

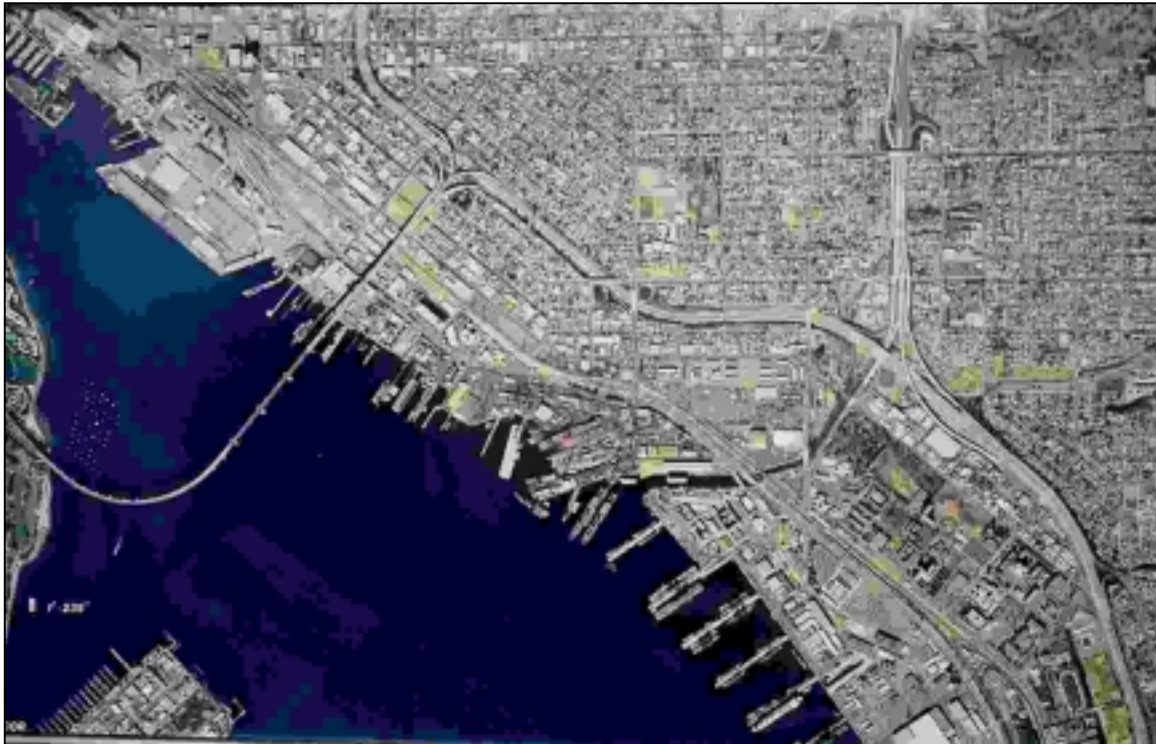
California Environmental Protection Agency



Air Resources Board

Barrio Logan Report

A Compilation of Air Quality Studies in Barrio Logan



November 2004

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INTRODUCTION

CHAPTER 1 - INTRODUCTION

In 1999, the Air Resources Board (ARB) established the Neighborhood Assessment Program (NAP). This program was designed to develop assessment tools for evaluating and understanding air quality in California communities. To support the NAP, ARB began to develop monitoring and modeling methodologies that would enable us to evaluate the cumulative impacts of air pollution at the community level. This included evaluating new ways of monitoring neighborhood facilities and developing enhanced local emission inventories, evaluating micro-scale and regional models for toxic air pollutants, and developing a method of combining regional and micro-scale air dispersion models.

In the same timeframe, several other events occurred that influenced the NAP. First, the Environmental Health Coalition (EHC), an organization representing the residents of the Barrio Logan community in San Diego, requested that the ARB conduct an air monitoring study at Memorial Academy Charter School (Memorial Academy). This location was selected because of concern the community had about localized impacts from air pollution. Also, the Legislature passed the Children's Environmental Health Protection Act (Senate Bill 25, Escutia 1999 (SB25)) requiring the ARB to look at the air that children are exposed to in places where they live and play.

As a result, the ARB selected Barrio Logan to begin its Neighborhood Assessment Program and SB25 efforts. Barrio Logan is a small community located in San Diego bordered on the north and east by State Routes 94 and 15, respectively, on the west by Highway 5, and on the south by the San Diego Bay. It is a community zoned for mixed use with small neighborhood businesses such as chrome platers and autobody shops interspersed among the homes. It is also close to the ship repair facilities and naval shipyards.

As part of the Barrio Logan effort, we worked with community representatives to identify and address residents' concerns about poor air quality in the area. The residents' concerns included cumulative impacts from ship repair yards, naval activities, and from smaller facilities such as chrome platers, welding, furniture strippers, and auto body shops.

The monitoring at Memorial Academy Charter School ran from October 1999 through February 2001. This was followed by a short, but intensive, air monitoring effort in and around two chrome plating facilities in Barrio Logan, which was prompted by community concerns about the impact of these chrome platers on the neighboring residences. In addition to the monitoring studies discussed above, limited short term toxic monitoring was also done during some of the model validation work. The results of the ambient air monitoring are only summarized in this report because they have been described in detail in earlier reports.

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In addition to the air monitoring studies, the ARB staff developed, for the first time, micro-scale emission inventories and tested them using several models to determine if localized hot spots could be predicted through air quality modeling. Validation of these local scale models was done with tracer gas studies conducted by the University of California, Riverside (CE-CERT). The ARB staff also performed regional air quality modeling using photochemical grid models to predict toxic air pollutant concentrations on an annualized basis. The model development was shared periodically with a Community Modeling Working Group that consisted of academicians, community groups, industry, state and local agency representatives, and consultants. The protocol for the modeling in Barrio Logan, including the emission inventory and selection of the meteorological models used, was peer reviewed by a group of four experts in the field.

This report summarizes and discusses the work done in Barrio Logan and the lessons learned. Many aspects of this study have been completed and reported in other documents. The results of these studies are summarized in this report, but the reader is encouraged to consult the original reports for more detail. The lessons learned from the Barrio Logan experience will be used and refined in the neighborhood assessment of Wilmington, a community in Los Angeles, as we continue our work to develop methodologies and tools for the Neighborhood Assessment Program.

The information in this report is organized into six additional chapters and presents the findings from the ambient air quality studies, the model development for cumulative impacts, the lessons learned in Barrio Logan, and the challenges that remain in our efforts to develop neighborhood assessment tools. A summary of each chapter is presented below.

Chapter 2 – Air Monitoring Studies in Barrio Logan. Chapter 2 describes the ambient air monitoring that was conducted in Barrio Logan. There were three air monitoring efforts conducted in Barrio Logan. Most of the ambient air quality monitoring has been discussed in the detailed reports for these studies. Therefore, these results are only summarized in this report. The three studies and references to the reports are listed below.

- Ambient Air Quality Measurements at Memorial Academy Charter School. This study was conducted from October 1999 through February 2001. A summary of the findings are contained in Chapter 2, but more information can be found in the data analysis report entitled “Air Quality at Memorial Academy Charter School in Barrio Logan, a Neighborhood Community in San Diego” (June 2002), and in the Technical Support Document to that study (June 2002). These documents can be found on the ARB website at:
<http://www.arb.ca.gov/ch/communities/studies/barriologan/barriologan.htm>
- Special Hexavalent Chromium Study. The special hexavalent chromium study was conducted December 2001 through May 2002, and was done in response to

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community concerns about two chromium plating facilities on Newton Avenue. For detailed information regarding this study, the reader is directed to the final report developed by ARB's Monitoring and Laboratory Division entitled "Ambient Monitoring for Hexavalent Chromium and Metals in Barrio Logan" (October 2003). Also, the ARB staff published a paper on the findings of this study in the AWMA proceedings entitled, "Neighborhood Scale Monitoring in Barrio Logan" (June 2003). This paper along with numbers, fact sheets and data summaries from all of our hexavalent chromium work are posted at <http://www.arb.ca.gov/ch/communities/studies/barriologan/barriologan.htm>.

- University of California, Riverside Short-Term Toxic Air Monitoring. Additional short term toxic monitoring was conducted by UC Riverside's College of Engineering-Center for Environmental Research and Technology (CE-CERT) to support validation of the emissions inventory and dispersion modeling effort. Although conducted for modeling purposes, this information also contributed to our overall understanding of the air quality in the community. The final report, "Measurement of Toxic Air Pollutants for the Neighborhood Assessment" (August 2003), can be found at <http://www.arb.ca.gov/ch/communities/studies/barriologan/barriologan.htm>

Chapter 3 – Conceptual Modeling Approaches for Assessing Cumulative Impacts.

