CHAPTER 3

DEVELOPMENT OF THE TOXICS EMISSIONS INVENTORY

Chapter 3. Development of the Toxics Emissions Inventory

3.1 Introduction

An emissions inventory of air pollutants and their sources is essential in order to identify the major contributors of air contaminants and the measures required to reduce air pollution. Information necessary to produce an emissions inventory for the Basin is obtained from the SCAQMD and other government agencies including: California Air Resources Board (ARB); California Department of Transportation (Caltrans); and Southern California Association of Governments (SCAG).

Each of these agencies is responsible for collecting data (e.g., industry growth factors, socio-economic projections, travel activity levels, emission factors, emission speciation profiles, etc.) and developing methodologies (e.g., model and demographic forecast improvements) required to generate a comprehensive emissions inventory. SCAQMD is solely responsible for developing the point source inventory, and the area source inventory is developed jointly by SCAQMD and ARB. ARB is the primary agency responsible for developing the emissions inventory for all mobile sources. SCAG is the primary agency for projecting population and activity growth in the Basin. ARB provides on-road and off-road inventories from their EMFAC and OFF-ROAD Models, respectively. Caltrans provides SCAG with highway network, traffic counts, and road capacity data. SCAG incorporates these data into their Travel Demand Model for estimating/projecting vehicle miles traveled (VMT) and speed. ARB's on-road inventory also relies on SCAG's VMT estimates.

3.2 Overview

The toxic emissions inventory for MATES III consists of four components: (1) point sources; (2) area sources; (3) on-road mobile sources; and (4) off-road (or other) mobile sources. Point source emissions are from facilities having one or more pieces of equipment registered and permitted with the SCAQMD and with emissions above certain threshold levels. Area sources represent numerous small sources of emissions that can collectively have significant emissions (e.g., dry cleaners, retail gasoline stations, auto body shops, residential heating, etc.). On-road mobile sources include cars, trucks, buses, and motorcycles. All mobile sources not included in the on-road mobile source inventory are considered as "off-road" mobile sources, which include aircraft, ships, commercial boats, trains, recreational vehicles, construction equipment, etc.

The 2007 Air Quality Management Plan (AQMP)[1] is the basis for the toxics emissions inventory developed for MATES III. A 2002 baseline emissions inventory is used for projecting the future year inventories in the 2007 AQMP and the 2005 inventory used for MATES III modeling analysis. A "top-down" approach is used to develop the toxics inventory, that is, toxic emissions are calculated by applying the latest ARB speciation profiles[2] to the hydrocarbon and particulate matter emissions. Speciation profiles provide estimates of the emission's chemical composition. The ARB maintains and updates the chemical composition and size fractions of particulate matter (PM) and the chemical composition and reactive fractions of total organic gases (TOG) for a variety of emission source categories. The source type (e.g., equipment and fuel) is used to identify the appropriate speciation profile.

A top-down approach is preferable for a regional modeling risk analysis, such as MATES III, for the following reasons:

- Speciating the VOC and PM inventory affords consistency with the 2007 AQMP.
- The photochemistry algorithms in the MATES III modeling system require the complete speciation of the VOC emissions to insure their correct application. An inventory of just reported toxic species would be insufficient.
- Lastly, the computer programs used to grow and control the VOC and PM emissions into the future for the 2007 AQMP can also be used for projecting the toxic emissions in MATES III. Thus, the future cancer risk reductions resulting from the 2007 AQMP can be estimated.

3.3 Point Sources

The 2002 point source emissions inventory is based on the emissions data reported by the point source facilities in the 2002/2003 Annual Emissions Reporting (AER) Program and is the basis for the 2005 inventory used for MATES III modeling analysis. This program applies to facilities emitting four tons or more of VOC, NOx, SOx, or PM or emitting more than 100 tons of CO per year. Facilities subject to the AER program calculate and report their emissions primarily based on their throughput data (e.g., fuel usage, material usage), appropriate emission factors or source tests, and control efficiency (if applicable). Under the 2002/2003 AER program, approximately 3,200 facilities reported their annual emissions to the SCAQMD. Emissions from smaller industrial facilities not subject to the AER Program, which represent a small fraction of the overall stationary source inventory, are included as part of the area source inventory (see Section 3.3).

