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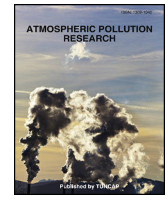

Modeling of VOCs and criteria pollutants from multiple natural gas well pads in close proximity, for different terrain conditions: A Barnett Shale case study

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ABSTRACT

Despite potential advantages in spatial/temporal coverage compared to measurement studies, few modeling studies have been conducted of non-methane air pollutants associated with natural gas. The objective of this study was to model volatile organic compound (VOC) and criteria pollutants from natural gas production, considering multiple well pads under different terrain conditions, using the Texas Barnett Shale as a case study.

Primary criteria pollutants from compressor engines (carbon monoxide, CO; nitrogen oxides, NO_x; particulate matter, PM10; sulfur dioxide, SO_2) were modeled using AERMOD, along with benzene as a VOC with potential worst health impacts, from condensate tanks, fugitive sources, and compressor engines. Modeling was conducted for level, moderate, and strong sloping terrain, with well pad densities of 1.4–1.9 well pads/km^2, exemplifying common maximum densities in the Barnett Shale.

In most cases, well pads were far enough away from each other that maxima at individual well pads were not influenced by other pads. When the same well pad arrangement and emission rates were modeled in different terrain types, strong sloping terrain gave the highest maximum concentrations.

For the well pad arrangements and emission scenarios modeled, CO, NO_x, PM10, and SO_2 maximum concentrations were less than the 1-h National Ambient Air Quality Standards (NAAQS). Benzene concentrations, however, exceeded the 1-h effect screening level (ESL) for level and strong sloped terrain, and the annual ESL for all terrain types. The maximum benzene emissions modeled likely represent a reasonable worst-case for the Barnett Shale but underestimate emissions for areas with wetter gas.

1. Introduction

Production of natural gas from hydrocarbon-rich shale formations, or shale gas, is bringing drilling and production operations to urban areas of the United States that have seen little or no similar activity in the past (Alvarez and Paranhos, 2012; Lev-On and Levy, 2012; Mueller, 2012). Over the past decade, natural gas drilling and production have become commonplace in U.S. shale formations such as the Marcellus Shale in Pennsylvania, the Barnett and Eagle Ford Shales in Texas, and the Niobrara Shale in Colorado (Alvarez and Paranhos, 2012; Mueller, 2012). Although natural gas drilling and production have occurred in sparsely populated areas for decades, their widespread occurrence in close proximity to large population centers has generated considerable interest in potential environmental impacts (Alvarez and Paranhos, 2012; Kuryla and Craft, 2012; Dickman, 2012; Mueller, 2012).

Air pollutants associated with natural gas drilling and production include 1) criteria air pollutants nitrogen oxide, carbon monoxide, and particulate matter from diesel compressor engines; 2) volatile organic compounds, which are constituents of natural gas itself and condensate, and a number of which are hazardous air pollutants; and 3) greenhouse gases, which include methane, the dominant constituent of natural gas itself, and carbon dioxide from compressor engines (Alvarez and Paranhos, 2012; Armendariz, 2009; Bar-Ilan et al., 2008; Boyer, 2010; Eastern Research Group and Sage Environmental Consulting, 2011; Hendler et al., 2009; Olaguer, 2012; Pring et al., 2010; Safitri et al., 2011; XTO Energy, 2010). During extraction, processing, and transport of natural gas, fugitive emissions of methane and volatile organic compounds can unintentionally leak to the atmosphere as a result of malfunctions and equipment wear and tear from sources such as compressors, valves, pumps, flanges, gauges, and pipe connectors. In

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addition, vented emissions of varying volumes occur by design, via routine venting of pneumatic valves, storage tanks, dehydrators, and wells after hydraulic fracturing (Alvarez and Paranhos, 2012).

A large number of studies have evaluated methane emissions in particular from natural gas drilling and production sites; these studies have been summarized by Allen (2014) and Moore et al. (2014). Several studies have assessed the impact of natural gas drilling and production on urban and regional air quality (Ahmadi and John, 2015; Cheng et al., 2015; Pacsi et al., 2013; Roohani et al., 2017; Swarthout et al., 2015; Vinciguerra et al., 2015), or national air pollutant emissions (Chang et al., 2014). Several studies have developed frameworks for using regional monitoring data to assess potential health impacts (Boyle et al., 2016; Meng, 2018; Esterhuyse et al., 2018). In terms of non-methane air pollutants, several measurement studies have been conducted in the local proximity of urban natural gas drilling and production, to assess potential citizen exposures (Pennsylvania Dept. of Environmental Protection, 2010, 2011 a&b; 2013; Macey et al., 2014; Goetz et al., 2015; Paulik et al., 2018). In the Barnett Shale in particular, ambient measurement studies have been conducted by the Texas Commission on Environmental Quality (TCEQ) (2010), Eastern Research Group and Sage Environmental Consulting for the City of Fort Worth in the Fort Worth Natural Gas Air Quality Study (FWNGAQS) (2011), Zielinska et al. (2014), Rich et al. (2014), Eapi et al. (2014), and Eisele et al. (2016); in addition, Bunch et al. (2014) evaluated data from existing monitors to assess VOC exposure. One limitation of measurement/monitoring studies is that measured concentrations are functions of meteorology and location, and may not be worst-case, depending on the conditions at the time and location of measurement.

Several studies have estimated emissions from various components of the natural gas drilling and production system, but have not included dispersion modeling to estimate concentrations to which nearby residents might be exposed (Alvarez et al., 2013; Armendariz, 2009; Hendler et al., 2009; Pring, 2012). Few modeling studies have been conducted of non-methane air pollutants in the proximity of urban natural gas drilling and production in the Barnett Shale. Zavala-Araiza et al. (2014) modeled VOC emissions from natural gas production in the Barnett Shale using AERMOD. Since the purpose was to compare measured concentrations with modeled concentrations, only one receptor location was modeled. The FWNGAQS modeled impacts from one gas well pad and compressor engine station, with several layouts. Impacts of surrounding terrain were not considered, with the justification being that Fort Worth is predominantly flat. However, as noted in Table 3 below, we found areas with moderate (up to 10%) and strong slopes (up to 30%), according to standard slope descriptors (Barcelona Field Studies Centre, 2018). In addition, given the fact that the sources at the well pad have generally low release heights (less than 10 feet, with the exception of the compressor engine stack, as shown in Table 1), we think that situations could exist where receptor elevations in close proximity are above the release heights. Complex terrain, depending on the site configuration, can block air flow and lead to reduced dispersion and higher pollutant concentrations (Georgiana et al., 2012).

In both Zavala et al. and FWNGAQS studies, dispersion modeling was limited to volatile organic compounds; dispersion modeling of criteria pollutants was not performed. When a new source or modified facility requests a New Source Review Permit, the TCEQ and equivalent agencies in other states may require dispersion modeling to ensure that the new/modified source will not cause adverse air quality impacts (TCEQ, 2018). However, TCEQ permits many new facilities through permits by rule (PBRs), which do not require modeling but rather a simple engineering estimate of annual emissions presuming the estimate is below 25 (short) tons per year. Even for cases where modeling of individual pads may have been done as part of the permitting process, the impact of multiple pads in close proximity may not have been evaluated, if the pads belonged to different owners or were permitted at different times.