Chapter 3 describes the development of both regional and micro-scale emission inventories. Emission inventories help researchers understand what are the sources of emissions, the mass of emissions emitted into an area, and the kinds of pollutants. The emission inventories are also an essential input to the air quality modeling.

Chapter 4 – Modeling Emission Inventory Development. Chapter 4 contains an overview of air quality modeling – both regional and micro-scale – and of the meteorological models available for this study. Part of the Barrio Logan effort was to consider and test different models. The models, their uses, and limitations are discussed in the overview. The rest of the chapter discusses the regional model used for this study, the micro-scale modeling efforts, and suggestions on integration of the two. Integration of two different scale models is technically challenging and there are issues of duplication of the inventory numbers. Much of our effort here was to explore how that might be done and provide recommendations as we assess other communities. This effort has continued in Wilmington, our second community assessment.

Chapter 5 – Modeling Results for Barrio Logan. This chapter describes the application of specific micro-scale and regional models in Barrio Logan and how they perform using the Neighborhood Assessment Protocol approach.

Chapter 6 – Findings and Conclusions. This chapter summarizes the findings from each of the technical chapters and discusses the conclusions from our work in Barrio Logan.

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Chapter 7 – References. This chapter presents a comprehensive list of references used throughout the report.

Appendix A - The appendix contains the conceptual modeling protocol for the NAP.

CHAPTER 2 - AIR MONITORING STUDIES IN BARRIO LOGAN

ARB's Monitoring and Laboratory Division established a monitoring station at Memorial Academy Charter School in October 1999 and monitored multiple criteria and toxic pollutants. The monitoring was the first step in our assessment of this community. The monitoring at Memorial Academy Charter School was extended and incorporated into the SB25 efforts.

In addition to the monitoring at Memorial Academy Charter School, community representatives also asked ARB to monitor hexavalent chromium levels on a street that had residences mixed with commercial and small industrial facilities. In particular, the community was concerned about the impact of two chrome platers. Monitoring for hexavalent chromium was conducted from December 2001 to May 2002. Additional short term toxic monitoring was primarily done to support the emission inventory and dispersion modeling validation. These studies are summarized below.

A) Ambient Air Quality Measurements at Memorial Academy Charter School

In order to evaluate the air pollution levels in Barrio Logan, an ambient air monitoring study was conducted at Memorial Academy Charter School in Barrio Logan (Figure 2.1). The monitoring site was selected by a local advisory group, which consisted of community representatives, and local businesses. The protocol for the monitoring can be found in The Barrio Logan Toxics Monitoring Sampling Protocol (November 1999) at www.arb.ca.gov/ch/reports/bl.pdf.

The objectives of the study were:

- To determine the ambient levels of toxic air contaminants and other pollutants at Memorial Academy Charter School;
- To assess the differences in air pollutants between Memorial Academy Charter School and other long-term air pollutant monitoring sites in the San Diego area; and
- To evaluate the potential cancer and non-cancer health risk of toxic air contaminants at Memorial Academy Charter School and compare it to routine monitoring sites in the San Diego area.

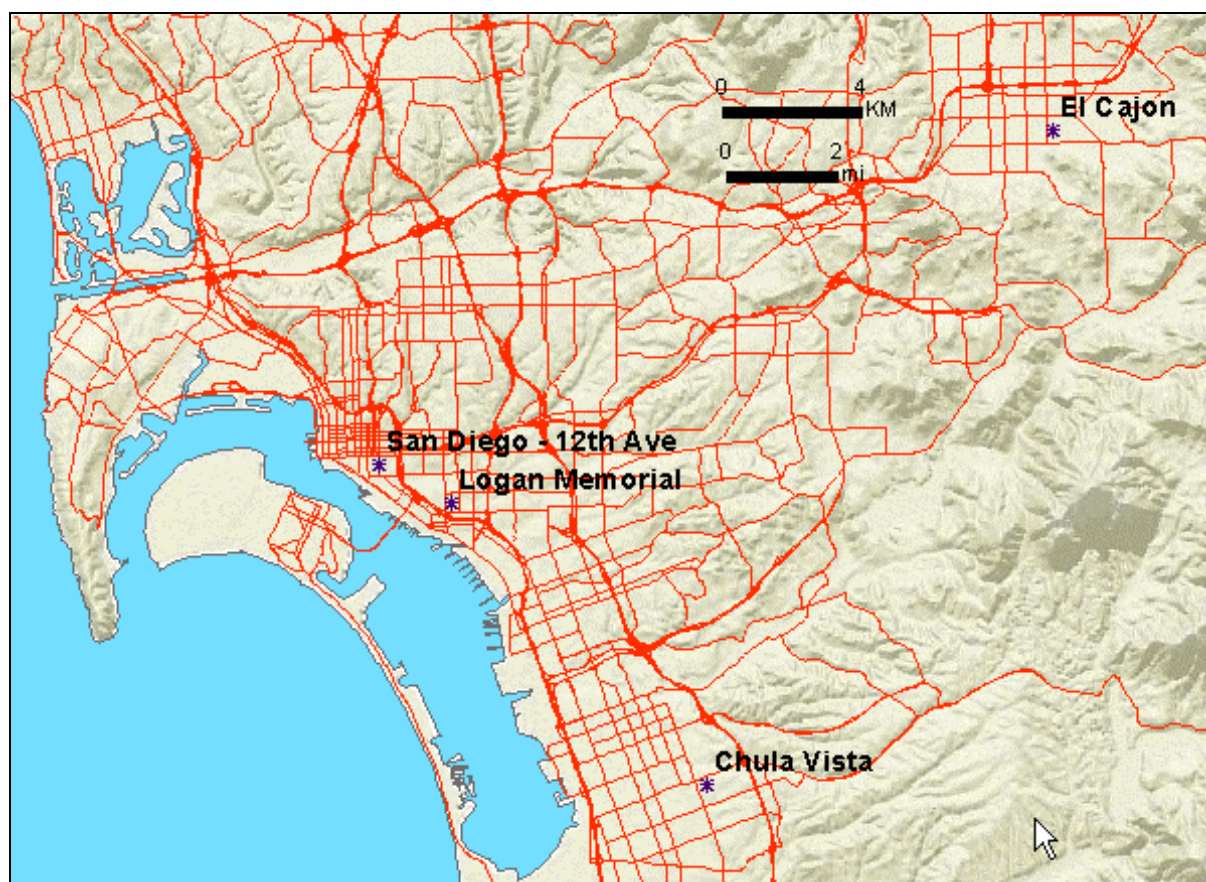
The monitoring study was conducted for 17 months from October 1999 through February 2001. Measured pollutants included ozone, carbon monoxide (CO), oxides of nitrogen (NO_x), PM₁₀, and a number of toxic air pollutants, including 1,3-butadiene, benzene, formaldehyde, and hexavalent chromium. Meteorological parameters included wind speed, wind direction, and ambient temperature.

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The gaseous criteria pollutants (ozone, CO, and NO_x) and PM_{2.5} were monitored continuously for the full duration of the project. Toxic air pollutants were collected every fourth day from October 1999 through March 2000. From April 2000 through September 2000, aldehydes and hexavalent chromium were collected once every twelve days.

The data collected at Memorial Academy Charter School were compared to the three long-term routine monitoring sites in the San Diego area. These long term air monitoring sites were Chula Vista (six miles southeast of Memorial Academy), El Cajon (thirteen miles northeast of Memorial Academy), and San Diego - 12th Avenue (two miles northwest of Memorial Academy). Toxic air pollutants are measured routinely at Chula Vista and El Cajon, and criteria pollutants are measured at all three sites.

Figure 2.1 - Toxic & Criteria Monitoring Sites 2000



Tables 2.1, 2.2, 2.3, and 2.4 summarize results from October 1999 to September 2000, for particulate matter, ozone, NO_x, and CO at Memorial Academy, Chula Vista, El Cajon, and San Diego 12th Avenue. The particulate matter results shown in Table 2.1 indicate that about one out of eight days measured at Memorial Academy were higher than the State standard of 50 ug/m³. Levels were higher than the State standard in about one out of 30 days measured at Chula Vista, and in about one out of 20 days

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measured at El Cajon. Although the number of days with levels above the standard may differ between Memorial Academy and the other three sites, the average and maximum levels are comparable.

