4.b: SMOKE Emissions Modelling

Introduction

For processing anthropogenic emissions for air quality model input, Utah DAQ used SMOKE v3.6. SMOKE is software actively developed by Community Modeling & Analysis System (CMAS)[1]. SMOKE (Sparse Matrix Operator Kernel Emissions) is a state-of-the-art emissions model whose purpose is to temporally and spatially allocate inventoried pollutants. SMOKE also speciates inventoried volatile organic carbon's (VOC) and particulate matter.

Inputs for SMOKE consist of inventory data in the form of county-wide criteria pollutant (CAP) totals (NOx, VOC, direct PM10, direct PM2.5, NH3, SO2, and CO). Inventory data exists for four distinct sectors: area, nonroad, mobile, and point.

For area, nonroad, and mobile sectors, inventory input consists of CAPs totaled by county and EPA Source Classification Code (SCC). The SCC is an eight-to-ten digit number that identifies the technology or process that directly emitted the associated pollutants.

Point sources encompass large emitters such as oil refineries, power plants, and big mining operations. Inventory input is comprised of CAPs totaled for each component of a large emitter (e.g., electric generators, storage tanks, etc.). Unlike other sectors, point source emissions are placed at precise locations using latitude and longitude information.

Other inputs for SMOKE include spatial, temporal and speciation profiles. A profile is assigned to an individual source in the inventory by linking its SCC to a profile code. These references are important for correctly characterizing the time, space, and VOC/PM composition for a given emissions source.

SMOKE output consists of gridded four-dimensional (3-D space and time) emissions. SMOKE gridded emission outputs are then input into the air-quality model (CMAQ v4.7.1).

Modeling Domain

UDAQ used a modeling domain that is a 4 km x 4 km grid with 79 columns, 97 rows, and 14 vertical layers. The horizontal extent of the domain is shown below:

[1] https://www.cmascenter.org/smoke/

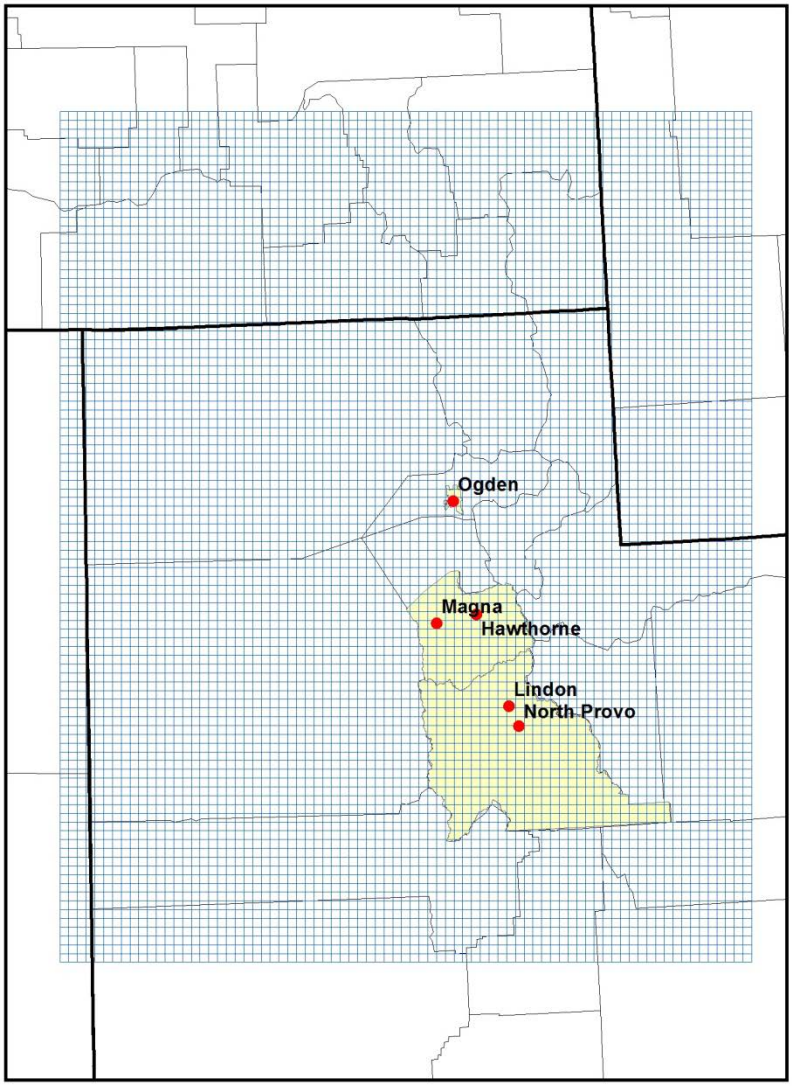

Figure 4.b.1: *PM10 SIP modeling domain shown with county and state boundaries. Red dots denote PM10 monitor locations Shaded green areas depict PM10 maintenance regions.*

The PM10 SIP modeling domain grid was constructed and initialized via the WRF meteorological model. Grid parameters from WRF were passed into SMOKE using the Meteorology-Chemistry Interface Processor (MCIP)[2]. MCIP's purpose is to propagate grid and meteorological information to SMOKE and CMAQ.

Stack plumes were modeled in SMOKE. The vertical extent of the domain is important for placing point source stack (or release point) emissions at the correct height. Other sectors' emissions are modeled at ground level.

Inventoried Emissions

[2] https://www.cmascenter.org/index.cfm?model=mcip

This section provides an overview of the inventory data used for emissions modeling. How the inventory was created for the modeling domain depends on the sector.

Area and Nonroad

For Weber, Davis, Salt Lake, and Utah counties, Utah DAQ created 2011 baseline and projected inventories (for years: 2019, 2024, 2028, and 2030). For counties outside of this four-county region, EPA's 2011 NEI version 2 data (http://www.epa.gov/ttnchie1/net/2011inventory.html) was used. This data-set was used for projected inventories as well. The inventory was held constant outside of the four-county area.

Past regulations on residential wood burning have been established for Salt Lake, Utah, Weber, and Davis counties. For these four counties, residential wood burning was reduced by 80% for 2011 modeling. Since 2014, new stricter regulations have established a mandatory residential wood-burning ban for days where forecasted 24-hour average PM2.5 concentrations exceed 15 $\mu g/m^3$. Given this criteria, projected residential wood burning has been reduced by 95% for future-year modeling.

Mobile

For the aforementioned four-county area, Utah DAQ worked with the metropolitan planning organizations that serve those counties. A four-county mobile inventory was created for the baseline and projection years. Mobile emissions were calculated using the MOVES 2014 model. These emissions were then input into SMOKE as precomputed mobile inventory numbers.

Like the area and nonroad sectors, 2011 NEI data was used for mobile emissions outside the four-county area. Mobile projections were not made outside of the four-county region.

Point

UDAQ made 2011 baseline and projected point source inventories for 23 point sources. These sites are largely in Salt Lake and Utah counties. However, three refineries in Davis County were also inventoried and projected by Utah DAQ. These three refineries are near the Salt Lake County border and are officially a part of the Salt Lake PM10 maintenance area.

Outside of these 23 sites, 2011 NEI data was used to populate all of the other point sources in the modeling domain. These 2011 NEI point sources were held constant for future-year projections.

Spatial Allocation

For spatial processing, SMOKE requires text files that describe relevant geographical information as a function of normalized grid-cell values. With respect to each county in the modeling domain, these normalized grid-cell values sum up to one. Arc GIS software was the primary tool used for translating various geographical data-sets to the required text format.

Population density at a gridded 4 km resolution for 2008 was developed using three separate data sets. For the four Wasatch Front counties (Weber, Davis, Salt Lake, and Utah), population by traffic analysis

zone is provided by the two metropolitan planning organizations: Wasatch Front Regional Council (WFRC) and Mountainland Association of Governments (MAG). The remaining counties in the domain relied on population estimates provided by the Utah Governor's Office of Management and Budget (GOMB).

Population by traffic analysis zone is very high-resolution data, especially in densely populated areas. The data is first converted to densities at 25-meter resolution to capture the fine scale boundaries of the traffic analysis zones. It is then aggregated to a four-kilometer resolution to create the population surrogates.