Table 1
Well pad source characteristics.

Source	Source Type	Height, ft. (m)	Diameter, ft (m)	Exit velocity (m/sec)	Temp. (°C)	Number of sources modeled per pad	Basis
Storage tanks	Pseudo-point (circular building & point source)	10 (3.0)	15 (4.6)	0.001	Ambient	3–5	ERG & Sage (2011); Aerial photos
Fugitives	Area	6 (1.8) (average height of piping)	Dimensions of actual pad (rectangular)	N/A	Ambient	1	ERG & Sage (2011)
Compressor Engines	Point	25 (7.6) (stack)	0.875 (0.267) (stack)	50	600	1–3	Caterpillar, aerial photos

Modeling studies have advantages over measurement studies in being able to assess concentrations 1) at hundreds or thousands or receptor locations, providing a more complete spatial assessment; 2) for several years of hourly meteorological data, which can in some cases provide more complete temporal assessment, and 3) due to the particular source of interest only, in this case natural gas drilling and production facilities, which eliminates confounding concentrations due to other sources. However, previous modeling studies have been limited to one well pad or one receptor location, and have not included criteria pollutants.

Thus, the **objective** of this study was to model potential air pollutant concentrations to which the public might be exposed in close proximity to natural gas well pads during natural gas production, considering multiple well pads under different terrain conditions, and including criteria pollutants. We anticipate that modeled concentrations from multiple well pads in close proximity will be higher compared to a scenario in which only one well pad is modeled, due to contributions from multiple sources. We also expect that complex terrain associated with strong slopes will limit dispersion of pollutants and lead to higher concentrations.

This research considers natural gas production only; drilling and fracturing are not considered, because those processes happen at the beginning of natural gas exploration. Drilling of a new well is typically a two to three week process from start to finish and involves several large diesel-fueled generators.

The Barnett Shale in Texas was chosen for the study. The Barnett Shale is one of the United States' largest onshore natural gas fields, comprising 5000 square miles, with a well count of over 22,000 (Natural Gas Intelligence, 2014). Although other production regions in the U.S. are larger than the Barnett Shale and have higher well counts, the Barnett Shale was chosen for this study due to its proximity to the authors and their familiarity with input data needed for the modeling.

2. Methodology

AERMOD View Gaussian dispersion model software version 9.0 developed by Lakes Environmental was used for estimating pollutant concentrations. Modeling inputs/assumptions are described below.

Source characteristics and emission rates: base case. The base cases include natural gas well pads modeled in their actual terrain (as opposed to well pads placed on terrain on which they do not actually sit, which occurs for later cases). Oil wells were not modeled. Three types of sources typically located at natural gas well pads were modeled, with characteristics shown in Table 1:

1. Condensate Storage Tanks: Volumes in Barnett Shale range from 10,000 to 20,000 gal. (Armendariz, 2009). A mid-range 13,200 gallon volume was modeled. Based on the City of FWNGAQS (ERG and Sage, 2011), typically each well pad has 3 - 10 storage tanks. In the base case, 3 - 5 storage tanks were modeled, based on the actual number of storage tanks shown on the aerial photos of the pads in the areas modeled.

2. Compressor Engines: Caterpillar engines G3406 (255 hp) & G3306 (145 hp) were modeled. Compressor engines range from 145 to 1890 hp in Fort Worth; 145 hp is the most common size, and 255 hp is also relatively common (ERG and Sage, 2011). Based on the FWNGAQS, 2/3 of the well pads have 0 compressor engines; the rest have from 1 to 6 compressor engines (lift compressors used to increase a well's gas production rate). In the base case, we modeled the compressor engines based on the actual number of compressor engines shown aerial photos (1–3 per pad). If a well pad did not contain a compressor engine, then one was added as a worst case.

Arrangement of the storage tanks and compressor engines on well pads was determined using real locations, based on aerial photos, with the exception that compressor engines were added to well pads that did not contain them, to model the worst case.

3. Fugitive Sources: All well pad sources excluding storage tanks and compressor engines (wellheads, valves, flanges, connectors, pneumatic controllers), were grouped as one source per pad, following the methodology used in the FWNGAQS. Since our emission factors for fugitives came from those used for the FWNGAQS, our study includes devices which vent by design, such as pneumatic controllers, in the category of fugitives.

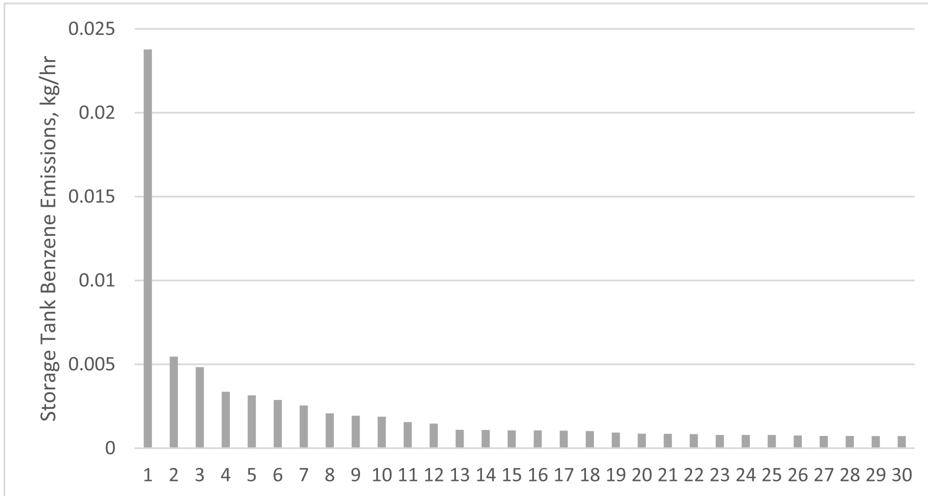
For VOCs, benzene was selected for modeling, because is a Hazardous Air Pollutant (HAP) and is generated from all emission sources modeled in this study. In addition, the ratio of the benzene ambient modeled level to Effects Screening Level (ESL) was higher than for the other 90 organics modeled in the FWNGAQS, which means it has the potential to cause higher health impacts. Modeling was conducted for three of the 6 criteria pollutants - carbon monoxide (CO); nitrogen oxides (NO_x), which includes the criteria pollutant nitrogen dioxide (NO_2), and particulate matter (PM10). Compressor engines were the only source of these emissions. Ozone was not modeled because it is not emitted directly from compressor engines, but is formed in the atmosphere from reactions between VOCs and NO_x. Lead and sulfur dioxide were not modeled because they are not emitted in significant quantities from the compressor engines modeled (Caterpillar engines G3406 and G3306), and thus emission factors were not available.

Source emission rates provided in Table 2 were taken from the FWNGAQS (2011). Storage tank and fugitive emission values came from field measurements at 375 well pads, which comprised around 10% of the 3700 well pads in the Barnett Shale. Sites were selected for surveying randomly, and city gas inspectors were only told of the next scheduled site upon departure, to avoid the possibility of site owners learning of the schedule in advance. Measurements at the 375 well pads may have included intermittent high emissions, but this is not known for certain. For compressor engines, emission rates were not measured, but were calculated from emission factors based on the models and horsepower of the 225 compressor engines found on the 375 well pads.