In order to prepare the point source inventory, emissions data for each facility are categorized based on U.S. EPA's Source Classification Codes (SCCs) for each emission source category. Since the AER collects emissions data on an aggregate basis (i.e., equipment and processes with the same emissions factor are grouped and reported together), facility's equipment permit data are used in conjunction with the reported data to assign the appropriate SCCs and develop the inventory at the SCC level. For modeling purposes, facility location is specified in Universal Transverse Mercator (UTM) coordinates. The business operation activity profile is also recorded so that the annual emissions can be distributed temporally throughout the day, week, and year.

Toxic emissions are calculated by applying the latest ARB speciation profiles[2] to the hydrocarbon and particulate matter emissions. The SCC is used to identify the appropriate speciation profile for the source.

3.4 Area Sources

The area source emissions developed for the 2007 AQMP and projected to the year of interest (i.e., 2005) are used for MATES III. SCAQMD and ARB shared the responsibility for developing the 2002 area source emissions inventory for approximately 350 area source categories. Specifically, SCAQMD developed the area source inventory for about 93 categories and ARB developed the remaining area source categories (of which 239 categories are associated with consumer products, architectural coatings, and degreasing). For each area source category, a specific methodology is used for estimating emissions. Emissions are spatially allocated to 2 km by 2 km grids using spatial surrogates. Some commonly used spatial surrogates are listed in Table 3-1. As with the point source inventory, toxic emissions are calculated by applying the latest ARB speciation profiles to the hydrocarbon and particulate matter emissions.

3.5 On-Road Mobile Sources

On-road emissions are the product of emission factors and vehicular activity. The emissions developed for the 2007 AQMP and projected to calendar year 2005 are used for MATES III. For the 2007 AQMP, ARB's EMFAC2007 (v2.3) emission factors[3] were used and link-based traffic volumes and speeds were obtained from the SCAG regional transportation modeling. The Direct Travel Impact Model (DTIM) was used to link emission factors and transportation modeling results and generate hourly gridded emissions of criteria pollutants (i.e., TOG, NOx, PM, CO, and SOx). Toxic emissions are calculated by applying the latest ARB speciation profiles for mobile sources to the hydrocarbon and particulate matter emissions. A flow chart illustrating this process is provided in Figure 3-1. Some of the key steps in the process are discussed in more detail below.

EMFAC stands for EMission FACtor. It is a FORTRAN computer model that estimates the on-road emissions of hydrocarbons (HC), CO, NOx, PM, lead (Pb), SO_2, and CO_2 for calendar years 1970 to 2040. EMFAC considers 1965 and newer vehicles powered by gasoline, diesel, or electricity and reports for 13 broad vehicle classes as shown in Table 3-2. Over 100 different technology groups are accounted for within each class (e.g., catalyst, non-catalyst, three-way catalyst, carbureted, multi-port fuel injection, LEV, TLEV, SULEV, etc.).

EMFAC currently considers the following county-specific information when calculating emissions:

- Ambient air temperature (denoted by T in Figure 3-1);
- Relative humidity (denoted by RH in Figure 3-1);
- Vehicle population;
- Fleet composition;
- Fleet growth rates;
- Mileage accrual rates;
- Vehicle age distribution;
- Distribution of VMT by speed;
- Smog check regulations;
- Fuel properties; and
- Altitude.

Some on-road activity information for the four counties in the Basin is summarized in Table 3-3. Four of the top seven counties in California in terms of vehicle population, VMT, and trips are in the Basin.

The output from EMFAC is a text file containing HC, CO, NOx, PM, lead, SO_2, and CO_2 emission rates for 45 model years for each vehicle class within each calendar year, for 24 hourly periods, and for each month of the year for each county/air basin specified. Processing continues with the DTIM modeling system, which prepares gridded hourly on-road emissions for photochemical grid modeling.

The DTIM processing system consists of three FORTRAN program modules: CONVIRS4, IRS4, and DTIM4. The main function of CONVIRS4 is to re-format the emission rate file output from EMFAC into a form compatible with IRS4. IRS4 creates fleet average emission rates by ambient air temperature, relative humidity, and vehicle speed.

