD website¹⁴.

As part of the 2008 Denver ozone SIP modeling, a model performance evaluation was performed¹⁵ that compared observations with predictions from the CAMx June-July 2006 base case simulation. This evaluation included the comparison of predicted and observed VOC and NOX concentrations and their ratios using special field study VOC samples collected by the CDPHE/APCD. The VOC sampling collected morning 3-hour grab samples at two sites in metropolitan Denver and two sites in the oil and gas producing region in Weld County (Fort Lupton and Platteville), as well as a few afternoon samples at downwind monitoring sites. The comparisons of the predicted and observed VOC concentrations found that CAMx underestimated the observed VOC concentrations.

Additional analysis was performed to investigate whether VOC emissions are understated in the current modeling system and investigate which source categories may be responsible for the understatement. Further details of this analysis can be found in the technical report¹⁶. This analysis consisted of the following activities:

- Further investigation of the CAMx June-July 2006 base case model performance in order to identify the potential geographic source locations of emissions when the overestimation is greatest.
- The VOC underestimation bias was greatest in the Weld County O&G producing region suggesting that VOC emissions from O&G sources may be underestimated. Thus, a CAMx sensitivity test was performed that multiplied the oil and gas VOC emissions in Colorado by a factor of 5.
- Chemical Mass Balance (CMB) receptor modeling was used to analyze the speciated VOC samples and perform VOC source apportionment modeling of the samples. The Positive Matrix Factorization (PMF) receptor model was also used to obtain alternative VOC source apportionment.
- Deterministic emissions based VOC source apportionment modeling was conducted using CAMx for the June-July 2006 period and the results compared with the OBM modeling to try and reconcile the VOC observations and predictions and identify potentially missing VOC sources.

VOC Model Performance Evaluation

During the summer of 2006, the CDPHE/APCD collected grab canister samples at several sites in the DMA/NFR region. Morning 3-hour VOC samples were collected at the CAMP and Welby sites in metropolitan Denver as well as at Fort Lupton and Platteville in Weld County. A few afternoon VOC samples were collected at the Rocky Flats North and Fort Collins West high ozone (downwind) monitors. It is expected that the VOC samples at the two Denver sites (CAMP and Welby) will be dominated by on-road mobile source emissions inventory, whereas the morning samples at the two Weld County sites will be dominated by the oil and gas VOC emissions so the VOC model performance evaluation should provide an indication of the accuracy of the VOC emissions inventory for these two source sectors. The VOC canister samples were speciated to obtain individual VOC species concentrations along with total nonmethane hydrocarbon (TNMHC) concentrations that were compared against the modeling results to determine how well the model predicted total VOC concentrations, concentrations of individual VOC species as well as predicting the key VOC/NOx indicator species ratios. The VOC speciation samples were speciated to the CB05 chemical mechanism VOC species used in the modeling. Weld County sites so we can only make model-observed comparisons for total CB05 VOC and Ethane (the VOC comparison is shown in Figure 9). At Fort Lupton, the modeled VOC ranges from 40 to 226 ppbC, whereas the observed values range from 122 to 981 ppbC. Most modeled VOC values at Fort Lupton are between 100-200 ppbC, whereas most observed values are over twice as high ranging from 250 to 700 ppbC. Similar results are seen at Platteville where the modeled VOC ranges from 50 to 200 ppbC, whereas the observed values are much higher ranging from 200 to 2,000 ppbC.

The model is also underpredicting the observed ethane concentrations at the two Weld County sites. At Fort Lupton the observed ethane values range from 24 to 240 ppbC, with average values of around 150 ppbC. Whereas the model ethane predictions range from 6 to 43 ppbC, with average values of approximately 25 ppbC that are over a 100 ppbC lower than observed on average. Even larger ethane underprediction bias is seen at Platteville with observed values of 35 to 600 ppbC and modeled values of 9 to 80 ppbC.