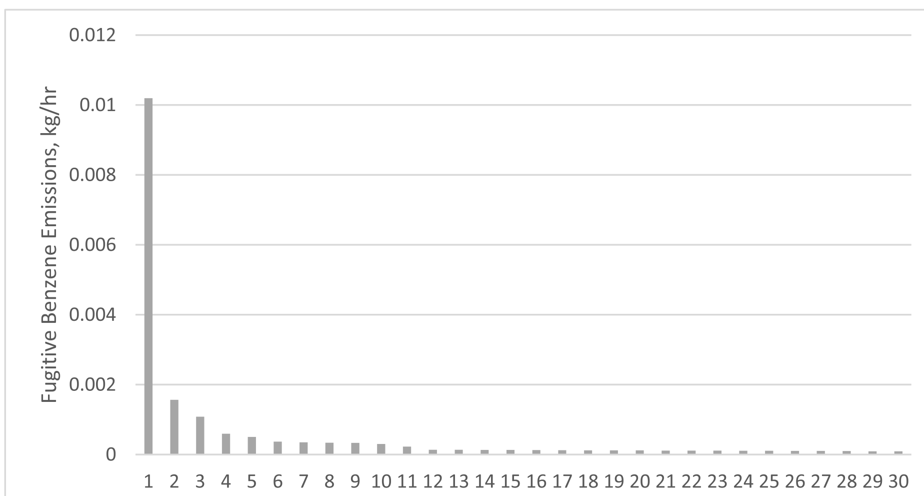
Fig. 1 shows the 30 highest storage tank, fugitive, and compressor engine benzene emission values from the FWNGAQS. When multiple identical compressor engines occurred at the same site, duplicate values were not plotted. The maximum storage tank benzene emission rate (highest of 380 tank values) is 4.4 times the 2nd highest value, and 45 times the average value. The maximum fugitive benzene emission rate

Table 2
Well pad source emission rates from Fort Worth Natural Gas Air Quality Study.

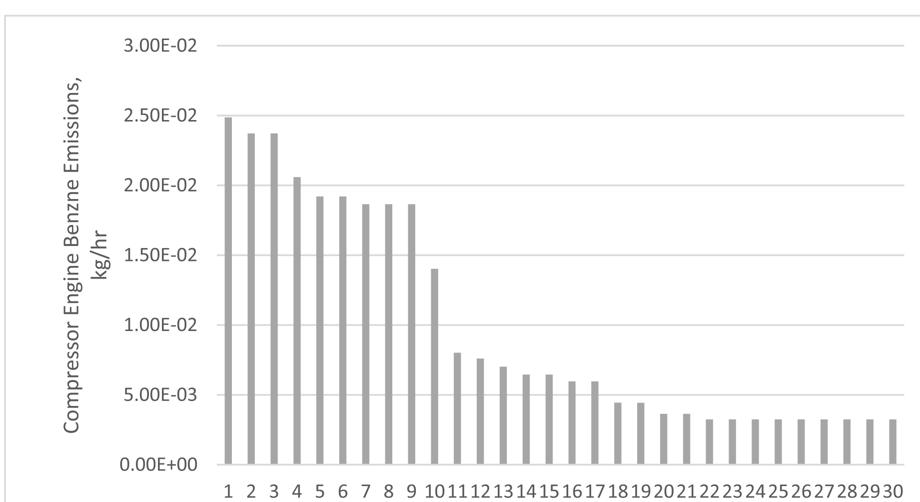
Source	Emission Rate (kg/hr)												
	Benzene			Methane		CO		NO_x		PM10		SO_2	
	Max.	2nd highest	Avg.	Max.	Avg.	Max.	Avg.	Max.	Avg.	Max.	Avg.	Max.	Avg.
Storage Tanks	0.0239	0.00546	5.27E-04	45.1	3.80	N/A	N/A	N/A	N/A	0.477	N/A	N/A	N/A
Fugitives	0.0102	0.00157	4.86E-05	33.0	1.64	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Compressor Engines	0.0249	0.0237	3.43E-03	N/A	N/A	18.55	1.28	0.926	0.152	0.05466	0.00773	0.00338	0.00057



(a) Storage tanks



(b) Fugitives



c) Compressor engines

Fig. 1. Top 30 benzene emission rates from the Fort Worth Natural Gas Air Quality Study for a) Storage tanks, b) Fugitives, and c) Compressor engines.

(highest of 375 site fugitive values) is 6.5 times the 2nd highest value, and 210 times the average value. The maximum compressor engine value is only 5% higher than the 2nd highest value, and 7 times the average value. Since the maximum benzene values were so much higher than the 2nd highest values for storage tanks and fugitives (and thus represent worst-case values, but cases reasonably unlikely to occur), the 2nd highest values were also modeled.

The maximum emission rates for the 375 sites included in the FWNGAQS are likely lower than the maximum rates that exist among the 3700 sites in the Barnett Shale. However, we assumed that maximum emissions from storage tanks, fugitives, and compressor stations occurred on the same well pad, which is probably overly conservative. Hence, our maximum rates when modeled together likely represent a reasonable worst-case for the Barnett Shale.

By way of comparison, Marrero et al. (2016) measured concentrations downwind of 31 natural gas well pads, some of which housed separators, condensate tanks, or compressors in addition to the well heads. The maximum benzene flux was about 0.005 kg/hr, which is on the order of the 2nd highest emissions from storage tanks in the FWNGAQS. Fluxes were measured an average of 34 m downwind, however, where some dilution would likely have occurred. The benzene flux from wet gas was over twice as high as from dry gas. The Barnett Shale does not belong to the shale areas with high aromatic compound contributions, and can thus be considered a comparatively low emitter of these compounds based on condensate composition.

Terrain scenarios and source locations. Level, moderate, and strong sloping terrain scenarios were modeled, as shown in Table 3 and Fig. 2. The categories of level, moderate, and strong slopes used in this study - 1, 10, and 30 foot maximum vertical elevation difference per 100 foot horizontal distance, or 1%, 10%, and 30%, respectively – are consistent with standard slope descriptors (level or nearly level, 0–2%; moderate, 9–15%, strong, 15–30%) (Barcelona Field Studies Centre, 2018).

For each terrain category, an example area containing multiple well pads in close proximity was selected within the City of Fort Worth. Dimensions of these areas are shown in Table 3. Selection of an area with strong slopes as large as the level and moderate areas was not possible. Within each selected terrain area, locations of actual well pads were determined, based on aerial photos and Texas Railroad Commission information. Fig. 3 shows the well pad locations, along with the number of storage tanks and compressor engines, for each selected terrain area. The number of well pads per square kilometer, shown in Table 3, ranged from 1.4 for strong sloped terrain to 1.9 for level terrain, exemplifying common maximum densities in the Texas Barnett Shale. Again, finding example areas of each of the terrain categories with the identical number of well pads per square kilometer was not possible. Under Texas Statewide Rule 38, the drilling unit size for wells subject to state rules is 40 acres, although special field rules may set different density requirements (Durrett, 2014). The number of acres per well pad is shown in Table 3, although the number of wells per pad is not known.