The DTIM4 module prepares gridded, hourly on-road emissions of HC, CO, NO_X, PM, lead, SO_2, and CO_2 link by link in the transportation network. SCAG's Travel Demand Model provides the following for each link in the transportation network: the number of vehicles, their average speed, and time on the link. Separate files containing hourly gridded temperature (T in Figure 3-1) and relative humidity (RH in Figure 3-1) are provided as input to DTIM4. Knowing the air temperature and relative humidity representative of the link and the average vehicle speed on the link, DTIM4 looks up the fleet average emission rate in the file prepared by IRS4, and multiplies these by the number of vehicles and the average time on the link.

ARB speciation profiles are used to speciate the on-road HC and PM emissions into its toxic components. Several important HC and PM speciation profiles are contained in Appendix VIII.

3.6 Off-Road Mobile Sources

The off-road emissions developed for the 2007 AQMP are used for MATES III. For the 2007 AQMP, ARB's OFF-ROAD model[4] was used to estimate emissions for all off-road categories (100+ source categories) except commercial ships, aircraft, locomotive, and recreational vehicles. This model incorporates various aspects of off-road elements, such as the effects of various adopted regulations, technology types, and seasonal conditions on emissions. The model combines population, activity, horsepower, load factors, and emission factors to yield the annual equipment emissions by county, air basin, or state. Spatial and temporal features are incorporated to estimate seasonal emissions. Aircraft and ship emissions for the 2007 AQMP were developed by SCAQMD and SCAG sponsored studies. Emissions are spatially allocated to 2 km by 2 km grids using spatial surrogates. Toxic emissions are calculated by applying the latest ARB speciation profiles for off-road mobile sources to the hydrocarbon and particulate matter emissions.

3.7 Summary of Toxic Emissions

Table 3-4 presents the emissions from selected compounds apportioned by the on-road, off-road, point, and area source categories. Chemicals that are considered potential or known human carcinogens are denoted with a check mark. Toxic emissions by major source categories are provided in Appendix VIII.

Species and source apportionment are shown in Table 3-5 and Figure 3-2, respectively. In those illustrations, the emissions of the carcinogenic pollutants in Table 3-4 are weighted by the ratio of their cancer potency to the cancer potency of diesel particulate matter (DPM). Thus, emissions from species less potent than DPM (e.g, benzene, perchloroethylene, etc.) are weighted less, while emissions from species more potent than DPM (e.g., hexavalent chromium, arsenic, etc.) are weighed more. DPM has a weighting factor of one.

As shown in Table 3-5, DPM emissions account for over 85% of the overall cancer risk. The other significant compounds (i.e., contributions >1%) are 1,3-butadiene, benzene, and perchloroethylene. On-road and off-road mobile sources contribute about 92% of the weighted carcinogenic risks and stationary sources contribute about 8% of the risk (Figure 3-2).

Carcinogenic emissions have decreased by 15% since MATES II (1998 inventory year) as shown in Figure 3-3. Carcinogenic emissions from on-road, point, and area source categories decreased by 13%, 65%, and 43%, respectively and off-road carcinogenic emissions are essentially unchanged (an increase of 1%). To perform the comparison, the 2002 on-road and off-road inventories were back-cast to 1998 in order to account for changes to the EMFAC and OFF-ROAD models that have occurred since MATES II.

3.8 Selected Emissions and Air Quality Changes Since MATES II

Table 3-6 compares emission and air quality changes since MATES II for selected toxics. The air quality change is compared to the MATES year one average from the 10 fixed monitoring sites. Emissions have decreased and air quality has improved since the MATES II (i.e., 1998 timeframe). It should be noted that the difference for some pollutants, such as cadmium and arsenic, are also due to lower method reporting limits in MATES III, as discussed in Chapter 2.

Several caveats are appropriate when comparing the changes in inventory emissions and ambient measurements. For example, weather and dispersion of emissions are not considered, which can influence the relationship between emissions and ambient concentrations. Also, the inventory is a regional estimate of total emissions throughout the Basin, whereas ambient measurements are from the ten fixed monitoring locations where there may be influences from local sources. Another difference is that secondary formation or degradation of substances are not accounted for. Nonetheless, comparing emissions estimates with air quality measurements can provide information on whether expected emissions changes are reflected in ambient measurements, can be used to help calibrate emissions, and may suggest where emissions inventory methods can be improved.