The ozone data presented in Table 2.2 show that over a 12-month period Memorial Academy measured ozone levels comparable to the San Diego region, with only one day above the State standard of 90 ppb.

Table 2.3 shows that Memorial Academy annual levels of NO_x are slightly higher than those at Chula Vista and El Cajon, but they are similar to San Diego 12th Avenue. Currently, carbon monoxide levels in most areas of California are below the State standard of 9 ppm. Table 2.4 shows Memorial Academy, like other sites in San Diego, is no exception.

Table 2.1 - Particulate Matter (PM₁₀) in a 12-Month Period

Location	Average*	Maximum*	Number of Days Above State Standard**
Memorial Academy	35	61	6 of 46 days
Chula Vista	31	59	2 of 55 days
El Cajon	32	60	3 of 58 days
San Diego - 12th Ave.	35	64	7 of 57 days

* Units of measure are micro-grams per cubic meter (ug/m³) for 24 hours.

** State PM₁₀ standard is 50 ug/m³

Table 2.2 - Ozone in a 12-Month Period

Location	Average*	Maximum*	Number of Days Above State Standard**
Memorial Academy	42	96	1
Chula Vista	50	91	0
El Cajon	49	106	5
San Diego - 12th Ave.	43	118	1

* Units of measure are parts-per-billion (ppb) for one-hour averages. Average and maximum are based on daily one-hour maximum values.

** State ozone standard is 90 ppb for one-hour average.

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Table 2.3 - Nitrogen Oxides in a 12-Month Period

Location	Average*	Maximum*
Memorial Academy	61	234
Chula Vista	31	137
El Cajon	43	184
San Diego - 12th Ave.	54	276

* Units of measure are parts-per-billion (ppb) for one-hour averages. Average and maximum are based on daily one-hour maximum values.

No State or Federal Standards have been established for oxides of Nitrogen; the State Standard for NO₂ is 250 ppb for a one-hour average; the federal annual average standard for NO₂ is 53 ppb.

Table 2.4 - Carbon Monoxide in a 12-Month Period

Location	Average*	Maximum*	Number of Days Above State Standard**
Memorial Academy	1.0	2.7	0
Chula Vista	0.9	2.1	0
El Cajon	Not Monitored	Not Monitored	Not Monitored
San Diego - 12th Ave.	1.2	4.1	0

* Units of measure are parts-per-million (ppm). The State standard and the daily maximum values are determined for an 8-hour average.

** State CO standard is 9 ppm for an 8-hour average.

Concentrations of toxic air pollutants were also measured at Memorial Academy and compared to the two toxic routine monitoring sites in San Diego – Chula Vista and El Cajon. The values were also compared to other toxic monitoring sites in California.

Toxic air pollutants are pollutants for which there are no standards or safe thresholds, and can cause long-term health problems such as cancer. In order to compare multiple toxic air pollutant concentrations at Memorial Academy to the concentrations at the two routine toxic monitoring stations in San Diego, we estimated the total potential cancer risk for nine toxic air pollutants. These nine toxic air pollutants are chosen for risk calculations because they account for the highest potential cancer health risk. Cancer risk estimates represent the chances of developing cancer assuming a person is continuously exposed to the average concentration for a 70-year lifetime.

As shown in Figure 2.2, the potential risk levels at Memorial Academy were slightly higher than those at Chula Vista, similar to El Cajon and the statewide average, and much lower than urban Los Angeles.

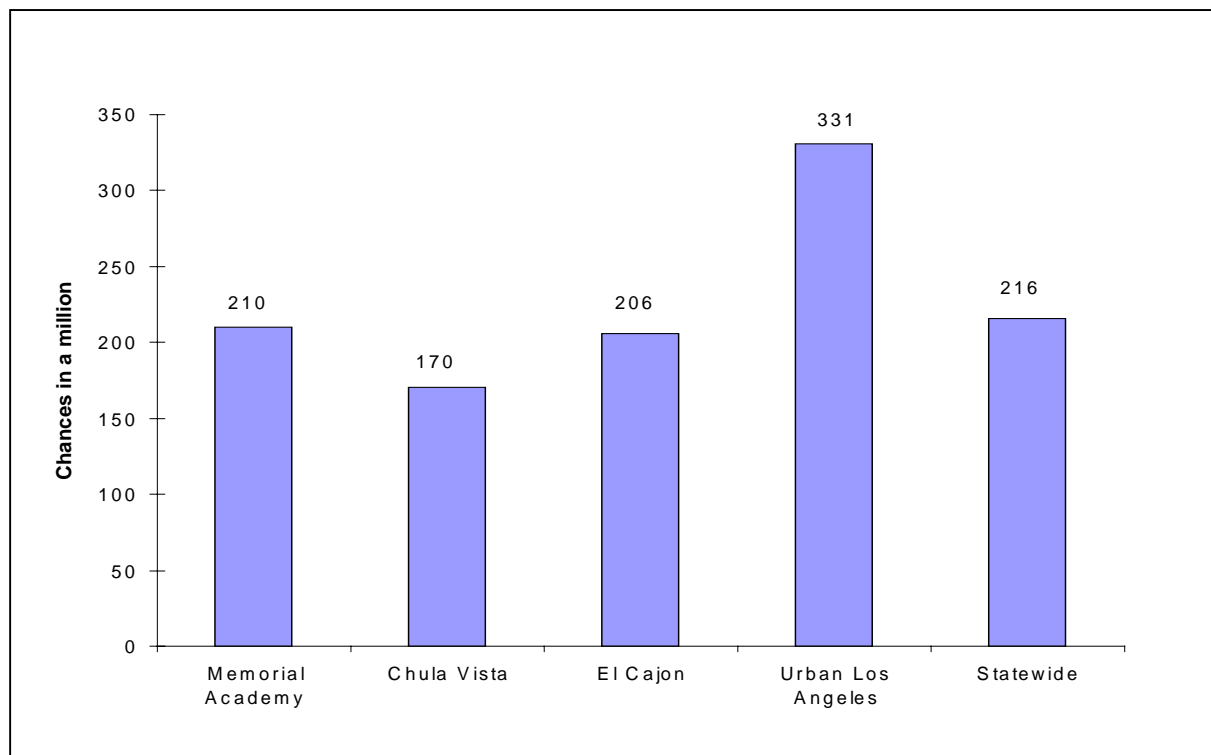
It is important to note that PM from the exhaust of diesel-fueled engines (diesel PM) is the primary contributor to potential cancer risk in urban areas from toxic air pollutants. Although diesel PM risks have been calculated from emissions and modeling, it has proven difficult to measure in the atmosphere. The difficulty in measuring diesel PM is

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that it is composed of literally hundreds of compounds, and many are not unique to diesel engines. Elemental carbon was the first compound to be used as a diesel marker but as diesel technologies improved and the diesel fleet became cleaner, it was clear that elemental carbon alone was not a good marker for diesel PM. This is also supported in the Health Effects Institute's Diesel Epidemiology Working Group report entitled, "Research Directions to Improve Estimates of Human Exposure and Risk from Diesel Exhaust."

Diesel PM was not measured in this study because no acceptable peer reviewed monitoring method exists. Therefore, the risk values presented here and in the corresponding reports on air quality in Barrio Logan do not include the potential cancer risk from this source. We are working on methodologies to measure diesel PM and there is already an aggressive risk reduction program underway to reduce diesel PM emissions.

Figure 2.2* Potential Cancer Risk (Without Diesel PM) at Memorial Academy Compared to Statewide and Local Areas (Based on Annual Averages)



* Figure does not include estimated risk from diesel PM. The potential risk estimates assume a lifetime exposure through breathing pathway only. Estimates for Memorial Academy, Chula Vista, and El Cajon are based on October 1999 – September 2000 data; urban Los Angeles and statewide averages are based on October – September from 1998-2000.

For a number of toxic air pollutants, emissions are produced directly or indirectly by cars and trucks. Two of these pollutants – 1,3-butadiene and benzene – were noticeably higher at Memorial Academy than at Chula Vista. The differences between these two pollutants led to the differences in potential cancer risk between the two sites. Levels of

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two other pollutants – formaldehyde and acetaldehyde – were similar at Memorial Academy, Chula Vista, and El Cajon. The average levels for the four pollutants were comparable to the statewide average levels, and the observed differences were not large compared to the range of levels across the State. Gasoline-powered engines are the major source of these four pollutants, but formaldehyde and acetaldehyde can also be formed through chemical reactions of other air pollutants in the atmosphere. Industry-related releases of these pollutants account for approximately 15 percent of the emissions of these pollutants.