Altogether, 47 well pads were modeled. The Barnett Shale contains over 22,000 wells; dividing this number by the average number of wellheads per well pad given in the FWNGAQS (6) gives 3700. Hence, 47 of the approximately 3700 well pads in the Barnett Shale were modeled.

In addition to the level, moderate, and strong sloping terrain scenarios with the actual well pad locations, a 4th scenario was modeled in which the 6 well pads from the strong sloping terrain were placed on the level and moderate terrains. This enabled us to evaluate the impact of terrain alone, keeping the sources identical.

Topographic information and elevations, NED GEOTIFF and NED 1/3 (USA – 10 m), were taken from www.WebGIS.com.

Meteorological Data. 8760 hourly values of meteorological data from Dallas-Fort Worth International Airport (station number 03927) (surface) and Stephenville (upper air) for 1992 were modeled. Stephenville is the closest station to DFW region with upper air data. 1992 is the latest of 11 years of meteorological data currently applied for air quality permit application modeling in Texas. According to a study by

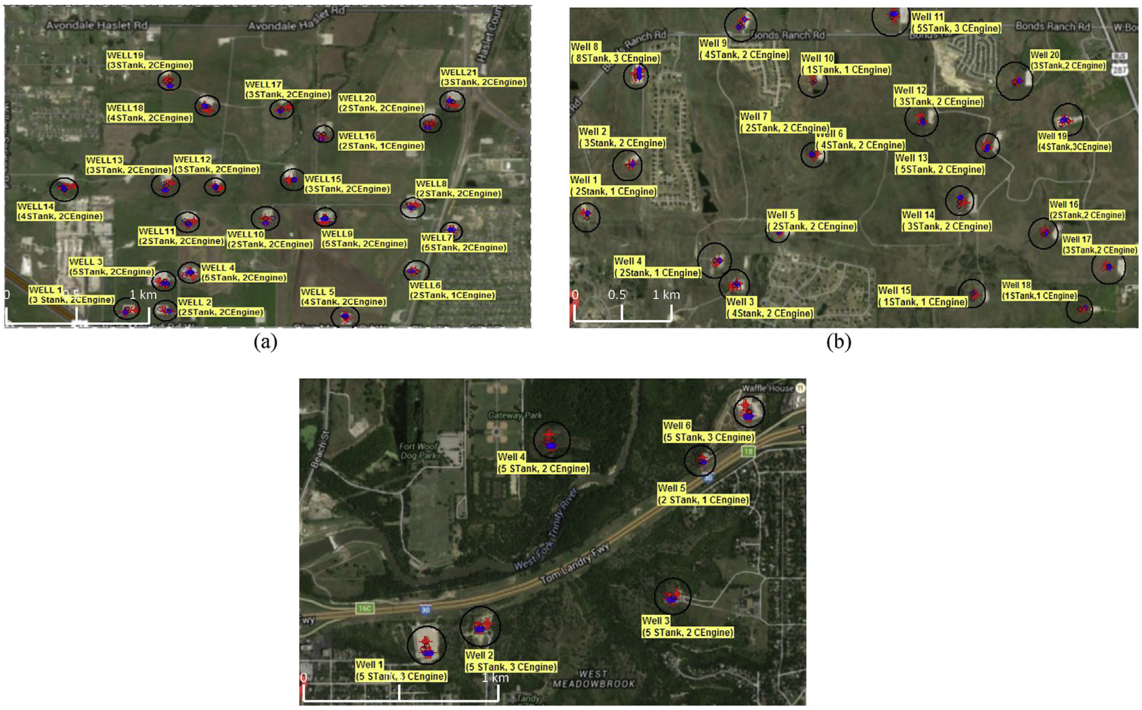
(a) Level (b) Moderate

(c) Strong sloping

Fig. 2. Elevation maps for (a) level, (b) moderate, and (c) strong sloping terrain.

Table 3
Terrain scenarios modeled and well pad densities.

Terrain Slope Category	Max. Vertical Elevation Difference (per 100′ horizontal)	Dimensions of Area Modeled	Number of Well Pads Modeled Within the Area	Number of Well Pads/km^2	Number of acres per well pad
Level	1’ (1%)	3.9 km × 2.9 km = 10.9 km^2	21	1.9	130
Moderate	10’ (10%)	5.1 km × 2.7 km = 13.8 km^2	20	1.5	165
Strong	30’ (30%)	2.6 km × 1.7 km = 4.4 km^2	6	1.4	176



(c)

Fig. 3. Locations of well pads, including numbers of storage tanks and compressor engines, modeled for (a) level terrain, (b) moderate terrain, (c) strong sloping terrain.

Sattler and Devanathan (2007), the 1992 dataset gives maximum concentrations similar to those of the 1988, 1989, and 1991, and thus is likely representative of meteorological conditions in the DFW region. Meteorological data was obtained from the Lakes Environmental web site (www.weblakes.com). AERMET was used to preprocess the data for AERMOD.

Other Model Options. A Cartesian receptor grid with uniform spacing was used for each site domain, with grad spacing ranging from 79 to 98 m. Concentrations were modeled at 1271, 1590, and 616 receptor locations for level, moderate, and strong sloping terrain, respectively. The modeling domain was chosen to be large enough that plumes from the natural gas wells were contained within it.

Plumes entering the domain from other sources were not modeled. In other words, background concentrations were assumed to be zero, and modeled concentrations thus represent concentrations above background. This assumption is very common in Gaussian dispersion modeling.

Regulatory default mode, rural dispersion coefficients, elevated terrain, and simple + complex terrain were used. No significant removal was assumed due to wet deposition, dry deposition, or gravitational setting.

Averaging times of 1-h and annual were selected. AERMOD modeled hourly concentrations at each receptor location, and then averaged 8760 hourly values to determine the annual average concentration at each receptor.

3. Results and discussion

3.1. Effect of well pads in close proximity on modeled concentrations

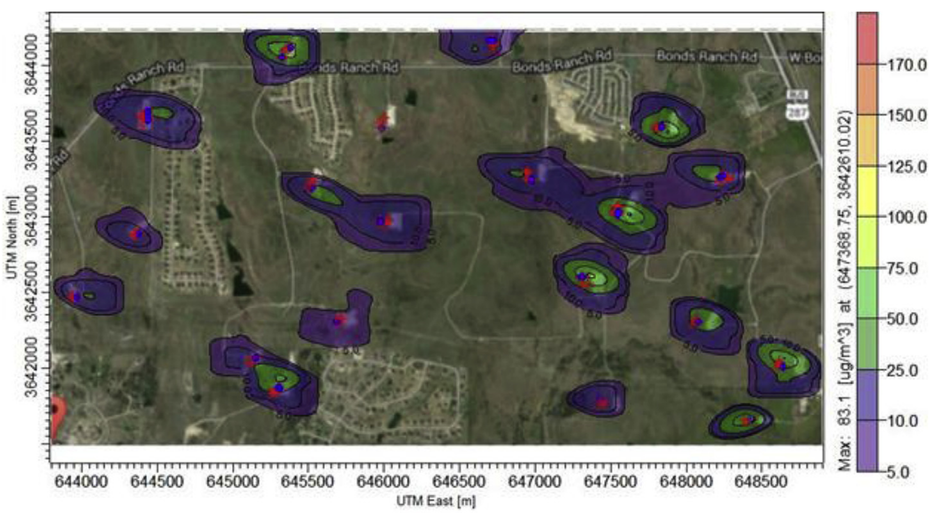
Fig. 4 shows 1-hr benzene isopleths for modeling of maximum benzene emission rates for actual well pads in level, moderate, and strong sloping terrain. Isopleths for the other air pollutants are available from the authors. As is standard for AERMOD output, the plots show the highest 1-h concentration at each receptor location out of the year of meteorological data modeled, even though the highest concentrations occurred at different hours for different receptors.