The model systematic underprediction of ethane in Denver and Weld County may suggest that there are missing sources of natural gas in the inventory. Or it may just be due to horizontal and vertical spatial gradients in the observed VOC and ethane concentrations that are not captured by the model grid cell average concentration. VOC species at the two Weld County monitors are dominated by ethane (ETHA) and paraffin (PAR). Table 6 compares the predicted and observed PAR and ETHA concentrations at Fort Lupton and Platteville. The large underprediction of PAR and ETHA at these sites (typically -70% to -80%) indicate that natural gas emissions may be missing in the inventory (Table 6). In addition to underestimating FORM and ALD2, as seen at the two Denver monitoring sites, the aromatic species are also underestimated at the Weld County sites, which suggest that gasoline combustion VOC emissions may be underestimated in the inventory as well.

		Observed	Predicted	Difference	Difference			
Site	Date	(ppbC)	(ppbC)	(ppbC)	(%)			
PAR								
Ft. Lupton	June 19	403	119	284	-70%			
Ft. Lupton	July 13	321	67	254	-79%			
Ft. Lupton	July 28	455	105	350	-77%			
Platteville	June 19	484	224	260	-54%			
Platteville	July 28	779	267	512	-66%			
		ET	HA					
Ft. Lupton	June 19	88	18	70	-80%			
Ft. Lupton	July 13	41	9	32	-77%			
Ft. Lupton	July 28	96	13	83	-77%			
Platteville	June 19	97	31	66	-68%			
Platteville	July 28	161	34	127	-79%			

Table 6. Comparison of predicted and observed morning paraffin (PAR) and ethane (ETHA) concentrations at the Weld County monitoring sites.

Figure 9. Comparison of the predicted and observed morning CB05-VOC concentrations at the Ft. Lupton and Platteville sites in Weld County.

VOC is underestimated at the Weld County monitoring sites in the oil and gas (O&G) production region. There are no NOX measurements at these monitoring sites so VOC/NOX ratio comparisons could not be made. The underestimation is particularly great for CB05 paraffin (PAR) and ethane (ETHA). The predicted PAR concentrations tend to be 29-50% of the observed values, whereas the predicted ETHA concentrations tend to be 20-30% of the observed values. As PAR and ETHA are markers for natural gas VOC, these results suggest that the O&G VOC inventory may be underestimated.

Back trajectories were performed from the VOC monitoring sites on high and low VOC concentration days to better understand the source regions that contributed to VOCs on those days. The back trajectories were run using the 4 km MM5 fields used in the CAMx modeling and were designed to arrive at the monitoring site at the time of the morning VOC sample (5-8am MST) and at 10 m above ground level. The back trajectory and ambient VOC observation analysis suggests that VOC emissions and especially alkanes (PAR) and ethane from oil and gas sources in the D-J Basin may be understated. On days when the back trajectories have a larger residence time over the D-J Basin O&G production region, the VOC underestimation bias is greater. Whereas on low VOC days when there was little or no

residence time over the D-J Basin O&G producing area there is better agreement between the predicted and observed VOC concentrations.

Oil and Gas VOC Sensitivity Simulation

The model performance evaluation and back trajectory analysis using measurements at the Weld County Fort Lupton and Platteville monitoring sites suggests that oil and gas volatile organic compound (VOC) and ethane emissions may be understated in the photochemical modeling database. To investigate this issue, we performed an oil and gas (O&G) VOC emissions sensitivity test using the CAMx photochemical grid model and the June-July 2006 base case database. For the O&G VOC emissions sensitivity test, VOC emissions from O&G sources were increased by a factor of five. The factor of 5 O&G VOC emissions are underestimated by such a factor. The sensitivity test was designed to see how sensitive ozone formation is to the level of O&G VOC emissions and whether increasing the O&G VOC emissions would improve ozone and VOC model performance. Thus, we wanted to perturb them by a large factor to make sure the change in ozone is above model noise.