The report on the ambient measurements at Memorial Academy Charter School concluded that levels of most toxic air pollutants were higher in the winter than for other seasons during the study, as is the case for most locations in the State. In addition, the annual average levels of toxic air pollutants observed at Memorial Academy Charter School are similar to those found in other parts of San Diego.

Due to industrial sources such as chrome-plating facilities near the Barrio Logan community, several metals were of particular interest in this study. Manganese, nickel, and zinc are some of the metals measured at Memorial Academy; however, their levels were not determined to pose a health risk.

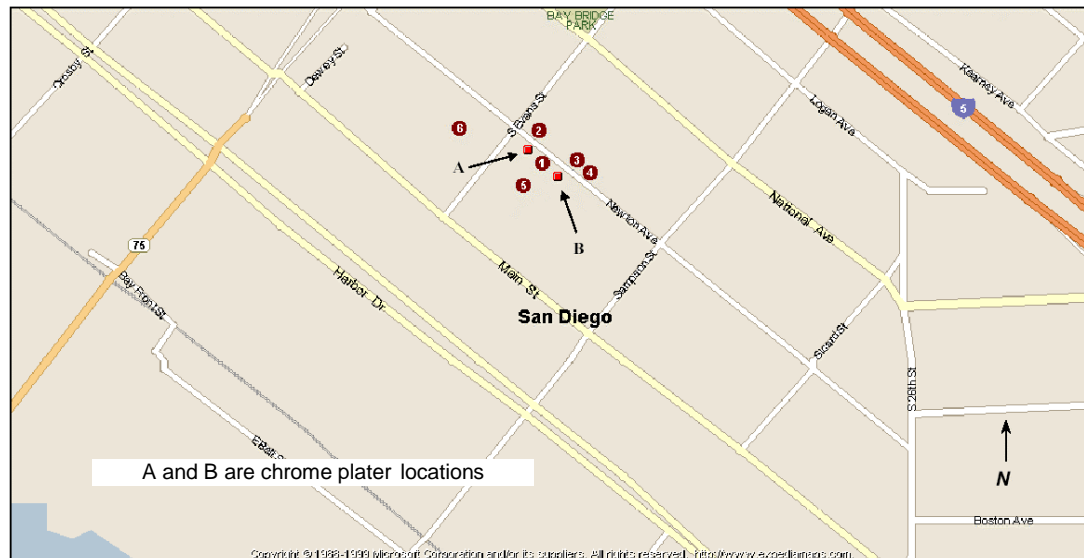
A complete evaluation of the ambient data collected at Memorial Academy Charter School and surrounding sites is available in the Technical Support Document to the report entitled, “Air Quality at Memorial Academy Charter School in Barrio Logan” (CARB 2002a).

B) Special Hexavalent Chromium Monitoring Study

Although we did not find ambient levels at Memorial Academy Charter School substantially different than the rest of the San Diego area, community members still had concerns about hexavalent chromium emissions on Newton Avenue, a mixed use area of Barrio Logan. This area had both residences and chrome platers in close proximity to each other.

In 2001, we initiated a study specifically aimed at looking at near source impacts of two chrome platers on the adjacent residences. In this study, monitoring for hexavalent chromium was conducted at a variety of locations in and around the two chrome platers between December 3, 2001 to May 12, 2002. The project began as a two week hexavalent chromium monitoring pilot study to understand the exposure of neighborhood residents to air pollution. The outdoor air was initially sampled at six locations for 24-hour periods near a hard chrome and a decorative chrome plater as shown in Figure 2.3. Community residents participated in the project and several of the ambient air monitors were placed in resident's yards.

Figure 2.3 - Hexavalent Chromium Monitoring Sites (CARB 2002b)



A and B are chrome plater locations

All sampling locations are approximate.

Chrome Platers

A = Master Plating (Decorative Chrome), 2109 Newton
B = Carlson & Beauloye (Hard Chrome), 2141 Newton

Proposed Ambient Sampling Sites

- 1 = 2121 Newton Avenue
- 2 = Vacant Lot (collocated + met station)
- 3 = 2144 Newton Avenue
- 4 = 2152 Newton Avenue
- 5 = Alley
- 6 = Mercado Apartments

Hard chrome plating refers to the applications of a relatively thick layer of chrome to industrial parts and equipment for corrosion and wear resistance. Decorative chrome plating refers to the applications of a thin layer of chrome to smaller parts for decorative purposes. Each facility has different emission control requirements.

The hard chrome plater was a larger, well-controlled facility that used fume suppressants, ventilation systems, and high efficiency filters to control their hexavalent chromium emissions. The decorative chrome plater was a smaller facility that used fume suppressants as their only control technique. Even though each facility used different types of emission controls, they both met all air quality regulations applicable for each type of facility.

In January 2002, the preliminary results of the initial two weeks of monitoring were received, and unexpectedly high levels of hexavalent chrome were found at a number of the monitoring sites. The concentrations ranged from 1 to 22 ng/m³ as shown in Table 2.5. The statewide average is 0.1 ng/m³. If the levels seen in these two weeks in December 2001 were to continue for 70 years, the annual risk would be 150 chances of cancer in million.

Upon receipt of the December monitoring results, the ARB and the San Diego County Air Pollution Control District notified local health officials and began planning the next monitoring phase to determine the source of the high hexavalent chromium

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concentrations. The monitoring resumed in February 2002, with strong community support, and continued through May 2002. Monitoring was conducted inside the facilities and outdoors in the community to help understand the source and magnitude of the emissions, air dispersion modeling was used to determine maximum source impact, and source testing was conducted to ensure that the control equipment was functioning properly.

Table 2.5 - Hexavalent Chromium Measurements in Barrio Logan 12/01-5/02.

Hexavalent Chromium Measurements, Barrio Logan, Dec. 3, 2001 – May 12, 2002 (CARB 2002b)					
Location	# of samples	Average Cancer Risk	Hexavalent Chromium (ng/m ³)		
			Average(a)	Highest	Date of Highest Concentration
1	107	114	0.76	21.0	Apr 6
2	45	33	0.22	3.6	Dec 7
2c ^(b)	43	31	0.21	3.2	Dec 7
3	44	50	0.33	7.9	Dec 7
4	43	43	0.28	4.8	Dec 7
5	107	69	0.46	22.0	Dec 13
6	42	23	0.15	1.0	Dec 12
Avg.			0.42		

a. Average values include ½ the limit of detection (LOD) for non-detects. LOD for hexavalent chromium is 0.2 ng/m³ (During this study).

b. Location 2c is a co-located sampler.

As additional monitoring results became available, it was apparent that there was a strong relationship between the emissions at the decorative chrome facility and the high outdoor concentrations at one of the residences. It was also evident that the impact of the chrome plater was greatest at the residence next door and that the impact dropped off quickly as one got further away from the sources. In addition, monitoring that was conducted during a period when the plating facility was not operating its plating tank indicated that there was another source of the hexavalent chromium emissions besides the plating tank. Fugitive dust being kicked up by housekeeping activities such as sweeping and moving material around resulted in much higher concentrations of hexavalent chromium both indoors and at the outdoor monitoring sites. Dust samples were tested and in fact contained high levels of hexavalent chromium.

Based on the findings from the special hexavalent chromium study, we had a high degree of confidence that the hexavalent chromium levels were associated with the decorative plating operating, and that the impact was very localized.

San Diego County used the results of this monitoring study and other hazardous material violations and obtained a temporary restraining against the decorative chrome plater in March 2002. The facility closed permanently in October 2002 pursuant to a settlement agreement with the San Diego Superior Court.

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Additional information on the hexavalent chromium study and the data collected can be found at <http://www.arb.ca.gov/ch/communities/studies/barriologan/barriologan.htm>.

C) University of California, Riverside Short-Term Toxic Air Monitoring

To learn more about the emissions inventory and dispersion model performance in Barrio Logan, we sponsored an additional short-term toxic monitoring study. The study was conducted by UC Riverside's College of Engineering-Center for Environmental Research and Technology (CE-CERT). A portion of this study was carried out at the same time as the hexavalent chromium study discussed above and a tracer study for dispersion model performance, which is discussed later. In this way, the CE-CERT study was intended to provide additional information to evaluate the emissions inventory and dispersion modeling developed for Barrio Logan. Secondary objectives of the CE-CERT study were to identify pollutant concentrations at receptors in the community and conduct limited source apportionment.