As shown in Fig. 4, the highest concentrations of pollutants surround the well pads, as anticipated. In most cases, the well pads were far enough away from each other (> 200 m) that maxima at individual well pads appear not to be substantially influenced by other well pads. This is shown by the separated green contours, although there are exceptions. For example, the maxima at the lower left of Fig. 4 (a) may have contributions from the 3 well pads in close proximity (approximately 200 m spacing between pads), shown by the blending of the 3 green contours. The green contours do not, however, indicate an exceedance of the 1-h ESL (170 μg/m^3, shown in red).

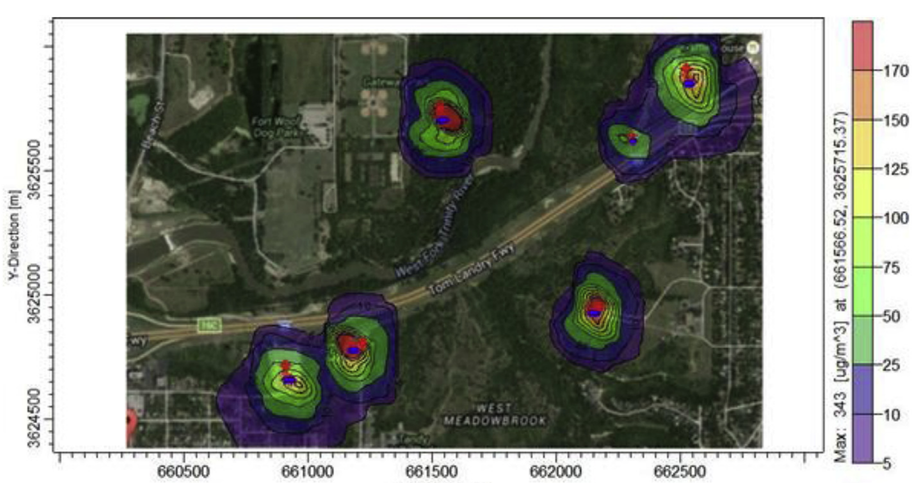
3.2. Effect of emission rates and terrain on modeled concentrations

Tables 4 and 5 show the maximum 1-h and annual average concentrations, respectively, of all 5 pollutants for all emission rates

(a) Level



(b) Moderate



(c) Strong sloping

Fig. 4. 1-hour benzene isopleths for actual well pads in (a) level, (b) moderate, and (c) strong sloping terrain (concentrations shown are above background).

Table 4
Maximum 1-h modeled pollutant concentrations for actual well pads in 3 types of terrain [d].

Pollutant	1-h NAAQS or ESL ($\mu g/m^3$)	Maximum concentration ($\mu g/m^3$)								
		Modeling of Max. Emission Rate			Modeling of 2nd Highest Emission Rate (Benzene)			Modeling of Avg. Emission Rate		
		Level Terrain	Moderate Terrain	Strong Sloping Terrain	Level Terrain	Moderate Terrain	Strong Sloping Terrain	Level Terrain	Moderate Terrain	Strong Sloping Terrain
Benzene	170	715[a]	83.1	343[b]	163	18.9	78.1	15.7	1.8	7.5
CH_4	–	1,356,000	157,569	649,632	N/A			114,708	13,208	54,574
CO	40×10^3	1088	1305	1619	N/A			75.2	90.2	112
NO_x	188 (NO_2)	54.4	65.2	80.8	N/A			8.9	10.7	13.3
PM	150[c] (PM10)	3.2	3.9	4.8	N/A			0.45	0.54	0.68
SO_2	196	0.20	0.24	0.29	N/A			0.03	0.04	0.05

[a] ESL exceeded for 951 h per year (918 h at one receptor location, and 10, 9, 8, and 6 h at 4 other locations).
[b] ESL exceeded for 61 h per year (27 h per year at one receptor location, 26 h per year at a second location, and 8 h per year at a 3rd location).
[c] 24-h averaging time.
[d] Concentrations shown are above background.

modeled for the three terrain scenarios with actual well pads. The maximum 1-h concentrations are maxima in terms of time (highest 1-h out of 8760 h per year) and space (highest of all the receptor locations). The highest annual concentrations are the highest in terms of space (highest of all the receptor locations).

The highest 1-h and annual concentrations of benzene and methane, for all emission rates, occur in level terrain. The highest 1-h concentrations of CO, NO_x, PM, and SO_2 occur in strong sloping terrain, and the highest annual concentrations of CO, NO_x, PM, and SO_2 occur in level terrain. Most of these cases do not agree with the hypothesis that strong slopes would produce the highest concentrations; however, this could be due to the fact that the well pads modeled in each type of terrain were different in terms of dimensions, number and location of storage tanks, and number and location of compressor engines, since these numbers and locations were taken from aerial photographs of actual well pads in each terrain location.

To test whether the high concentrations for level and moderate terrain were actually due to the terrain or due to the different well pads modeled, the same 6 well pads from the strong sloping terrain were modeled in the level and moderate terrain, using maximum emission rates for benzene, as shown in Fig. 5 (the strong sloping terrain case is repeated here for comparison). The maximum benzene concentration (343 μg/m^3) occurred in strong sloping terrain, which is consistent with the hypothesis that strong sloping terrain can limit pollutant dispersion. The maximum concentration for level terrain (161 μg/m^3), however, was slightly higher than for moderate terrain (126 μg/m^3), which is surprising.

3.3. Comparison of modeled concentrations to ESLs and NAAQS

In Tables 4 and 5, the maximum 1-h and annual average concentrations of benzene are compared to the short-term (1-h averaging time) and long-term (annual averaging time) TCEQ Effect Screening Levels (ESLs) for benzene, respectively. The TCEQ uses ESLs in their air permitting process to evaluate air dispersion modeling's predicted impacts. If modeled concentrations of a pollutant do not exceed the screening level, adverse health or welfare effects are not expected. If modeled concentrations of a pollutant exceed the screening levels, it does not necessarily indicate a problem but rather triggers a more in-depth review.

In Table 4, benzene concentrations exceeded the 1-h effect screening level for level and sloping terrain for the maximum emission rate case. In Table 5, for the maximum emission rate case, benzene exceeded the annual ESL for all terrain types. For the 2nd highest emission rate case, benzene exceeded annual ESL for level terrain.