CAMx Version 4.51 with the vertical velocity (VV) enhancement was used in the O&G VOC sensitivity test. Previously CAMx VV was used to make a revised 2006 base case and 2020 ozone projections as part of the post Denver 2008 ozone SIP model improvements. The revised CAMx VV 2006 base case simulation (Run22) was compare to the 5 times O&G VOC emissions sensitivity simulation (Run23) to determine the sensitivity of the CAMx VOC and ozone predictions to the level of O&G VOC emissions. Figure 10 compares the daily time series of the predicted and observed morning VOC concentrations at the four monitoring sites for the CAMx base case (Run22) and 5xVOC O&G emissions sensitivity test (Run23). The VOC comparisons in Figure 10 used the sum of the CB05 VOC species, including ethane, to obtain the observed and predicted VOC concentrations. Note that technically these are really total nonmethane organic compound (TNMOC) concentrations because they include ethane, but will call them CB05 VOC concentrations. At the two Weld County monitoring sites, the 5xVOC sensitivity test results in substantial increases in the modeled VOC concentrations so that they match the observed VOC concentrations much better. For example, at the Platteville site, the average observed VOC concentration (970 ppbC) is underestimated in the CAMx Run22 base case simulation (162 ppbC) by a factor of approximately 6. Whereas in the 5xVOC O&G emissions sensitivity test The CAMx Run23 simulation only underestimates the average observed VOC value by -30%.

Figure 10. Observed and predicted TNMOC concentrations for the CAMx base case (Run22) and 5 x VOC O&G emissions sensitivity test.

Similarly a comparison was conducted between the base case (Run 22) and 5x sensitivity run (Run 23) for predicted ozone model performance at the three monitoring sites for four 3-day episode periods during the June-July 2006 modeling period. The three monitoring sites are the Rocky Flats North (RFNO) monitor, which over the last decade has had the highest ozone Design Value in the DMA/NFR region, the Fort Collins West (FTCW) monitor which also observed high ozone but is improving, and Weld County Tower (WCTO) monitoring site that is near Greeley north of Platteville and within the D-J Basin O&G production region. During June 17-19, 2006 episode, the 5xVOC O&G emissions sensitivity test has no effect on the predicted ozone concentrations on the first two days (June 17-18). On June 19th there is a slight (~2 ppb) increase in the hourly ozone between 6am and noon at the RFNO and FTCW monitoring sites, but little to no effect the remainder of the time. During the June 26-28, 2006 episode the CAMx hourly ozone peak at RFNO on June 26 increases from 66.0 to 69.7 ppb due to the 5xVOC sensitivity test with slightly higher ozone also seen at RFNO on June 27 but no change on June 28. Very small ozone increases are also seen at FTCW and WCTO. There is essentially no change in the predicted ozone at RFNO and FTCW due to the 5xVOC sensitivity test during the July 13-15, 2006 episode. At the WCTO monitor, small increases in ozone are seen due to the 5xVOC sensitivity test. This includes the model trying to replicate a sharp rise in the observed morning ozone on July 15th where the ozone increases 6 ppb at 10am from 69 to 75 ppb due to the 5xVOC sensitivity simulation. The July 27-29, 2006 episode has slow wind speeds, consequently the largest changes in ozone occur at the WCTO monitoring site. The hourly ozone peaks at WCTO are increased from 81 to 85 ppb (+4 ppb) and from 82 to 87 ppb (+5 ppb) on, respectively, July 28 and 29 due to the 5xVOC O&G emissions sensitivity test better matching the observed ozone peaks on these two days.

The five times oil and gas VOC emissions sensitivity test produced slightly improved ozone model performance on some days at some of the monitoring sites. However, it resulted in significant improvement in VOC model performance at the two Weld County monitoring sites. These results suggest that VOC emissions may be understated in the D-J Basin, however the results are inconclusive as the VOC underestimation could also be due to spatially variability in the VOC concentrations that is not captured by the model grid cell average predictions.

The single largest source of VOC emissions from O&G sources in the D-J Basin are flash emissions from condensate tanks. Large condensate tanks are required to control these emissions, but smaller tanks are not. There is a lot of spatial variability in VOC emissions and consequently VOC concentrations across the D-J Basin. The model fails to capture all of this spatial variability due in part to use of the 4 km grid resolution. The model is also using average emissions rates that fail to capture the real-world temporal variability in emissions, including O&G production emissions. Some of the highest observed VOC concentrations (e.g., July 1, 2006 at Platteville) are likely due in part to temporal variations in the real-world emissions not captured in the emissions modeling. If the monitors are located close to some of these VOC sources then that could be a source of a model VOC underestimation bias, when in reality it is just an artifact of the averaging that is done in the model. The ozone increases due to the 5xVOC O&G emissions sensitivity test are small in the context of an ozone model performance evaluation that compares predicted and observed ozone concentrations. However, in

the context of emissions control strategy evaluation in attainment demonstration modeling, a few ppb change in ozone is quite significant.