For outlying counties, population is developed from 1) estimates of population within corporate boundaries and 2) the remaining population in the unincorporated areas of the county. Town populations are placed within corporate boundaries in the GIS. Remaining population is assumed to be spread evenly across the rest of the area of the county. Gridded population in the outlying counties is then created in the same manner as that done for the four Wasatch Front counties. Finally, all three data sets are combined into one gridded population data set for the entire modeling domain.

Mobile source emissions data is distributed to the modeling grid using a combination of link-based data and county totals. The data based on county-wide VMT is distributed using population density as a surrogate. As with the population data, the VMT distribution is based on several different data sources. The MPO's provided link based data for VMT on arterial roads and freeways for the four Wasatch Front counties. UDOT provided link based VMT for state roads and interstates in the outlying counties as well as estimates of VMT driven on local roads.

Because link based VMT does not exist for VMT on local roadways, the distribution of local VMT was created by the use of population surrogates. This was done for all counties in the modeling domain.

Spatial surrogates for urban, forest, and water areas were developed using U.S. Geological Survey (USGS) land use and land cover data[3].

The following table provides a full list of the spatial surrogates used for emissions allocation:

[3] http://www.usgs.gov/science/science.php?term=628&type=theme

20	Interstate Highways
40	Arterial Roads
50	Population
51	Normalized Population
55	Urban Area
60	Area
61	Forest Area
62	Agriculture
63	Water Area
71	Airports
74	Railroads
80	Publically Owned Treatment Works
81	Landfills

Table 4.b.1: List of spatial surrogates used by Utah DAQ.

The *Normalized Population* (51) surrogate was created specifically for spatially allocating banked emissions in Salt Lake and Utah counties. *Normalized Population* was constructed by modifying the *Population* (50) surrogate. This modification results in distributing banked emissions equally amongst grid-cells where population information exists.

For area and nonroad sources where spatial surrogate assignments were not obtainable, *Population* was used as the spatial surrogate. In other words, *Population* was used as the default spatial surrogate for area and nonroad sources. Mobile sources were fully specified in terms of spatial surrogate assignment.

Temporal Allocation

Temporal profiles are meant to characterize large-scale emissions behavior over time. Emissions were distributed in time according to temporal profiles and source assignments gathered from the EPA's 2011v6 modelling platform (http://www.epa.gov/ttn/chief/emch/index.html#2011). For the few instances where temporal profiles didn't exist in the 2011v6 modeling platform for a given SCC, temporal profile assignments were assigned based on SCC description.

We used three components of temporal allocation in SMOKE:

1. Monthly
2. Weekly
3. Hourly ("ALLDAY")

Monthly profiles determine how emissions are distributed month-to-month, January through December. For example, we produce less lawnmower emissions in winter months. However, we elevate snow blower emissions during that same period. Next, weekly profiles determine how emissions are distributed day-to-day, Monday through Sunday. We reduce business-related emissions on weekends for instance. Finally, hourly profiles set the hour-by-hour behavior of emissions sources for a given day.

One example is that we reduced mobile emissions late at night while increasing them during times of rush hour traffic.

Below, is a visual example of the three temporal components we used for residential natural gas usage:

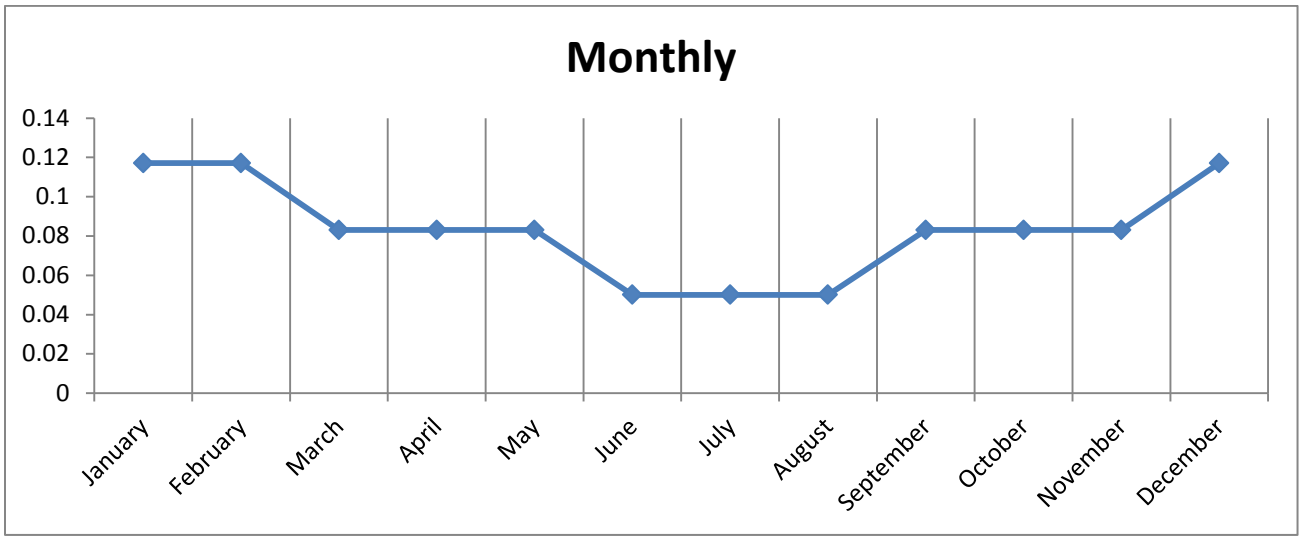

Figure 4.b.2: Monthly allocation of residential natural gas emissions.

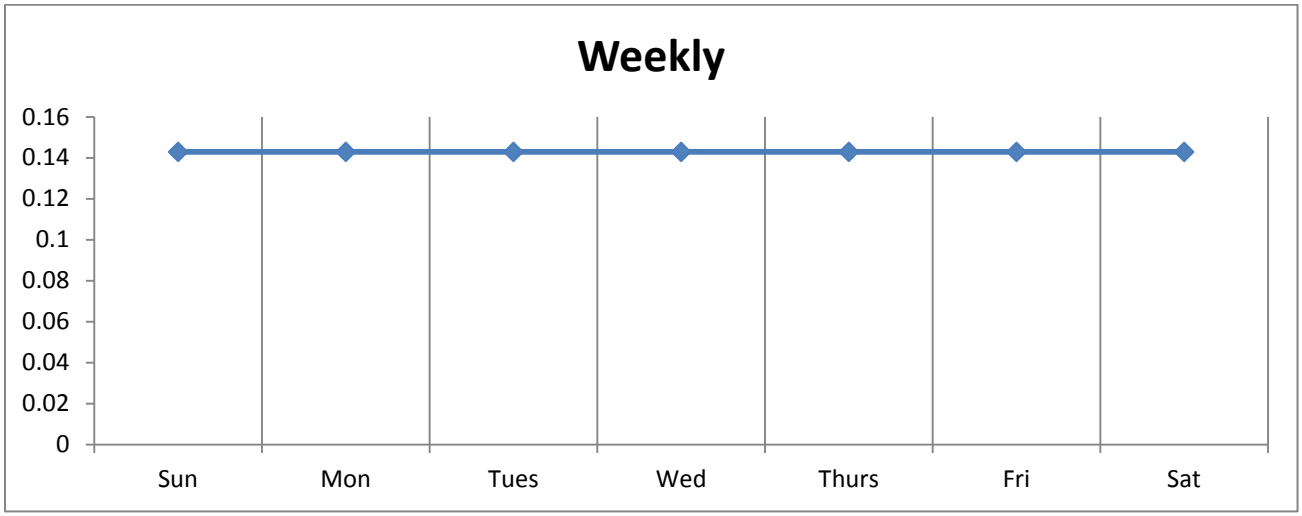

Figure 4.b.3: Weekly allocation of residential natural gas emissions.