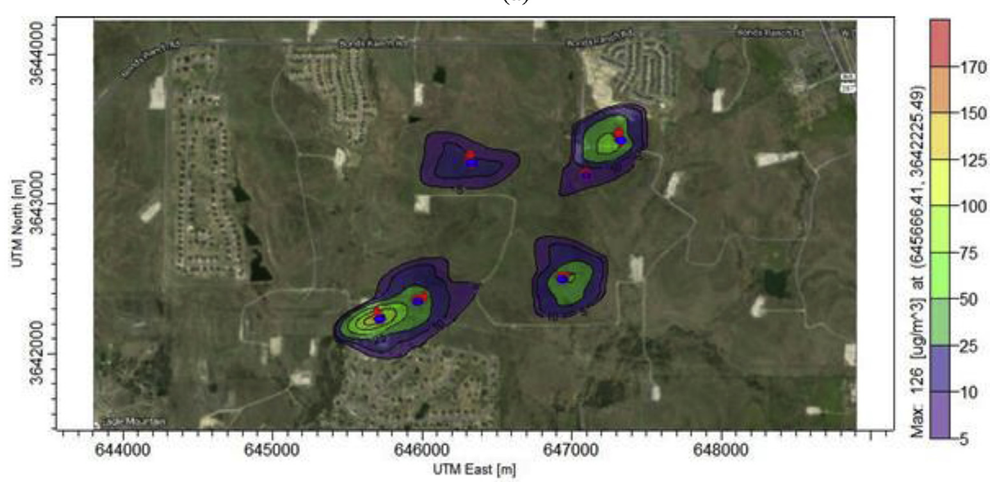
The maximum benzene emissions modeled likely represent a reasonable worst-case for the Barnett Shale but underestimate benzene emissions for shale areas with wetter gas. It should be noted, also, that background levels of benzene in this study were assumed to be zero. However, urban benzene levels at some locations can be as high as 30–50% of ESL values. If the well pads were to undergo New Source Review permitting, ambient background levels would have to be added to the modeled values before an ultimate permit decision were to be made. ESL exceedances with background addition would be spatially more extensive, and may ultimately lead to the denial of a permit unless

Table 5
Maximum annual modeled pollutant concentrations for actual well pads in 3 types of terrain.[d].

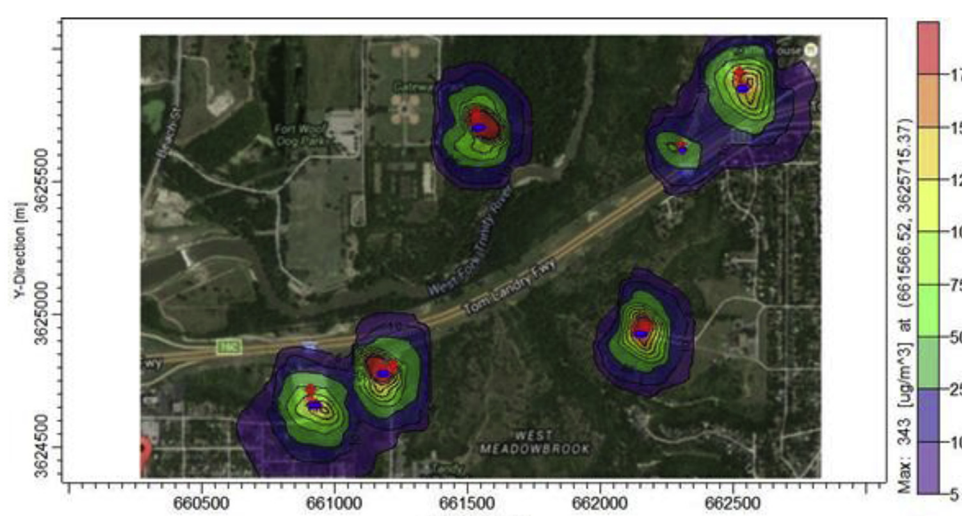
Pollutant	Annual NAAQS or ESL ($\mu g/m^3$)	Maximum concentration ($\mu g/m^3$)								
		Maximum Emission Rate Modeled			2nd Highest Emission Rate Modeled (Benzene)			Average Emission Rate Modeled		
		Level Terrain	Moderate Terrain	Strong Sloping Terrain	Level Terrain	Moderate Terrain	Strong Sloping Terrain	Level Terrain	Moderate Terrain	Strong Sloping Terrain
Benzene	4.5	78.8[a]	7.9[b]	19.4[c]	18.0[c]	1.6	4.4	1.76	0.14	0.45
CH_4	–	149,495	18,845	37,763	N/A			12,506	1246	3071
CO	N/A	245	232	204	N/A			16.9	16.0	14.1
NO_x	99.7 (NO_2)	12.2	11.6	10.2	N/A			2.0	1.9	1.7
PM	N/A	0.72	0.68	0.60	N/A			0.10	0.10	0.09
SO_2	N/A	0.044	0.42	0.037	N/A			0.008	0.007	0.006

[a] ESL exceeded at more than 10 receptor locations.
[b] ESL exceeded at one location only.
[c] ESL exceeded at 7 receptor locations.
[d] Concentrations shown are above background.

(a)



(b)



(c)

Fig. 5. 1-hour benzene isopleths for identical 6 well pads modeled in (a) flat, (b) moderate, and (c) strong sloping terrain (concentrations shown are above background).

emission mitigation measures were taken.

Since there are no ESLs for CO, NO_2, PM10, and SO_2, the maximum 1-h concentrations for these compounds were compared to National Ambient Air Quality Standards (NAAQS), although the short-term NAAQS are actually statistical measures. Despite the presence of multiple well pads in close proximity, the maximum concentrations for CO, NO_2, PM10, and SO_2 in Table 4 were below NAAQS, for all emission rate cases. According to EPA's evaluation of sites without downwash, AERMOD's overall predicted-to-observed ratio for short-term averages was 1.03 (with a range among sites from 0.73 to 1.35) and 0.76 for annual averages (with a range among sites from 0.30 to 1.64). For sites with downwash, AERMOD's overall predicted-to-observed ratio for short-term averages was 0.97 (EPA, 2003). Even if our estimates for CO, NO_2, PM10, and SO_2 are multiplied by the largest predicted-to-observed ratio found in the evaluation - 1.35 - the results are still below NAAQS.

In Table 5, the only criteria pollutant with an annual NAAQS was NO_2. The highest modeled NO_x concentration was well below this value.

For the FWNGAQS, the worst-case well pad modeled included 10 storage tanks and 2 compressor engines, which is more storage tanks than we modeled, but fewer compressor engines than some of the sites we modeled. Maximum emission rates were used for storage tanks and fugitives, but average emission rates were used for compressor engines. Concentrations were estimated for locations outside the property line only. The maximum 1-h and annual benzene concentrations were 59.5 and 3.99 ppb, respectively, equivalent to 190 and 12.7 $\mu g/m^3$. These values are slightly higher than the 1-h and annual ESLs for benzene, which are 170 and 4.5 $\mu g/m^3$, respectively. In comparison, maximum 1-h and annual values modeled in this study were 715 and 78.8 $\mu g/m^3$. The fact that we modeled concentrations within the property line likely accounts for the higher values.