CMB and PMF Receptor Modeling

In this section we discuss the application of receptor models to the measured VOC species concentrations in the Denver area during the June-July 2006 modeling episode for the purpose of trying to resolve differences between the measured ambient VOC concentrations and the VOC emissions inventory used in the photochemical grid modeling.

Receptor models, also called observation based models (OBM), use measured concentrations and estimate what source types contributed to them. In this study we used detailed speciated VOC measurements of numerous individual VOC species and receptor models to estimate source contributions to the VOC measurements. The two receptor models used were the Chemical Mass Balance (CMB) and the Positive Matrix Factorization (PMF). In the CMB receptor model, speciated VOC source profiles (source VOC finger prints) are provided and the CMB tries to fit those source profiles to the VOC measurements and estimate VOC source contributions to the measured VOC concentrations. The PMF receptor model decomposes the VOC measurements into "factors" that have different key VOC species and then the user examines the factors' VOC speciation profiles to infer what types of sources emit those types of VOC profiles (i.e., what source category do the factors represent). In CMB, accurate and representative source profiles specific to the region of interest are needed as input in order to obtain reliable VOC source apportionment. CMB has a disadvantage in that potentially a large amount of the VOC measurement may be unidentifiable if it does not fit any of the provided source profiles. PMF has an advantage in that you do not have to a prior define the source profiles and it determines the factors based on the speciated VOC measurements. This can be an important attribute if there is a strong source signature for a source type that you don't have source profiles for when CMB is used. However, PMF has a disadvantage in that it requires many more speciated VOC measurements than CMB to develop its factors and that the PMF factors may be nonsensical or represent multiple source types so are difficult to interpret.

In this study we first applied the CMB model to obtain preliminary CMB VOC source apportionment. We then made a preliminary application of PMF using just the VOC species in the CMB VOC source profiles and compared it with the CMB source apportionment. The PMF application helped identify additional VOC source profiles that were then used in a revised CMB application. We also performed a revised PMF application using all of the measured VOC species in the measurement, rather than just the VOC species in the CMB VOC speciation profiles used in the preliminary PMF application. Detailed technical formulations of both the CMB and PMF models can be found in the technical report for the study¹⁶.

The preliminary CMB modeling was applied to the morning (5-8am) VOC samples at the two Weld County monitoring sites. The preliminary CMB receptor modeling used the following VOC source profiles:

- Compressed Natural Gas (CNG)
- Geogenic Natural Gas (GNG)
- Liquid Petroleum Gas (LPG)
- Gas Evaporative (Gas Evap)
- Vehicle Exhaust (Gasoline Combustion)
- Biogenic

The leftover VOC mass classified as "unidentified" represents the unknown species from the measured VOC that are not represented in the input VOC source profiles. The CNG, GNG, LPG and Gas Evap profiles correspond to oil and gas sources. This would include oil and gas exploration and productions, as well as oil and gas processing and use. The Vehicle Exhaust profile corresponds to gasoline combustion within on-road mobile sources, as well as non-road gasoline engines and stationary

source gasoline combustion. The biogenic profile is keyed in on isoprene that is primarily emitted by deciduous trees.

The CMB model was applied to the morning speciated VOC measurements at the two Weld County sites using samples from the June-July 2006 period and the six VOC source profiles discussed above. There were 14-16 morning samples at each monitoring site. Figure 11 displays the source category contributions estimated by CMB averaged across the 14-16 sample days at the Fort Lupton and Platteville monitoring sites. As expected, the VOC contributions attributable to vehicle exhaust is relatively small at the two Weld County sites (6% and 2%), and the contribution of source categories associated with oil and gas sources is relatively high at the two Weld County sites (94% and 98%). The biogenic contribution was extremely low for all sites.

Figure 11. Average source contribution to measured VOC concentrations at four monitoring sites estimated using the preliminary CMB receptor modeling.