To meet these objectives, more than 50 pollutants were measured at four sites in Barrio Logan and at one background site for 12 days in winter 2001-2002. In addition, monitoring for the tracer gas released during the tracer study was conducted. A cursory review of the toxic data from the CE-CERT report shows no significant difference in observed concentrations between monitoring locations for most pollutants. This information also contributes to our overall understanding of the air quality in the community.

However because of the realization that there really was a limited amount of toxic data collected, further analysis of these data were not conducted. The final report, "Measurement of Toxic Air Pollutants for the Neighborhood Assessment" (August 2003), can be found at <http://www.arb.ca.gov/ch/communities/studies/barriologan/barriologan.htm>

D) Findings from the Ambient Air Monitoring Studies

Memorial Academy was chosen for this project because we and the community members believed it would provide information on the impact of local sources on the neighborhood and particularly the school. When we began this project, we thought that this school might represent high concentrations due to its location between many neighborhood sources.

Based on the 17 months of ambient air measurements, we found the air quality at Memorial Academy Charter School to be similar to measurements made at other routine data collection locations in the San Diego urban region. The toxic air pollution levels at Memorial Academy Charter School were similar to the levels at El Cajon and statewide averages, but slightly higher than Chula Vista. However, the potential cancer risks at Memorial Academy and Chula Vista are not statistically different. As we found with other SB25 studies, the monitoring was adequate for assessing the regional impact

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from air pollution, but not adequate for assessing very near source impacts. The final report “Assessment of California’s Statewide Air Monitoring Network for the Children’s Environmental Health Protection Act (SB 25)” (October 2003) can be found at <http://www.arb.ca.gov/ch/programs/sb25/adequacyreport.pdf>.

The hexavalent chromium study taught us that community involvement is important to identifying localized hot spots and that partnerships between the communities and the other government agencies involved are critical to success. We also found sources in close proximity to residences may have a high near source impact that is very localized, but the impact of the source drops off quickly as the emissions disperse. In addition, we also found that chrome platers may emit chromium not only as part of the plating process but also because of housekeeping activities. These were significant findings since none of it would have been discovered with regional ambient air monitoring or modeling. This information will be used as we review and consider revisions to our chrome plating air toxic control measure to ensure health protection.

In order to find this community’s greatest risk to air pollutants we needed to move our monitors closer to sources of emissions. This may vary in other neighborhoods, depending on the types of sources (e.g. industries), pollutants emitted from each source, and other details (e.g. spatial distribution, release characteristics, operating schedules, and size of the sources).

It is also important to remember that diesel PM is the largest contributor to known air pollution risk and is not included in the risk estimates because there is no peer reviewed accepted method to measure diesel PM.

Today, all of California attains the health based air quality standards for lead, sulfur dioxide, and nitrogen dioxide and most areas attain the CO standard. Annual averages of PM concentration have declined over 20% and the statewide cancer risk from toxic air pollutants has been reduced by about 50%. Despite these successes, air pollution continues to be a public health issue. Most areas in California continue to exceed the State’s health-based air quality standards for ozone and PM. Federal air quality standards for these pollutants are also exceeded in a number of areas. Air monitoring shows that over 90% of Californians still breathe unhealthy levels of one or more air pollutants during some part of the year. And while regional exposure to air toxics is declining, health risk remains high.

CHAPTER 3 - CONCEPTUAL MODELING APPROACH FOR ASSESSING CUMULATIVE IMPACTS

The modeling analysis in Barrio Logan represents ARB's initial, research approach to use modeling to assess the cumulative impacts of air pollution at the neighborhood-scale under its Neighborhood Assessment Program (NAP). The lessons learned from this pilot study will be applied to the next generation of NAP studies, including the current modeling study in Wilmington and, in the future, the conduct of cumulative assessments statewide.

This chapter contains a summary of the NAP draft conceptual modeling approach. Chapter 4 provides a more in depth discussion of developing the emissions input data for modeling, and Chapter 5 describes the application of specific models in Barrio Logan and the associated modeling results.

A) NAP Modeling Protocol

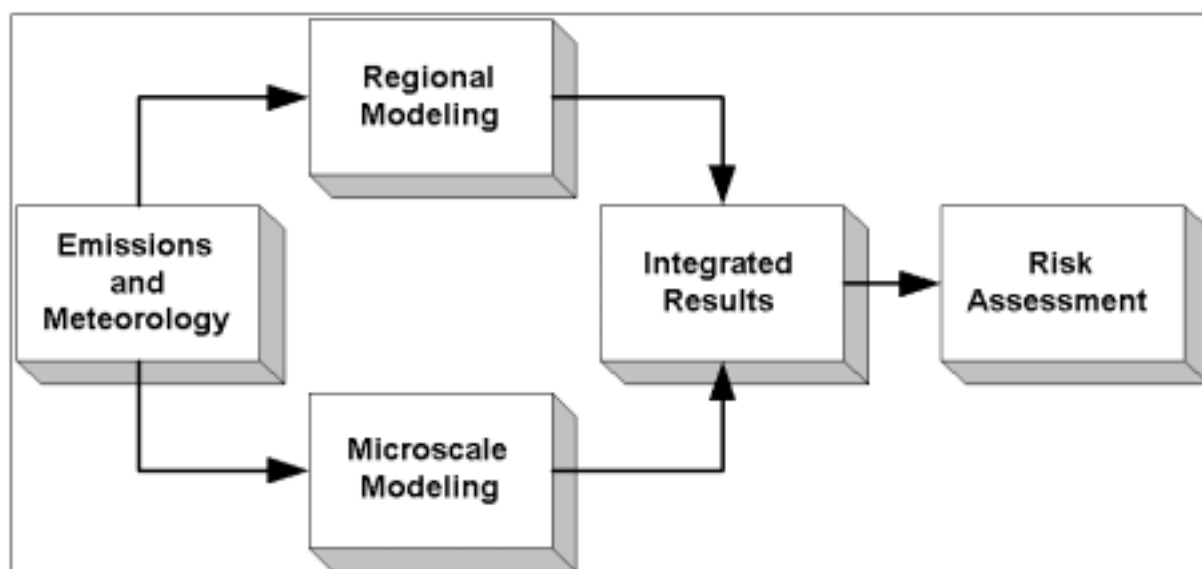
ARB staff along with the Community Modeling Working Group drafted the first NAP Conceptual Modeling Protocol (NAP Protocol; Appendix A) that describes a process to investigate air pollution impacts at the neighborhood level. The Community Modeling Working Group includes over 40 participants from government agencies, universities, industry, and environmental groups. The NAP Protocol was also peer reviewed by members of the academic community including, Mr. John Irwin, Dr. Michael Kleeman, Dr. Christian Seigneur, and Dr. Akula Venkatram.

The hypothesis of the methodology proposed in the NAP Protocol (diagrammed below in Figure 3.1) is that the assessment of cumulative emissions at the neighborhood scale can be accomplished using two types of air quality models. Micro-scale dispersion modeling is needed to determine the spatial distribution of pollutant concentrations above background levels within the neighborhood and regional modeling is needed to determine the general background levels of pollutants in the neighborhood. Combining the results of both air quality models provides an assessment of cumulative impacts in the neighborhood. Common to both types of models are the needed meteorological and emissions inventory inputs.

The regional modeling estimate is based on emissions from the entire urban area as well as the community under study. Because the sources that are included in local scale modeling are also included in the regional scale modeling, the contribution of these emission sources would be counted twice if we simply superimposed the model results from the local scale modeling with the model results from the regional scale modeling. This problem is referred to as 'double counting'. A variety of approaches to

alleviate double counting are proposed in the NAP Protocol, but a final recommended approach is still under development.

Figure 3.1 - Schematic of Cumulative Impact Assessment



The overall objective of the work elements contained in the NAP Protocol is to test and develop tools and methodologies that can be applied to assess cumulative impacts in neighborhoods across California. Within this objective is the need to assess the adequacy of inputs, input data collection methods, and model performance metrics. This includes emissions and meteorological inputs to the models as well as the collection and use of representative, neighborhood scale air pollution measurements, against which model simulated concentrations will be compared. Successful modeling (i.e. adequate model performance) will require inputs with sufficient accuracy for the modeling systems to produce air quality simulations that closely match real-life, measured conditions in neighborhoods. Initially, for practical purposes, some inputs and input collection methods will come from either routine data collection or existing special studies (like field data collection and modeling to support State Implementation Plans), while other inputs will require special data collection efforts. Thus, the adequacy of routine data and data collection methods will need to be considered.