4. Conclusions and recommendations for future research

In most cases, well pads were far enough away from each other that maxima at individual well pads were not influenced by other well pads. When the same well pad arrangement and emission rates were modeled in different terrain types, strong sloping terrain gave the highest maximum concentrations for all pollutants compared to level and moderate terrain.

For the well pad arrangement and emission scenarios modeled, CO, NO_x, PM10, and SO_2 maximum concentrations were less than the National Ambient Air Quality Standards (NAAQS) for 1-h averaging times. Benzene concentrations, however, exceeded the 1-h effect screening level for level and strong sloped terrain, and the annual effect screening level for all types of terrain. The maximum benzene emissions modeled likely represent a reasonable worst-case for the Barnett Shale but underestimate benzene emissions for shale areas with wetter gas.

Recommendations for future research include modeling worst-case emissions for CO and PM, as well as n-hexane, which is more abundant in product streams than benzene, and also toxic. Modeling should be conducted of the combined impacts of well pads and gathering stations in different terrains. We also recommend collecting field data on temporal variations in emissions, which could be used to model temporal variations in atmospheric concentrations.

Competing Interests

There are no competing interests.

References

Ahmadi, M., John, K., 2015. Statistical evaluation of the impact of shale gas activities on ozone pollution in North Texas. Sci. Total Environ. 536, 457–467.

Allen, D.T., 2014. Atmospheric emissions and air quality impacts from natural gas production and use. Annu. Rev. Chem. Biomol. Eng. 5, 55–75.

Alvarez, R., Paranhos, E., 2012. Air pollution issues associated with natural gas and oil operations. Environ. Manag. 6, 22–25.

Alvarez, Y., Shah, T., Bar-Ilan, A., Lindhjem, C., Kemball-Cook, S., Yarwood, G., 2013. Gas Compressor Engine Study for Northeast Texas. Prepared for East Texas Council of Governments, Kilgore, TX.

Armendariz, A., 2009. Emissions from natural gas production in the Barnett shale area and opportunities for cost-effective improvements. Report for Environmental Defense Fund. On-Line Document. . http://www.edf.org/documents/9235_Barnett_Shale_Report.pdf.

Barcelona Field Studies Centre, 2018. Measuring Slope Steepness. https://geographyfieldwork.com/SlopeSteepnessIndex.htm, accessed 10/2018.

Bar-Ilan, A., Parikh, R., Grant, J., Shah, T., Pollack, A.K., 2008. Recommendations for Improvements to the CENRAP States' Oil and Gas Emissions Inventories. Report Prepared by ENVIRON International Corporation for the Central States Regional Air Partnership. . http://www.wrapair.org/forums/ogwg/documents/2008-11_CENRAP_O&G_Report_11-13.pdf (accessed August 2012).

Boyer, D., 2010. 2006/2012 DFW modeling update. In: Presentation Prepared by Texas Commission on Environmental Quality for the DFW Photochemical Modeling Technical Committee Meeting, Arlington, Texas, , Accessed date: 5 November 2010.

Boyle, M.D., Payne-Sturges, D.C., Sangaramoorthy, T., Wilson, S., Nachman, K.E., Babik, K., Jenkins, C.C., Trowell, J., Milton, D.K., Sapkota, A., 2016. Hazard ranking methodology for assessing health impacts of unconventional natural gas development and production: the Maryland case study. PLoS One 11 (1). https://doi.org/10.1371/journal.pone.0145368. e0145368.

Bunch, A.G., Perry, C.S., Abraham, L., Wikoff, D.S., Tachovsky, J.A., Hixon, J.G., Urban, J.D., Harris, M.A., Haws, L.C., 2014. Evaluation of impact of shale gas operations in the Barnett Shale region on volatile organic compounds in air and potential human health risks. Sci. Total Environ. 468, 832–842. 469. https://doi.org/10.1016/j.scitotenv.2013.08.080.

Caterpillar Engine Specifications Model G3408 http://s7d2.scene7.com/is/content/Caterpillar/LEHW0030-00. http://catoilandgas.cat.com/industries/gas-compression-power and general data available at:.

Chang, Y., Huang, T., Masanet, E., 2014. The energy, water, and air pollution implications of tapping China's shale gas reserves. Resour. Conserv. Recycl. 91, 100–108. https://doi.org/10.1016/j.resconrec.2014.07.015.

Cheng, H., Small, M.J., Pekney, N.J., 2015. Application of nonparametric regression and statistical testing to identify the impact of oil and natural gas development on local air quality. Atmos. Environ. 119, 381–392. https://doi.org/10.1016/j.atmosenv.2015.08.016.

Dickman, S.C., 2012. EPA's plan to study the potential impacts of hydraulic fracturing on drinking water resources. Environ. Manag. 3, 14–19.

Durrett, Brandon E., 2013-2014. A Primer on Oil and Gas Regulation in Texas: Spacing, Density, Permits, Exceptions. *Landman*, a publication of the American Association of Professional Landmen, Winter, pp. 35–45. https://www.dykema.com/media/site_files/120_NO_ADS_Durrett_Pub-NA.pdf accessed 10/2018.

Eapi, G.R., Sabnis, M.S., Sattler, M.L., 2014. Mobile measurement of methane and hydrogen sulfide at natural gas production site fence lines in the Texas Barnett Shale. J. Air Waste Manag. Assoc. 64 (8), 927–944. https://doi.org/10.1080/10962247.2014.907098.

Eastern Research Group, 2011. Sage Environmental Consulting. City of Fort Worth Natural Gas Air Quality Study. Final report prepared for City of Fort Worth.

Eisele, A.P., Mukerjee, S., Smith, L.A., Thoma, E.D., Whitaker, D.A., Oliver, K.D., Wu, T., Colon, M., Alston, L., Cousett, T.A., Miller, M.C., Smith, D.M., Stallings, C., 2016. Volatile organic compounds at two oil and natural gas production well pads in Colorado and Texas using passive samplers. J. Air Waste Manag. Assoc. 66 (4), 412–419. https://doi.org/10.1080/10962247.2016.1141808.

Esterhuyse, S., Avenant, M., Redelinghuys, N., Kijko, A., Glazewski, J., Plit, L., Kemp, M., Smit, A., Vos, A.T., 2018. Monitoring of unconventional oil and gas extraction and its policy implications: a case study from South Africa. Energy Policy 118, 109–120.

Environmental Protection Agency (EPA), 2003. AERMOD: Latest Features and Evaluation Results. EPA-454/R-03-003.

Georgiana, G., Cuculeanu, V., Tudor, G., Mocioaca, G., 2012. Air pollution dispersion modeling in a polluted industrial area of complex terrain from Romania. Rom. Rep. Phys. 64 (1), 173–186.

Goetz, D., Floerchinger, C., Fortner, E.C., Wormhoudt, J., Massoli, P., Knighton, W.B., Herndon, S.C., Kolb, C.E., Knipping, E., Shaw, S.L., DeCarlo, P.F., 2015. Atmospheric emission characterization of Marcellus shale natural gas development sites. Environ. Sci. Technol. 49, 7012–7020. https://doi.org/10.1021/acs.est.5b00452.