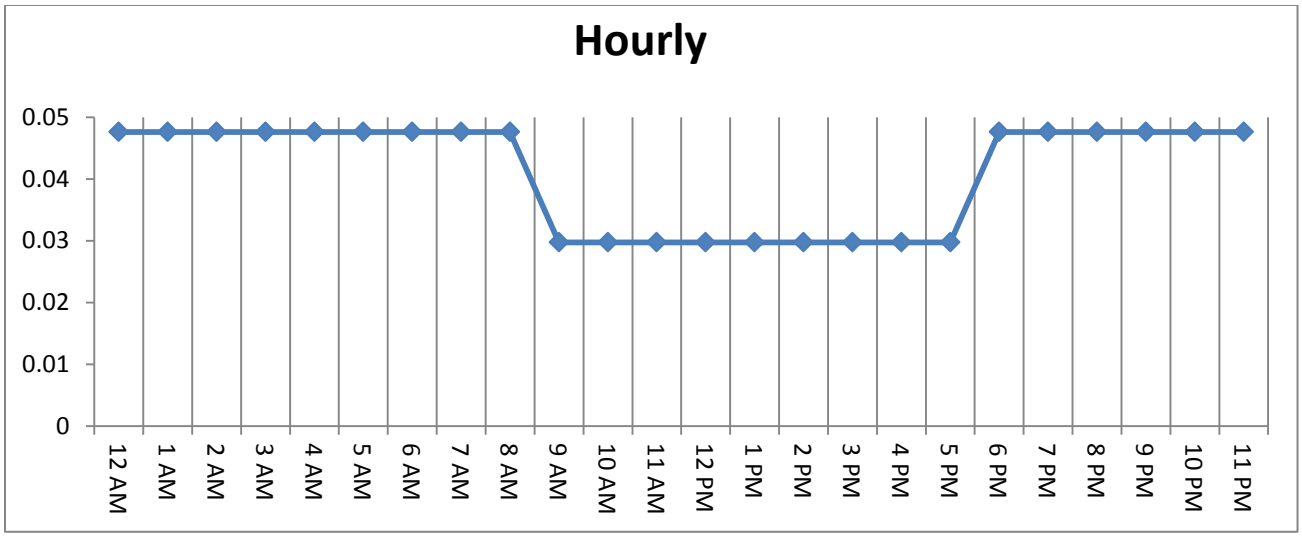

Figure 4.b.4: Hourly allocation of residential natural gas emissions.

Figure 4.b.2 shows residential natural gas emissions are reduced during the summer months, while these emissions are increased during the winter presumably due to home-heating. During the course of the week, Figure 4.b.3 presents the assumption that residential natural gas usage doesn't change day-to-day. Figure 4.b.4 illustrates that we reduce residential natural gas emissions during hours where people are often at work and not using their home appliances.

Since we are modeling a winter-time episode, several emission categories that have no relevance to winter-time emissions have effectively been eliminated. Some of these include:

- Biogenic emissions
- Unpaved road dust
- Agricultural harvesting and burning
- Wildfires

Speciation

Inventoried VOC estimates were converted to total organic gas (TOG) and then speciated according to source-specific TOG profiles. Speciation profiles and their associated SCC assignments generally came from EPA's 2011v6 modeling platform. When a source assignment wasn't found in the 2011v6 modeling platform, assignments were either based on SMOKE defaults or inferred from the source's SCC description.

VOC emissions were speciated for use with CMAQ's CB05 photochemical mechanisms. PM10 was speciated specifically for use with CMAQ's AERO6 aerosol module. An example speciation assignment and profile are shown below for degreasing solvent use:

SCC	VOC-to-TOG factor	Speciation Code
2415000000	1.45	8745

Table 4.b.2: Degreasing solvent use SCC, with VOC-to-TOG scaling factor, and speciation profile lookup code.

The above table suggests that inventoried VOC's associated with degreasing solvent usage are multiplied by 1.45 to account for the unreactive VOC's not explicitly inventoried. Then the TOG associated with degreasing solvent usage is speciated for CMAQ according to speciation code, "8745".

VOC species name (CB05)	% of "8745" TOG (mass)
Ethanol	6%
Ethene	2%
Parrafin Carbon Bond (C-C)	48%
Monoterpenes	9%
Toluene & Other Monoalkyl Aromatics	8%
Unreactives	19%
Xylene & Other Polyalkyl Aromatics	7%
**** smaller < 1% contibutors not shown***	

Table 4.b.3: TOG associated with speciation code, "8745", is split into the CB05 species (left column) by percentages (right column).

Quality Assurance

Reports generated by SMOKE that summarized emissions data by county, prior to temporalization and gridding, demonstrated agreement with MS Excel inventory totals from UDAQ's inventory team.

For spatial and temporal allocation, the largest emission sources were examined individually to determine that the correct profiles were assigned. A weighted sum was constructed by totaling NOx, VOC, SO2, and direct PM10 emissions for each source, across each sector.