The CMB-estimated CNG source contributions appear to be highest at Fort Lupton, although the unidentified fraction and Gas Evap contributions can also be high on some days. The signal of the four source categories associated with oil and gas is greatest at the Platteville monitoring site, which is consistent with its location in the center of the D-J Basin oil and gas producing area. On June 28, 2006, the CMB estimates that 1,600 ppbC of VOC is contributed by CNG, GNG, LPG and Gas Evap source categories.

The large fraction of measured VOC not speciated was a cause for concern indicating that there are additional VOCs which cannot be attributed to sources by the CMB receptor model. Another area of concern was the low biogenic VOC contribution estimated by the preliminary CMB modeling. To help identify potential additional source profiles that could be used, the PMF receptor model was applied. As noted previously, the PMF does not use source profiles as input but instead analyzes the VOC speciation data to obtain VOC speciation factors that may be attributable to a particular source category.

The PMF receptor model was used initially to try and better understand and potentially refine the preliminary CMB VOC source apportionment modeling results. The PMF was configured initially to use just the VOC species used in the preliminary CMB application. That is, the VOC species in the CNG, GNG, LPG Gas Evap, Vehicle Exhaust and Biogenic VOC speciation profiles were provided as input to PMF for the ~60 VOC measurements. The PMF was exercised using 4 and 5 factors. The 4 factor PMF application produced more recognizable source factors so is reported here. We examined the four factors produced by the PMF receptor modeling and found three of them produced a good match with the CMB VOC speciation profiles.

Figure 12 compares the four PMF factor VOC speciation profiles with VOC source profiles from the CMB collection. The first PMF factor is compared against the composite VOC source profile for CNG, GNG, LPG and Gas Evap, which is representative of VOC emissions from oil and gas production, processing and use. Both PMF and the composite VOC profile agree that N-Propane (N_PROP) is the largest component followed by Ethane (ETHANE) and then N-Butane (N_BUTA). There are also contributions of Iso-Butane (I BUTA) and Iso-Pentane (IPENTA) in the first factor.

The second PMF factor compares favorably with the cold start emissions VOC speciation profile (Figure 12, second panel). Although the match is not as good as seen with the PMF factor 1 oil and gas VOC profile, there are numerous key species associated with cold start VOC emissions that are present in the second PMF factor (e.g., aromatics species of Benzene, Toluene and Xylene or BTX). PMF factor 2 does overstate the contributions of Ethane and Iso-Pentane to the vehicle cold start VOC profile. Note that the vehicle cold start VOC emissions profile was not used in the preliminary CMB modeling because of concern it could be co-linear with the vehicle running exhaust VOC profile.

The third PMF factor VOC species contribution has a fairly good match with the vehicle running exhaust VOC profile (Figure 12, third panel). Ethane and N-Butane are matched well, although the PMF third factor understates N-Propane.

The final PMF factor does not appear to match any of the profiles very well. In Figure 12 (bottom) the fourth PMF factor is compared to a composite solvent and biogenic VOC speciation profile, as these are two of the largest remaining source categories not accounted for in the previous three PMF factors. However, PMF factor four has a poor match with biogenic and solvent VOC speciation profiles.

Based on the PMF modeling, we identified two additional VOC profiles (vehicle cold starts and solvent) for the revised CMB receptor modeling. The revised CMB modeling used the following VOC source profiles: CNG; GNG; LPG; Gas Evap; Gasoline Combustion; Bio; Veh Cold Start; and Solvent. The CMB-estimated VOC source contributions for CNG, GNG, LPG and Gas Evap were combined together to represent the oil and gas (O&G) source sector. Note that in the preliminary CMB application we were careful not to provide too many VOC source profiles as that can degrade the CMB source apportionment, especially when the VOC source profiles were co-linear. For example, specifying VOC source profiles for vehicle exhaust and vehicle cold starts could cause problems in the CMB modeling due to their co-linearity. However, the PMF modeling demonstrated that these two signals are sufficiently unique that this should not be a problem.

Figure 13 compares the daily VOC contributions estimated by the preliminary PMF and revised CMB receptor modeling using the source categories associated with the four PMF factors. With four sites and 14-16 days for each site this results in approximately 60 comparisons. Note that although the PMF factors were used to help identify additional VOC source profiles to use in the revised CMB modeling, the PMF and CMB VOC source apportionment receptor modeling are completely separate and independent calculations.