Hendler, A., Nunn, J., Lundeen, J., 2009. VOC Emissions from Oil and Condensate Storage Tanks. Final report prepared for the Texas Environmental Research Consortium. http://files.harc.edu/Projects/AirQuality/Projects/H051C/H051CFinalReport.pdf, Accessed date: August 2012.

Kuryla, M., Craft, Z., 2012. Shale production air emissions: key legal developments. Environ. Manag. 6, 26–31.

Lev-On, M., Levy, J.A., 2012. Environmental issues associated with shale oil and gas exploration and production, part 2: air emissions. Environ. Manag. 6, 7–13.

Macey, G.P., Breech, R., Chernaik, M., Cox, C., Larson, D., Thomas, D., Carpenter, D.O., 2014. Air concentrations of volatile compounds near oil and gas production: a community-based exploratory study. Environ. Health 13, 82. http://www.ehjournal.net/content/13/1/82.

Marrero, J.E., Townsend-Small, A., Lyon, D.R., Tsai, T.R., Meinardi, S., Blake, D.R., 2016. Estimating emissions of toxic hydrocarbons from natural gas production sites in the Barnett shale region of northern Texas. Environ. Sci. Technol. 50, 10756–10764. https://doi.org/10.1021/acs.est.6b02827.

Meng, Q., 2018. Rethink potential risks of toxic emissions from natural gas and oil mining. Environ. Pollut. 240, 848–857.

Moore, C.W., Zielinska, B., Pétron, G., Jackson, R.B., 2014. Air impacts of increased natural gas acquisition, processing, and use: a critical review. Environ. Sci. Technol. 48, 8349–8359 dx.doi.org/10.1021/es4053472.

Mueller, D., 2012. Environmental issues associated with shale oil and gas exploration and production—Part 1. Environ. Manag. 3, 6–7.

Natural Gas Intelligence. NGI's Shale Daily, https://www.naturalgasintel.com/topics/145-barnett-shale, accessed 12/2018.

Olaguer, E.P., 2012. The potential near-source ozone impacts of upstream oil and gas industry emissions. J. Air Waste Manag. Assoc. 62, 966–977. https://doi.org/10.1080/10962247.2012.688923.

Pacsi, A.P., Alhajeri, N.S., Zavala-Araiza, D., Webster, M.D., Allen, D.T., 2013. Regional air quality impacts of increased natural gas production and use in Texas. Environ. Sci. Technol. 47 (7), 3521–3527.

Paulik, L.B., Hobbie, K.A., Rohlman, D., Smith, B.W., Scott, R.P., Kincl, L., Haynes, E.N., Anderson, K.A., 2018. Environmental and individual PAH exposures near rural natural gas extraction. Environ. Pollut. 241, 397–405.

Pennsylvania Department of Environmental Protection, 2013. Technical Support Document for Long-Term Ambient Air Monitoring Project Near Permanent Marcellus Shale Gas Facilities Protocol. PA DEP, Philadelphia.

Pennsylvania Department of Environmental Protection, 2011a. Northeastern Pennsylvania Marcellus Shale Short-Term Ambient Air Sampling Report. PA DEP, Philadelphia.

Pennsylvania Department of Environmental Protection, 2010. Southwestern Pennsylvania Marcellus Shale Short-Term Ambient Air Sampling Report. PA DEP, Philadelphia.

Pennsylvania Department of Environmental Protection, 2011b. Northcentral Pennsylvania Marcellus Shale Short-Term Ambient Air Sampling Report. PA DEP, Philadelphia.

Pring, M., 2012. Condensate Tank Oil and Gas Activities. Eastern Research Group, Inc., Lexington, MA.

Pring, M., Hudson, D., Renzaglia, J., Smith, B., Treimel, S., 2010. Characterization of Oil and Gas Production Equipment and Develop a Methodology to Estimate Statewide Emissions. Final Report Prepared by Eastern Research Group for Martha Maldonado of the Texas Commission on Environmental Quality, Air Quality Division, November 24, 2010. . http://www.tceq.texas.gov/assets/public/implementation/air/sip/ozone/pAppA_AreaSourceOilGas.pdf.

Rich, A., Grover, J.P., Sattler, M.L., 2014. Air emissions from natural gas exploration and mining in the Barnett Shale Geologic Reservoir. J. Air Waste Manag. Assoc. 14, 61–72. https://doi.org/10.1080/10962247.2013.832713.

Roohani, Y.H., Roy, A.A., Heo, J., 2017. Impact of natural gas development in the Marcellus and Utica shales on regional ozone and fine particulate. Atmos. Environ. 155, 11–20.

Safitri, A., Gao, X., Mannan, M.S., 2011. Dispersion modeling approach for quantification of methane emission rates from natural gas fugitive leaks detected by infrared imaging technique. J. Loss Prev. Process. Ind. 24, 138–145. https://doi.org/10.1016/j.jlp.2010.11.007.

Swarthout, R.F., Russo, R.S., Zhou, Y., Miller, B.M., Mitchell, B., Horsman, E., Lipsky, E., McCabe, D.C., Baum, E., Sive, B.C., 2015. Impact of Marcellus shale natural gas development in southwest Pennsylvania on volatile organic compound emissions and regional air. Quality Environ. Sci. Technol. 49, 3175–3184.

Texas Administrative Code, Chapter 117, Subchapter D, Division 2, Rule §117.2110, http://txrules.elaws.us/rule/title30_chapter117_sec.117.2110 , accessed 10/2018.

Texas Commission on Environmental Quality, 2010. Barnett Shale Area Special Inventory. Phase One. https://www.tceq.texas.gov/assets/public/implementation/air/ie/pseiforms/Barnett%20Shale%20Area%20Special%20Inventory.pdf accessed 10/2018.

Texas Commission on Environmental Quality, 2018. Air Quality Modeling Guidelines APDG 6232. Air Permits Division.

Texas Railroad Commission, 2018. Barnett Shale Information. http://www.rrc.state.tx.us/oil-gas/major-oil-and-gas-formations/barnett-shale-information/ accessed 7/2018.

Vinciguerra, T., Yao, S., Dadzie, J., Chittams, A., Deskins, T., Ehrman, S.D., Russell, R., 2015. Regional air quality impacts of hydraulic fracturing and shale natural gas activity: evidence from ambient VOC observations. Atmos. Environ. 110, 144–150. https://doi.org/10.1016/j.atmosenv.2015.03.056.

XTO Energy, Inc, 2010. Permit by Rule for the Havener Tank Battery Located in Tarrant County, Texas. Attachment #7. XTO Energy, Inc. to the TCEQ Submitted by , Accessed date: 24 May 2010.

Zavala-Araiza, D., Sullivan, D.W., Allen, D.T., 2014. Atmospheric hydrocarbon emissions and concentrations in the Barnett shale natural gas production region. Environ. Sci. Technol. 48, 5314–5321 dx.doi.org/10.1021/es405770h.

Zielinska, B., Campbell, D., Samburova, V., 2014. Impact of emissions from natural gas production facilities on ambient air quality in the Barnett Shale area: a pilot study. J. Air Waste Manag. Assoc. 64 (12), 1369–1383. https://doi.org/10.1080/10962247.2014.954735.