Pollutant weights were inversely proportional of that pollutant's contribution to the entire inventory. This means that direct PM10 was weighted the highest since direct PM10 emissions, in total tons/year, are lower than the other three key pollutants.

We then ranked each source, in descending order, by their respective weighted sums. Then, the sources that comprised the top 80% in cumulative sum were checked for correctness in spatial and temporal assignment. The other sources (the bottom 20%) were much more numerous, but provided relatively small contributions to total emissions. Therefore, these small contributors were not individually examined. However, temporal assignments for *all* sources were based on EPA's 2011 v6 modeling platform. Plus, sensible default assignments were used for each sector.

This process was conducted for our 2011 inventory, with respect to Salt Lake County and Cache County, Utah. Cache County was chosen since its inventory is from the 2011 NEI and exhibits a more rural emissions profile than Salt Lake County.

Results

Below, emission summaries for 2011 and all future projection years are displayed for the three PM10 maintenance regions: Salt Lake, Utah, and Ogden City. These emissions are post-processed by SMOKE and have been temporally adjusted to reflect a typical winter-workday.

Salt Lake County		NOX	VOC	NH3	SO2	PM10
2011	**Area**	*9.1*	*30.4*	*3.8*	*0.4*	*5.5*
	Nonroad	*11.7*	*6.4*	*0.0*	*0.3*	*7.1*
	Point	*15.6*	*3.0*	*0.2*	*8.9*	*4.0*
	Mobile	*58.0*	*35.4*	*1.1*	*0.3*	*11.0*
	Year Total	*94.4*	*75.1*	*5.2*	*9.9*	*27.6*
2019	**Area**	*5.8*	*22.1*	*4.2*	*0.4*	*4.9*
	Nonroad	*9.1*	*5.9*	*0.0*	*0.4*	*8.3*
	Point	*22.2*	*3.8*	*0.3*	*7.7*	*11.3*
	Mobile	*25.8*	*21.2*	*0.9*	*0.3*	*10.9*
	Year Total	*62.9*	*52.9*	*5.3*	*39.2*	*35.3*
2024	**Area**	*5.4*	*22.8*	*4.5*	*0.5*	*5.0*
	Nonroad	*8.5*	*6.2*	*0.0*	*0.4*	*8.8*
	Point	*22.4*	*3.9*	*0.3*	*8.2*	*11.5*
	Mobile	*17.2*	*16.6*	*0.9*	*0.3*	*11.3*
	Year Total	*53.4*	*49.5*	*5.7*	*39.8*	*36.7*
2028	**Area**	*5.6*	*23.8*	*4.7*	*0.4*	*5.3*
	Nonroad	*8.4*	*6.5*	*0.0*	*0.4*	*9.3*
	Point	*22.6*	*4.0*	*0.3*	*8.6*	*11.7*
	Mobile	*13.9*	*13.9*	*0.9*	*0.3*	*11.8*
	Year Total	*27.9*	*48.2*	*5.9*	*40.2*	*38.1*
2030	**Area**	*5.6*	*24.3*	*4.8*	*0.3*	*5.4*
	Nonroad	*8.5*	*6.7*	*0.0*	*0.5*	*9.5*
	Point	*22.7*	*4.0*	*0.3*	*8.8*	*11.8*
	Mobile	*12.6*	*13.3*	*0.9*	*0.3*	*12.1*
	Year Total	*49.4*	*48.4*	*6.0*	*40.4*	*38.8*

Table 4.b.4: Emission summaries for Salt Lake County PM10 maintenance region.