3.9 References

1. A copy of the 2007 AQMP can be viewed or downloaded at the following SCSCAQMD link: http://www.SCAQMD.gov/aqmp/07aqmp/index.html.
2. ARB speciation profiles can be viewed or downloaded from the following ARB link: http://www.arb.ca.gov/ei/speciate/speciate.htm.
3. EMFAC2007 model and its documentation can be obtained at the following ARB link: http://www.arb.ca.gov/msei/onroad/latest_version.htm.
4. The OFF-ROAD Model and its documentation can be obtained at the following ARB link: http://www.arb.ca.gov/msei/offroad/offroad.htm.

Table 3-1. Commonly Used Spatial Surrogates.

Population	Total employment
VMT	Industrial employment
Length of rail per grid cell	Retail employment
Locations of unpaved rural roads	Single dwelling units
Total housing	Total housing
Agricultural land cover	Rural land cover – forest
National forest > 5000 ft	Rural land cover – range land

Source: http://eos.arb.ca.gov/eos/projects/surrogates/

Table 3-2. Broad Vehicle Classes Considered by EMFAC.

Vehicle Class	Weight (lbs)	Vehicle Class	Weight (lbs)
Passenger cars	All	Heavy-Heavy-Duty Truck	33,001 – 60,000
Light Truck I	0 – 3,750	Motorcycle	All
Light Truck II	3,751 – 5,750	Urban Diesel Bus	All
Medium-Duty Truck	5,751 – 8,500	School Bus	All
Light-Heavy-Duty Truck I	8,501 – 10,000	Other bus	All
Light-Heavy-Duty Truck II	10,001 – 14,000	Motor Homes	All
Medium-Heavy-Duty Truck	14,001 – 33,000		

Source: Adopted from the User's Guide for EMFAC2007.

Table 3-3. Vehicle Activity Information for the Counties in the Basin.

County	Vehicle Population	VMT/day	Trips/day	Miles per Vehicle-Day	Mean Age of Passenger Car Fleet (years)
Los Angeles	5,811,255	197,059,000	39,896,020	33.91	9.36
Orange	2,071,490	65,359,000	14,058,600	31.55	10.46
Riverside	1,014,703	42,170,000	6,890,676	41.56	11.91
San Bernardino	1,064,007	39,152,000	7,298,540	36.80	9.99

Source: http://www.arb.ca.gov/msei/onroad/briefs/activity.pdf

Table 3-4. 2005 Annual Average Day Toxic Emissions for the South Coast Air Basin.

	Pollutant	Emissions (lbs/day)				
		On-Road	**Off-road**	**Point**	**Area**	**Total**
√	Acetaldehyde*	4857.0	8622.4	125.8	505.1	14110.3
	Acetone**	4020.5	7189.1	552.4	28904.9	40666.8
√	Benzene	13244.8	7808.3	906.5	609.3	22568.9
√	1,3 Butadiene	2723.1	1755.6	537.1	108.7	5124.5
√	Carbon tetrachloride	0.0	0.0	11.2	0.0	11.2
√	Chloroform	0.0	0.0	206.9	0.0	206.9
√	1,1 Dichloroethane	0.0	0.0	0.5	0.0	0.5
√	1,4 Dioxane	0.0	0.0	0.8	0.7	1.5
√	Ethylene dibromide	0.0	0.0	2.2	0.0	2.2
√	Ethylene dichloride	0.0	0.0	67.2	0.0	67.2
√	Ethylene oxide	0.0	0.0	16.1	52.6	68.7
√	Formaldehyde*	12596.6	19889.0	1488.8	1302.0	35276.4
	Methyl ethyl ketone*	745.6	1366.0	1244.3	6466.7	9822.6
√	Methylene chloride	0.0	0.0	325.1	13548.3	13873.3
√	MTBE	0.0	4.4	89.6	0.0	93.9
√	Naphthalene	573.4	376.8	16.6	568.1	1534.9
√	p-Dichlorobenzene	0.0	0.0	115.4	5553.9	5669.3
√	Perchloroethylene	0.0	0.0	940.4	9685.4	10625.7
√	Propylene oxide	0.0	0.0	2.2	0.2	2.3
	Styrene	681.7	326.3	1332.5	76.5	2417.0
	Toluene	37707.9	15369.2	8724.3	21029.4	82830.8
√	Trichloroethylene	0.0	0.0	587.1	633.1	1220.1
√	Vinyl chloride	0.0	0.0	51.1	0.0	51.1
√	Arsenic	0.2	4.0	13.4	24.8	42.3
√	Cadmium	1.5	2.9	3.2	7.2	14.8
	Chromium	21.1	9.3	49.2	77.3	156.9
√	Diesel particulate	22164.6	37117.8	489.5	618.4	60390.1
	Elemental carbon***	10498.2	11685.6	4956.7	14331.6	41472.0
√	Hexavalent chromium	0.1	0.1	0.2	0.0	0.4
√	Lead	2.4	5.1	13.7	181.0	202.2
√	Nickel	15.3	6.0	44.2	23.4	88.9
	Organic carbon	19972.7	25503.9	707.4	69654.9	115838.9
	Selenium	0.5	0.6	41.4	2.2	44.6
	Silicon*	838.7	108.1	1210.6	218525.6	220683.0