B) Micro-Scale Dispersion Models

Several micro-scale dispersion models were used to assess localized air pollution impacts of sources in the community of Barrio Logan. These models were applied to estimate annual ambient concentrations for commercial and industrial stationary sources, and highways and roadways (line sources). Dispersion models are useful tools to estimate downwind concentrations at receptor distances of approximately one hundred meters to a few kilometers from local sources of emissions. Sometimes it is

necessary to use these models for receptors that are tens of meters from a source because few alternatives are available (e.g. due to the lack of representative input data that might drive more complex models). Because micro-scale model receptor spacing can be allocated to very dense grids around sources of emissions (e.g., 50-meter spacing) they are useful to assess whether hot spots might result from the cumulative emissions. However, the ability of the models to represent reality is highly dependent on whether the model is applied for its intended purpose as well as the quality and representativeness of the emissions and meteorological inputs that are used to 'drive' the model.

The majority of the utilized models are steady-state plume models that spatially distribute pollutants (via dispersion) based on statistical distributions. Steady state Gaussian models do not account for the meandering of a plume caused by changing wind direction. Rather, they assume a Gaussian distribution of the diffusion of the plume in the lateral directions of the plume travel. In the direction of the wind, the plume is diluted inversely proportional to the wind speed. Thus, these models generally are not suitable for winds speeds that approach zero. In addition, it is assumed that downwind plume travel is instantaneous and infinite. Generally, these models do not simulate dynamic atmospheric processes, like photochemistry, but assume all pollutants are non-reactive. One exception to these generalizations is the CALPUFF (Scire 2000). ref.) model, which is a non-steady state Gaussian puff model. CALPUFF takes into account plume meandering due to hourly variations in meteorology, and may also be used for long-range transport. The protocol also indicated that a Lagrangian particle dispersion model would be used to provide concentration estimates at scales of meters to tens of meters from a source, but the scope of the work plan was changed to ensure adequate resources for model validation, and the Lagrangian model work was not done.

1) Micro-Scale Model Selection

Emissions from stationary sources, such as facilities, are simulated with three separate models: ISCST3 (U.S. EPA 1995), AERMOD (U.S. EPA 1998), and CALPUFF. These models are well suited for simulating the dispersion of emissions from stationary sources such as stacks and fugitive sources such as evaporative emissions. The Industrial Source Complex Short Term, Version 3, model (ISCST3) is the most commonly applied U.S. EPA dispersion model for stationary sources. AERMOD is the American Meteorological Society/EPA Regulatory Model (Cimorelli et al., 1996). It is an advanced dispersion model that is being promoted by U.S. EPA to replace ISCST3. CALPUFF is also an advanced model on the U.S. EPA list of recommended models for assessing impacts in complex terrain and for long-range transport. The use of AERMOD and CALPUFF was minimal for this effort because of the iterative nature of developing the emissions inventory. CAL3QHCR (U.S. EPA 1995.) is used to simulate the dispersion of emissions from roadways.

2) Micro-Scale Data Requirements

Micro-scale models require hourly meteorological observations. Representative, on-site observations are preferred. For this project, meteorological data for ISCST3 dispersion modeling were constructed from both on-site and nearby representative meteorological data from the nearest National Weather Service (NWS) station. Hourly meteorological inputs required for the steady-state Gaussian models are:

- wind speed;
- wind direction;
- ambient temperature;
- atmospheric stability; and
- mixing height.

3) Micro-Scale Model Performance Evaluation

A tracer study was conducted to evaluate the capability of the micro-scale models to simulate transport and diffusion in Barrio Logan within two kilometers of a source. Tracer releases and observations were conducted on an hourly basis for limited time periods in the summer and winter. Additionally, field measurement programs were conducted to study the ambient levels of toxics in Barrio Logan. More information on the observational field studies is covered in Chapter 5.

C) Status of Micro-Scale Modeling NAP Work

Table 3.1 summarizes the status of micro-scale modeling work elements for ARB's overall NAP work that have been completed in Barrio Logan. Other elements will be continued in a companion case study in Wilmington, California. The text following the table discusses the final state of micro-scale modeling conducted as part of the Barrio Logan study. The remainder of this report addresses the work that was completed in Barrio Logan. Subsequent reports on efforts in Wilmington will address other elements of the work plan.

MODELING EMISSION INVENTORY DEVELOPMENT

Table 3.1 - Protocol Elements for Overall NAP Work

Work Elements (From Version 1 of NAP Conceptual Modeling Protocol)		Model				
		ISCST3	AERMOD	CALPUFF	CAL3QHCR	LAGRANGIAN
a	Estimate a detailed concentration field near emission sources.	+	✓	✓	+	Ø
b	Apply and test the models to estimate annual ambient concentrations.	+	+	+	+	Ø
c	Use on-site (Memorial Academy Charter School) meteorological observations and cloud data from the closest NWS station (Montgomery Field) to calculate Pasquill-Gifford stability categories required for modeling.	+			+	
d	Prepare source configuration inputs for more than 600 individual stationary sources for more than 100 individual pollutants and diurnal variation of emissions by hour of day and by day of week.	+	+	+		Ø
e	Prepare hourly traffic volumes for the roadway links from the 1999 travel demand model results and traffic network for San Diego County provided by SANDAG.				+	
f	Obtain the emission factors from EMFAC2000 version 2.02r for an average summer day of calendar year 1999. Base the composite emission factors on the default fleet for San Diego County. This output is generated using Caltrans' Impact Rate Summary (IRS) model.				+	
g	Conduct a performance evaluation for each model. Compare model estimates with measured hourly concentrations for criteria pollutants, and 24-hour and annual concentrations for toxic pollutants where measurements are available.	✓	✓	✓	✓	Ø
h	Evaluate the micro-scale models with a new database for short-range dispersion in urban areas. Data will be collected through a field monitoring study for a tracer gas and meteorological data.	+	+	✓		Ø
i	After evaluating the performance of each micro-scale and regional model, we will develop recommendations for guidelines, including technical protocols and methodologies.	⇒	⇒	⇒	⇒	Ø
j	Share our modeling results and recommendations with EPA's Emission Modeling and Analysis Division, OAQPS, which is currently developing guidelines for air dispersion modeling of toxic pollutants in urban areas.	⇒	⇒	⇒	⇒	Ø

Status Key:
 (+) Completed (⇒) To be considered for Wilmington
 (✓) Some testing; not completed (Ø) Change of Scope; not completed

ISCST3 was the primary micro-scale model used in Barrio Logan. Although all these models - ISCST3, AERMOD, and CALPUFF - were tested using an initial micro-scale stationary emission inventory, only ISCST3 was used for the subsequent emission inventory updates. Additional inventory refinements would have been needed to make additional runs using AERMOD and CALPUFF. Dispersion of emissions from major roadways, such as cars and trucks, were simulated with the CAL3QHCRCR model.

All models except the Lagrangian Particle Model were tested. CALPUFF was tested in Barrio Logan for only nine pollutants. The reason for this is that the feature used in ISCST3 to streamline the calculations for post-processing risk is not available in CALPUFF. Specifically, ISCST3 stores the output concentration based on a unit emission rate for each source at each receptor. This facilitates post-processing the

modeling output for estimating inhalation risk for each pollutant. CALPUFF does not store the output concentration for each source at each receptor without making multiple model runs or modifying the source code, thus making CALPUFF resource intensive or cumbersome to use.

An ARB contract with UC Riverside called for performing Lagrangian modeling in Barrio Logan. However, the scope of work for the contract was changed to allow resources for the tracer study for model validation; as a result the Lagrangian modeling was discontinued. Although Lagrangian particle modeling was not performed as intended, the University of California, Riverside's (UCR) College of Engineering-Center for Environmental Research and Technology (CE-CERT) did conduct a special study at UC Riverside for receptors very near a source (Venkatram 2003b). In this tracer study, a neutrally buoyant tracer gas, SF₆, was released from the top of a trailer in the parking lot at UC Riverside. Receptors were placed in two arcs at ten and twenty meters downwind. The tracer study showed that improvements in model predictions could be obtained by including a new dispersion algorithm with site-specific turbulence information. This new algorithm is proposed for inclusion in future releases of AERMOD.

Model performance was conducted by comparing model estimates with observations of long-term concentrations of TAC's at Memorial Academy Charter School; however, a comparison with criteria pollutants was not conducted. Completing this type of work in future projects, such as Wilmington, could lead to a better understanding of the criteria pollutant emissions inventory and the micro-scale model's ability to simulate dispersion in Barrio Logan.