Utah County		NOX	VOC	NH3	SO2	PM10
2011	**Area**	*5.6*	*13.0*	*6.6*	*0.3*	*3.9*
	Nonroad	*4.2*	*2.3*	*0.0*	*0.0*	*3.5*
	Point	*1.0*	*0.2*	*0.2*	*0.3*	*0.3*
	Mobile	*24.6*	*11.9*	*0.5*	*0.1*	*4.9*
	Year Total	*35.5*	*27.4*	*7.3*	*0.7*	*12.6*
2019	**Area**	*2.2*	*10.7*	*6.5*	*0.3*	*3.8*
	Nonroad	*3.0*	*2.0*	*0.0*	*0.0*	*4.8*
	Point	*3.2*	*0.9*	*0.4*	*0.4*	*0.9*
	Mobile	*13.8*	*6.4*	*0.5*	*0.2*	*6.0*
	Year Total	*22.2*	*19.9*	*7.4*	*0.9*	*15.5*
2024	**Area**	*1.8*	*11.7*	*6.0*	*0.4*	*2.8*
	Nonroad	*2.5*	*1.9*	*0.0*	*0.0*	*5.2*
	Point	*3.4*	*0.9*	*0.4*	*0.5*	*0.9*
	Mobile	*9.0*	*5.2*	*0.5*	*0.2*	*6.4*
	Year Total	*16.7*	*19.7*	*6.9*	*1.0*	*15.3*
2028	**Area**	*1.8*	*12.5*	*5.9*	*0.3*	*3.1*
	Nonroad	*2.2*	*1.9*	*0.0*	*0.0*	*5.7*
	Point	*3.6*	*1.0*	*0.4*	*0.5*	*1.0*
	Mobile	*7.3*	*4.6*	*0.5*	*0.2*	*7.0*
	Year Total	*11.3*	*20.0*	*6.9*	*0.9*	*16.7*
2030	**Area**	*1.8*	*12.9*	*5.9*	*0.2*	*3.2*
	Nonroad	*2.1*	*1.9*	*0.0*	*0.0*	*6.3*
	Point	*3.7*	*1.0*	*0.4*	*0.5*	*1.0*
	Mobile	*6.8*	*4.5*	*0.5*	*0.2*	*7.7*
	Year Total	*14.3*	*20.4*	*6.9*	*0.9*	*18.1*

Table 4.b.5: Emission summaries for Utah County PM10 maintenance region.

Ogden City		NOX	VOC	NH3	SO2	PM10
2011	**Area**	*2.1*	*5.7*	*0.9*	*0.1*	*0.9*
	Nonroad	*1.3*	*0.9*	*0.0*	*0.0*	*0.9*
	Point	*0.0*	*0.0*	*0.0*	*0.0*	*0.0*
	Mobile	*12.2*	*8.6*	*0.2*	*0.1*	*2.1*
	Year Total	*15.6*	*15.2*	*1.1*	*0.1*	*3.8*
2019	**Area**	*1.2*	*3.9*	*0.9*	*0.1*	*0.6*
	Nonroad	*0.8*	*0.8*	*0.0*	*0.0*	*1.0*
	Point	*0.0*	*0.0*	*0.0*	*0.0*	*0.0*
	Mobile	*6.7*	*5.3*	*0.2*	*0.1*	*2.1*
	Year Total	*8.7*	*9.9*	*1.1*	*0.1*	*3.7*
2024	**Area**	*1.2*	*4.2*	*1.0*	*0.1*	*0.7*
	Nonroad	*0.7*	*0.8*	*0.0*	*0.0*	*1.1*
	Point	*0.0*	*0.0*	*0.0*	*0.0*	*0.0*
	Mobile	*4.5*	*4.2*	*0.2*	*0.1*	*2.1*
	Year Total	*6.4*	*9.1*	*1.1*	*0.2*	*3.8*
2028	**Area**	*1.2*	*4.4*	*1.0*	*0.1*	*0.7*
	Nonroad	*0.7*	*0.8*	*0.0*	*0.0*	*1.1*
	Point	*0.0*	*0.0*	*0.0*	*0.0*	*0.0*
	Mobile	*3.1*	*3.4*	*0.2*	*0.1*	*2.2*
	Year Total	*5.0*	*8.6*	*1.2*	*0.2*	*4.0*
2030	**Area**	*1.2*	*4.5*	*1.0*	*0.1*	*0.7*
	Nonroad	*0.6*	*0.8*	*0.0*	*0.0*	*1.2*
	Point	*0.0*	*0.0*	*0.0*	*0.0*	*0.0*
	Mobile	*2.8*	*3.3*	*0.2*	*0.1*	*2.2*
	Year Total	*4.7*	*8.6*	*1.2*	*0.1*	*4.1*

Table 4.b.6: Emission summaries for Ogden City PM10 maintenance region.