√ Denotes potential or known human carcinogen.

* Primarily emitted emissions. These materials are also formed in the atmosphere as a result of photochemical reactions.

** Acetone and silicon are not toxic compounds. Their emissions are included here because they were measured in the sampling program and were subsequently modeled for the purpose of model evaluation.

*** Includes elemental carbon from all sources (including diesel particulate).

Table 3-5. Cancer Potency Weighted Species Apportionment for 2005 Emissions.

Toxic	Contribution (%)	Toxic	Contribution (%)
Diesel particulate	86.94	Ethylene oxide	0.03
1,3-butadiene	4.02	Vinyl chloride	0.02
Benzene	2.95	Trichloroethylene	0.01
Perchloroethylene	2.92	Lead	0.01
Formaldehyde	0.97	Ethylene dichloride	< 0.01
Arsenic	0.66	Chloroform	< 0.01
p-dichlorobenzene	0.30	Carbon tetrachloride	< 0.01
Cadmium	0.29	Ethylene dibromide	< 0.001
Hexavalent chromium	0.26	MTBE	< 0.001
Naphthalene	0.24	1,4-dioxane	< 0.0001
Acetaldehyde	0.18	Propylene oxide	< 0.0001
Nickel	0.11	1,1-dichloroethane	< 0.0001
Methylene chloride	0.06		

Table 3-6. Selected Emissions and Air Quality Changes Since MATES II.

Toxic Gases	Change in Emissions	Change in Air Quality	Toxic Particulates	Change in Emissions	Change in Air Quality
Acetaldehyde	-9%	-9%	Arsenic**	-20%	-48%
Benzene	-38%	-46%	Cadmium**	-19%	-74%
1,3-butadiene	-31%	-66%	Elemental carbon*	-2%	-28%*
Formaldehyde	-21%	-9%	Hex. chromium	-85%	-5%
Methylene chloride	-38%	-43%	Lead	-14%	-31%
Perchloroethylene	-58%	-77%	Nickel	-22%	-30%
Trichloroethylene	-65%	-79%			

*Adjusted for instrumentation changes in MATES III; see Section 2.6.3.