The agreement between the PMF factor 1 and CMB O&G VOC source apportionment is quite good (Figure 13, top panel). The day-to-day VOC contributions associated with vehicle cold start emissions estimated by PMF and CMB is not as good as seen for O&G sources, but they do tend to follow the trends in each other well at Fort Lupton (FLCO) (Figure 13, second panel). Agreement between PMF and CMB cold start VOC contributions is fairly good at Fort Lupton, but not as good at Platteville where CMB estimates higher contributions than PMF.

A comparison of the VOC contribution due to vehicle running exhaust emissions is given in the third panel in Figure 13 and shows good agreement in the day-to-day variations at Fort Lupton, with CMB estimating a much higher contribution than PMF. There is poor agreement in both the trends and magnitude in the VOC due to vehicle running exhaust emissions at Platteville with PMF estimating much higher contributions compared to CMB. Finally, the bottom panel in Figure 13 compares the PMF fourth factor VOC contributions with the CMB VOC contributions from solvent and biogenic sources. Not surprisingly given the poor agreement between the PMF and CMB VOC speciation profiles for this factor (see Figure 12, bottom), the VOC source contributions also has poor agreement.

Figure 14 displays the revised CMB VOC source apportionment modeling results averaged across all monitoring days at the two Weld County monitoring sites that can be compared with Figure 11 for the preliminary CMB modeling. The revised CMB modeling estimates slightly lower VOC at Fort Lupton due to oil and gas sources (89%) compared to the preliminary CMB modeling (94%), this appears to be due in part to the new solvent category as the motor vehicle (7%) remain approximately the same. At Platteville, the contribution of vehicle running exhaust emissions remained the same in the preliminary and revised CMB modeling (1%), but the vehicle cold start emissions added another 2% contribution to motor vehicles. The new cold start (2%) and solvent (3%) source categories appear to have reduced the O&G contributions from 98% to 94% in the revised CMB modeling.

The conclusions in the revised CMB modeling remain the same as the preliminary CMB modeling with the two Weld County monitoring sites seeing a large contribution from O&G sources. But the comparison of the PMF and CMB VOC source apportionment modeling results provide some confidence in the CMB and PMF VOC contributions of O&G and motor vehicle source sectors to the measured VOC concentrations.

Figure 14. Average source contribution to measured VOC concentrations at monitoring sites estimated using the revised CMB receptor modeling.

Emission Based VOC Source Apportionment Modeling

The CMB and PMF VOC source apportionment modeling presented two realizations of the "sources" that contributed to the morning VOC measurements collected during the June-July 2006 period. In the past, such receptor modeling based VOC source apportionment results have been compared against the emissions inventory to try an reconcile the differences between the VOC emissions inventory and the receptor modeling VOC source apportionment based on the VOC measurements. However, it is unclear how big an area around the monitoring sites should be included in the VOC emissions inventory comparison. Upwind sector averaging can be used to refine the selected VOC inventory area for comparison with the receptor modeling VOC contributions, but there are still issues with how far upwind to look and what to do when wind varies. To get around this issue we performed VOC source apportionment modeling using the CAMx probing tools. The Ozone Source Apportionment Technology (OSAT) was used to track VOC emissions from major source categories that were then extracted at the monitoring sites for the 5-8am MST period and compared with the CMB and PMF receptor modeling VOC source apportionment results. In this application we analyzed the VOC tracers to determine major source category contributions to VOC concentrations at the time and locations that the VOC measurements were made. The CAMx/OSAT VOC source apportionment modeling tracked ozone, VOC and NOX contributions during the June-July 2006 episode for the following source categories: Biogenic, On-Road Mobile, Non-Road Mobile, Oil and Gas Production, Area, and Point.

Figure 15 displays the relative contributions of VOC source contributions at the two Weld County monitoring sites averaged across the VOC morning sampling times estimated by the CAMx/OSAT emissions-based source apportionment modeling and the revised CMB and PMF receptor modeling. All three source apportionment techniques estimate that O&G is the largest contributor to VOC concentrations at Fort Lupton and especially Platteville. CAMx/OSAT estimates higher contributions of mobile, area/point and biogenic than the two receptor models. It is suspected that sources that CMB/PMF attributes to oil and gas are within the area/point and mobile source categories in the CAMx/OSAT modeling.