D) Regional Photochemical Models

The terms "photochemical models", "regional models", and "grid-based models" all generally refer to computer models that simulate the current scientific knowledge of how ozone and other pollutants are formed and transported in the atmosphere. These models are typically used within a region to study the relationship between emissions from different source categories (such as natural sources, motor vehicles, and stationary sources) and air quality. They are also used to assess the effectiveness of air pollution control strategies that might be used to achieve state and federal air quality standards in the future. In Barrio Logan, regional modeling is needed to determine the contribution of emission sources from the surrounding regions to cumulative air pollution impacts on the community.

1) Model Selection

Two state-of-the-science regional air quality models were selected for use in Barrio Logan and the NAP: CALGRID and the Community Multi-Scale Air Quality Modeling System Models3/CMAQ (CMAQ). CALGRID is the baseline model for this analysis and is used to simulate atmospheric processes on criteria and toxic pollutants for a period of

one year (January 1 to December 31, 1998). CMAQ is applied for the comparison of model results on selected months.

We originally proposed using the Urban Airshed Model with the Flexible Chemical Mechanism (UAM-FCM) together with CMAQ for annual toxics modeling. However, CALGRID was selected instead of UAM-FCM for the following reasons. The UAM-FCM is based on an older version of the UAM (UAM-IV), which is no longer supported by U.S. EPA and is poorly documented. CALGRID was developed under ARB funding (Yamartino, 1989), has a better formulation than UAM-IV, and is better documented. CALGRID is a state-of-the science model that has been used for estimating ozone and precursor gas concentrations. CMAQ represents a state-of-science model that has been developed by U.S. EPA over the past six years.

2) Regional Modeling Data Requirements

Regional air quality models require meteorological data, an emissions inventory, and initial and boundary conditions. Air quality data are also needed to evaluate the model's ability to reproduce 'real-world' observations. Both air quality models use the same emissions, initial conditions, and boundary conditions, but each model is driven by different meteorological inputs. CALGRID used the output from CALMET; CMAQ used the output from MM5.

Both CALGRID and CMAQ require the selection of a chemical reaction mechanism to represent the complex atmospheric chemical reactions. Several atmospheric reaction mechanisms are available, like Carbon Bond IV (CBIV) and SAPRC99. Previous annual toxics simulations have used a version of the CBIV (Whitten et al., 1980), and the TOX chemical mechanism (SCAQMD, 1999; CRC, 2002; U.S. EPA, 1992). In this study, a toxics application of SAPRC-99 (together with the TOX mechanism) was used to simulate the August 3-7, 1997 SCOS episode (CRC, 2002).

Annual average concentrations are computed by the air quality model for over 30 toxics compounds present in ambient air, including volatile organic compounds and particulate matter species. Explicit reactions were added to the SAPRC-99 host mechanism to represent the reactive toxics species. However, because of limitations in the models' code, pseudo reactions were used to incorporate the inert species. For the case of CMAQ, an artificial decay rate was used to represent deposition effects on the inert PM species and hexavalent chromium.

3) Regional Model Performance Evaluation

Once computer model simulations are completed, a model performance evaluation is used to assess the ability of the model to simulate atmospheric processes. This is done by comparing model estimates of concentrations with actual observations collected during the period represented by the inputs. Another component of a model

performance evaluation is to test the design and formulation of a model (e.g., whether a model behaves as expected under certain conditions).

Due to the extensive history of ozone modeling that has been conducted to support State Implementation Plans, statistical metrics and procedures to evaluate model performance for hourly ozone simulations have been developed over time and with a great deal of experience (e.g. ARB's Technical Guidance Document; 1992). However, the regional modeling component of the NAP modeling protocol requires model simulations to be conducted for toxic air pollutants and for every hour of an entire year. This represents a new problem for the regional photochemical modeling community for which little experience exists. As a result of this lack of history with simulating annual concentrations for toxic air pollutants, formal regional model performance metrics for annual simulations of any pollutant, including toxic air pollutants, do not currently exist.

The performance of the air quality models for simulating annual toxic air pollutant concentrations was evaluated by comparing the predicted average concentrations with measured ambient observations. For the Barrio Logan analysis and based on the long-term experience with ozone modeling and the associated performance standards that have been developed, hourly ozone model performance evaluations for each hour of the simulated year are calculated and assessed. The same statistics are also calculated for annual, monthly, and seasonal model estimates of toxic air pollutant concentrations. Because performance metrics for annual, monthly, and seasonal model estimates do not yet exist, first-cut statistical metrics are proposed for evaluating annual regional model performance for ozone and toxics. In addition, graphical displays, like scatter plots, are used for comparing simulated annual toxic concentrations against observed concentrations, while annual concentration contour plots are also used to qualitatively assess toxic species estimates generated by both CMAQ and CALGRID.

E) Meteorological Models

1) Regional Meteorological Model Selection and Input Data Requirements

Meteorological models are used to simulate meteorological conditions in the area of study and make use of real world meteorological data. Two different meteorological models, CALMET (Scire 1995) and MM5 (Grell 1995), are used to generate the hourly, three-dimensional meteorological inputs for regional models. CALMET (a diagnostic meteorological model) is used to generate meteorological data for CALGRID, whereas MM5 (a prognostic meteorological model) is used to generate meteorological data for CMAQ.

CALMET is a diagnostic model and is the simpler of the two models. It requires inputs from observational data for surface and aloft winds as well as temperature data. CALMET uses a diagnostic wind field generator with objective analysis and parameterized treatments of: slope flows; kinematic terrain effects; and terrain blocking

effects. CALMET also includes a divergence minimization procedure and a micro-meteorological model for over land and over water boundary layers.

CALMET requires hourly surface observations of:

- wind speed;
- wind direction;
- temperature;
- cloud cover;
- ceiling height;
- surface pressure;
- relative humidity; and
- precipitation type (e.g., snow, and rain).

The upper air data required by CALMET are twice-daily observations of vertical profiles of:

- wind speed;
- wind direction;
- temperature; and
- pressure.

MM5 is an advanced state-of-science prognostic meteorological model that solves the conservation equations to simulate winds and temperatures. This is a non-hydrostatic primitive equation model that uses the sigma coordinate system in the vertical dimension with equally spaced rectangular grid cells in the horizontal on an Arakawa-Lamb B grid. The MM5 simulations for this effort use:

- the Blackadar high-resolution planetary boundary layer scheme;
- the Grell cumulus scheme with explicit moisture that resolves mixed water-ice phase; and
- parameterization of long and short wave radiation parameterized using Dudhia's scheme.

The MM5 model (which is used by CMAQ) is applied with one coarse and one fine nested domain. Atmospheric circulation patterns that are prevalent over the region during the study period are numerically simulated using the coarse and fine nested grids with a two-way nested grid approach. In this approach, the effects of small-scale terrain on the evolution of the atmospheric circulation patterns are captured by the fine nested grid. The model is capable of capturing the major flow features observed within the study domain.

2) Regional Meteorological Model Performance Evaluation

There is a large volume of data involved in producing annual meteorological data sets. There is also an absence of an established protocol to evaluate hourly wind fields on an

annual basis. Therefore, the wind fields were not formally evaluated for the complete year. However, qualitative assessments were made. The wind roses for five observational sites for the months of January and August 1998 were compared to the CALMET and MM5 outputs. In addition, a review of CALMET and MM5 wind fields reveal that, generally, the model outputs capture some of the features of the observed wind speeds and wind directions. Comparisons between the CALMET and MM5 outputs did show some differences between the two meteorological models, which could lead to differences in model results between CMAQ and CALGRID.

F) Integration of Modeling Results

The modeling protocol calls for utilizing two different kinds of models, then integrating the results in order to estimate the combined impact of local and regional sources. Micro-scale dispersion models are used to simulate local-scale concentration gradients within a neighborhood that are caused by sources within the neighborhood. The impact from regional sources and secondary pollution formation are simulated with regional photochemical models. In combining the results from these models, there is a desire to minimize or avoid duplicating emissions where the domains overlap. To address this, the protocol proposes to remove non-reactive emissions from those modeling cells in which micro-scale modeling will also be performed. However, because photochemical mechanisms are very sensitive to sudden changes in conditions, it was decided to only remove non-reactive emissions, and keep reactive emissions, in those cells for regional modeling. This resulted in some level of double counting of emissions.

Sensitivity studies were conducted to estimate the net effect or 'magnitude' of emissions double counting on simulated concentrations. The sensitivity test consists of eliminating all of the emissions contained in the regional modeling grid cell where the Barrio Logan community is located.