**Difference in air quality likely in part due to lower laboratory reporting limits in MATES III.

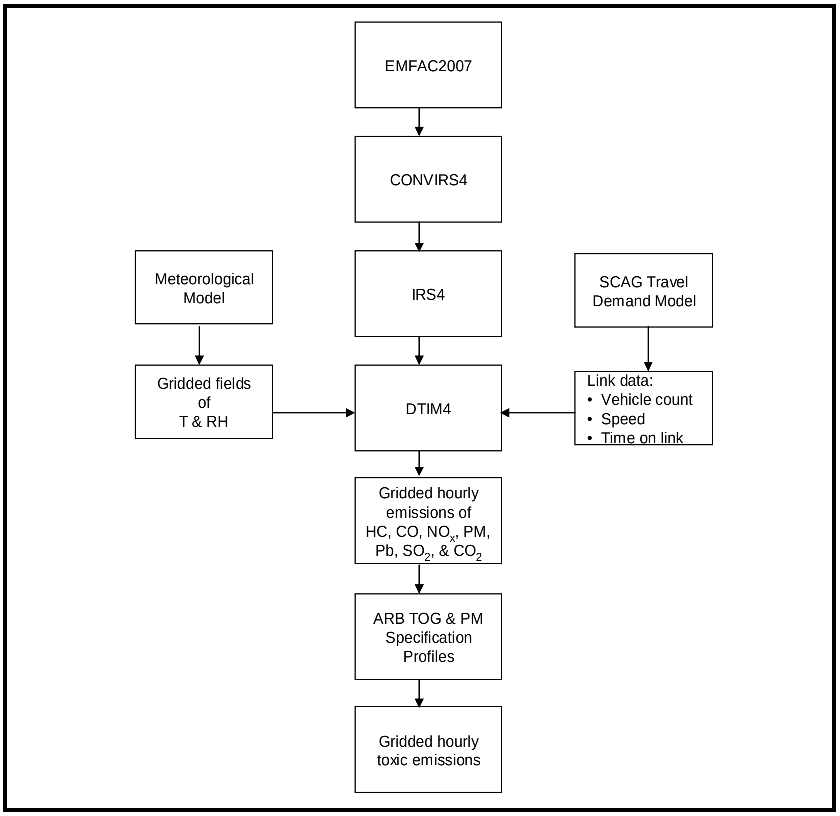


Figure 3-1. Flow Diagram for On-road Emissions Processing.

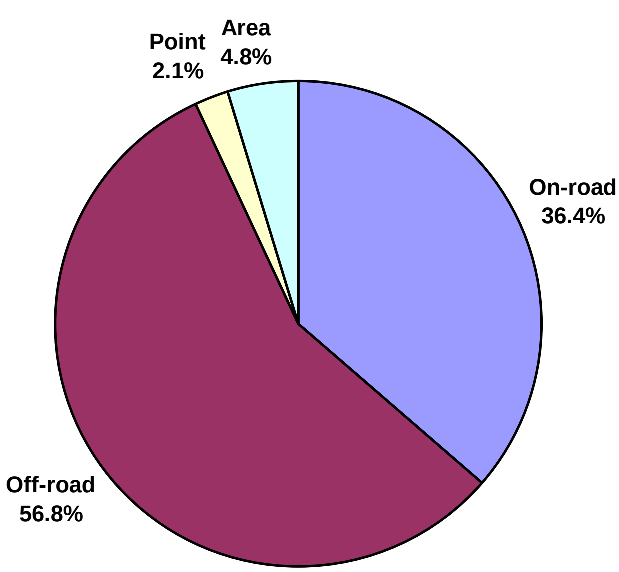
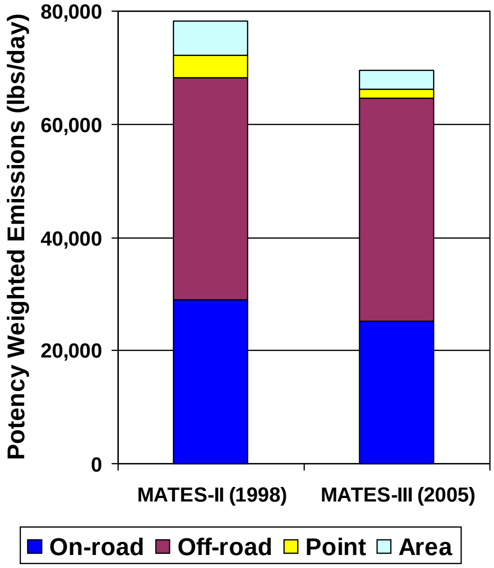


Figure 3-2. Cancer Potency Weighted Source Apportionment for 2005 Emissions.



Source Category	Percent Change
On-road	13% decrease
Off-road	1% increase
Point	65% decrease
Area	43% decrease

Figure 3-3. Cancer Potency Weighted Emission Comparison of MATES II and MATES III.