Figure 15. Comparison of the relative contributions of VOC source categories to the average VOC concentrations at the Fort Lupton and Platteville Weld County monitoring sites.

The comparison of the emissions based deterministic CAMx/OSAT VOC source apportionment modeling results with the observation-based CMB and PMF receptor modeling VOC source apportionment modeling results is inconclusive because of the following:

- The CAMx/OSAT, CMB and PMF VOC source categories do not represent the same sources so this is not an "apple-apple" comparison. The CAMx biogenic, mobile, oil and gas and area/point are well defined from the pre-merged emission files. But the PMF and CMB oil and gas category likely contains some sources in the CAMx/OSAT mobile and area/point categories.
- The PMF VOC source apportionment is not precise instead being mathematical factors that are interpreted as specific source categories. In reality they are mixture of sources (e.g., ethane in the biogenic source category).
- It is difficult to determine whether the CAMx VOC underestimation bias is due to insufficient VOC emissions or just differences between the surface-based point measurement versus the grid cell volume average model prediction.

Despite these limitations, there is evidence that VOC emissions in the oil and gas production area of Weld County may be under represented in the VOC emissions inventories. The largest source of VOC emission in the oil and gas production is flash emissions from the condensate tanks. Regulation 7 (Reg 7) requires large condensate tanks to have 95% control, which is what was provided in the Reg 7 reports used to develop the oil and gas emissions in the D-J Basin under WRAP Phase III. Note that a

small reduction in control efficiency would result in a large increase in VOC emissions from these sources.

FUTURE WORK

The work presented here shows that improvements have been made and implemented in the WRAP methodologies for basin level inventories. Despite this, a recent study of the reconciliation between measured VOC concentrations and model predicted concentrations suggests that these inventories are still underpredicting VOCs. Recent work by NOAA in taking aircraft-based flux measurements of methane in oil and gas basins also confirms the underestimation of emissions from oil and gas¹⁷. In response to this, the NETL has funded a research group comprised of NOAA, NREL, CSU and the Colorado School of Mines to study the reconciliation of top-down measurements and bottom-up inventories of methane from oil and gas.

The bottom-up inventory portion of the study will consist of further improvements to the methodologies initially used in the WRAP Phase III basin inventories. Some of these improvements include:

- Temporal resolution the inventory will focus on a time period concurrent with the topdown field measurements such that a highly temporally resolved inventory will be developed for direct comparison with the top-down measurements (order of several weeks).
- Episodic emission inventory the study will develop a survey for operators that is focused specifically on episodic emissions events, such as maintenance and upset conditions, well liquids unloading, well completions, and vessel and compressor blowdowns. The data gathered from the surveys will provide an enhanced set of activity data to estimate emissions from these non-routine events which have often been either missing from inventories or captured at a very coarse temporal resolution.
- Focus on midstream and transmission sectors building on the findings of the previous WRAP inventories, significant efforts will be made to identify and include midstream gathering and processing companies and transmission and distribution companies in the survey effort. Past work has shown that midstream gathering and processing facilities are often undercounted in oil and gas inventories, including gathering pipelines, compressor stations, liquid knockout, tank batteries and other similar sources. Both routine and episodic activity surveys will be developed for these sectors.
- Use of latest emission factors leveraging the extensive observation-based emissions factors developed as part of the EDF study of oil and gas emissions, the emission factors will include the latest data on pneumatic devices, fugitive components and other emission source factors reported as part of the EDF study.
- Uncertainty analysis variability in activity data and the uncertainty and probability distributions of the emissions factors from the EDF study will allow for a Monte Carlo-type uncertainty analysis to be performed on the resulting inventory. This will be the first basin-level oil and gas inventory to explicitly attempt to evaluate uncertainty for better comparison to the top-down measurements.

The study began in 2014 and is expected to continue through 2016. Results will be published in peer-reviewed journals once available, and will include presentations and outreach/educational efforts to broadly publicize the results of the work once available.

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KEY WORDS

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