CHAPTER 4 - MODELING EMISSION INVENTORY DEVELOPMENT

As mentioned in the previous chapter, both regional photochemical models and micro-scale dispersion models require inputs that properly characterize emissions and meteorology. This chapter describes the development of the emissions inputs required by the two modeling systems. Regional models require emission inputs for all reactive criteria and toxic pollutants within the modeling domain in order to account for the effects of atmospheric chemistry on toxic air pollutant concentrations. However, the micro-scale models used for the neighborhood-scale analyses only require source-specific emissions for the toxic air pollutants under consideration, since they treat all pollutants as inert. A detailed emission inventory was gathered for the micro-scale analysis, which included canvassing the Barrio Logan neighborhood on foot. The resources needed to carry out this element of the pilot study in Barrio Logan were extensive, but were necessary to evaluate all emission sources at the neighborhood level.

A) Background

In order to understand how the inventories for the regional and micro-scale modeling were developed, it is necessary to understand the basics of how a county-level, annual average emission inventory (i.e. regulatory inventory) is developed. California's emission inventory is an estimate of the amounts and types of pollutants emitted from thousands of industrial facilities, millions of motor vehicles, and of hundreds of millions of applications of other products such as paint and consumer products. Because emission inventories are estimates they should be used with an understanding of their limitations. These inventories are based on routine, annual air pollutant emissions including a variety of factors and assumptions, and are not an exact accounting of actual amounts. They do not include excess emissions resulting from process upsets or accidental releases. The emission estimates are generally based on a limited number of source tests, available emission factors, or material balance calculations for similar types of sources. Each emission inventory reflects the best information available at the time.

The development and maintenance of the inventory is a multi-agency effort involving the ARB, 35 local air pollution control and air quality management districts (districts), regional transportation planning agencies (RTPAs), and the California Department of Transportation (Caltrans). The ARB staff is responsible for the compilation of the final, statewide emission inventory, and maintains this information in a complex electronic database.

As stated in Chapter 3, the modeling analysis in Barrio Logan represents ARB's initial, research approach to use modeling to assess the cumulative impacts of air pollution at

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the neighborhood-scale under its Neighborhood Assessment Program (NAP). The primary focus of these modeling analyses are on the exposure to toxic air pollutants. As a result, emission estimates of toxic air pollutants are necessary inputs to the models that are utilized.

There are a variety of data sources from which toxic emission estimates can be collected. Some data sources, like formal Health Risk Assessments (HRAs), provide chemical-specie-specific estimates of a particular facility's emissions. Other data sources, like statewide emission inventories, are based on emission factors designed to estimate Total Organic Gas, or TOG. These estimates of TOG emissions are disaggregated into estimates of discrete toxic species using factors (i.e. discrete specie to TOG ratios) that have been developed from source-specific testing.

To produce regulatory, countywide emissions estimates, the basic principle for estimating emissions is to multiply an estimated, per-unit emission factor by an estimate of typical usage or activity. For example, on-road motor vehicle emission factors are estimated for a specific vehicle type and model year based on dynamometer tests of a small sample of that vehicle type and applied to all applicable vehicles. The usage of those vehicles is based on an estimate of such activities as a typical driving pattern, number of vehicle starts, typical miles driven, and ambient temperature. It is assumed that all vehicles of this type in each region of the State are driven under similar conditions.

Developing emission estimates for stationary sources involves the use of per unit emission factors and activity levels. Under ideal conditions, facility-specific emission factors are determined from emission tests for a particular process at a facility. More commonly, a generic emission factor is developed by averaging the results of emission tests from similar processes at several different facilities. This generic factor is then used to estimate emissions from similar types of processes when a facility-specific emission factor is not available. Activity levels from point sources are measured in such terms as the amount of product produced, solvent used, or fuel used.

ARB maintains an electronic database of emissions and other useful information. Annual average emissions are stored for each county, air basin, and district. The database is called the California Emission Inventory Development and Reporting System (CEIDARS). Emissions are stored in CEIDARS for criteria and toxic pollutants. The criteria pollutants are total organic gases (TOG), carbon monoxide (CO), oxides of nitrogen (NO_x), oxides of sulfur (SO_x), and total particulate matter (PM). Reactive organic gases (ROG) and particulate matter 10 microns in diameter and smaller (PM₁₀) are calculated from TOG and PM, respectively.

B) Regional Emission Inventory

Regional modeling emissions inputs developed under the Southern California Ozone Study (SCOS97) were adapted for use in this project. The inventory for SCOS97 was

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developed by the Emission Inventory Working Group, which consisted of members from ARB, various southern California air districts, and the U. S. Navy. We used the most current inventory data from the districts (base year 1997) and forecasted the data to 1998 using the California Emission Forecast System. Modeling inventories were developed for a weekday and a weekend day each in February, May, August, and November 1998. Following are more details on how emissions are estimated for point and area sources, on-road motor vehicles, and biogenics. Additional general information on California emission inventories can be found at <http://www.arb.ca.gov/ei/ei.htm>

The modeling domain for SCOS97 completely encompasses the South Coast Air Basin and San Diego County, almost all of the South Central Coast Air Basin (except a small piece of San Luis Obispo County), the California-Mexico Border regions, and most of the inland desert areas. This large domain was chosen to minimize the influence of boundary conditions on simulation results and allow the effects of recirculation and interbasin transport to be better represented by meteorological and photochemical models. Emissions of toxic air pollutants were calculated based on the speciation of 1997 base-year SCOS97 TOG and PM emissions for each source type. Other details of how the regional modeling inventory was developed, including adaptations of the SCOS97 emissions, are provided below.

1) Gridded Inventory Terminology

The terms “point sources” and “area sources” have had different meanings to the developers of ‘regulatory’ emission inventories and the developers of modeling inventories. The Table of Inventory Terms (Table 4.1) summarizes the difference in the terms. Both sets of terms are used in this document. In modeling terminology, “point sources” refers to elevated emission sources that exit from a stack and have a potential plume rise. “Area sources” refers collectively to area-wide sources, such as architectural coatings or consumer products, stationary-aggregated sources, such as emergency back-up generators, and other mobile sources. “Area sources” are low-level sources. In the development of the SCOS97 inventories, all point sources were treated as possible elevated sources. In other words, the use of the term “point sources” is the same whether using the modeling or emission inventory definition.

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Table 4.1 - Table of Inventory Terms

Modeling Term “Gridded Inventory”	Emission Inventory Term (Regulatory Inventory)	Examples
Point	Stationary – Point Facilities	Stacks at Individual Facilities
Area	Off-Road Mobile	Farm Equipment, Construction Equipment, Aircraft, Trains
Area	Area-wide	Consumer Products, Architectural Coatings, Pesticides
Area	Stationary - Aggregated	Industrial Fuel Use
On-Road Motor Vehicles	On-Road Mobile	Automobiles
Biogenic	Biogenic	Trees

2) Point and Area Source Emissions

Development of Base Year Point and Area Source Criteria Emissions

The 1997 base year point and area source criteria emissions were obtained from the statewide regional emission inventory. The stationary source component of the emission inventory is comprised of more than 13,000 individual facilities for this domain, called “point sources”. It includes about 140 categories of “aggregated point sources”. All districts report as point sources any facility with criteria pollutant emissions of 10 tons per year and greater. Some districts choose a cutoff smaller than 10 tons per year for reporting facilities as point sources. Any remaining sources are reported as aggregated point sources. Aggregated point sources are groupings of many small point sources that are reported as a single source category (gas stations, dry cleaners, and print shops are some examples). These emission estimates are based mostly on area source methodologies or emission models, and include emissions data for the entire category of point sources, not each specific facility.

The area-wide source component includes several hundred source categories and is made up of sources of pollution mainly linked to the activity of people. Examples of these categories are emissions from consumer products, pesticide applications, architectural coatings, and wind-blown dust from agricultural lands. The emissions for these categories are located mostly within major population centers. Some of the emissions in these categories come from agricultural centers and construction sites.

The off-road mobile source inventory is based on an estimate of the population, activity, and emissions estimate of the varied types of off-road equipment. The major categories of engines and vehicles include agricultural, construction, lawn and garden, and off-road recreation, and includes equipment from hedge trimmers to cranes. The OFFROAD model estimates the relative contribution of gasoline, diesel, compressed natural gas,

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and liquefied petroleum gas powered vehicles to the overall emissions inventory of the State. For more information, see <http://www.arb.ca.gov/msei/off-road/off-road.htm>.

The local air districts provide point source information to ARB to update the annual average CEIDARS database. Estimating emissions from area sources is a cooperative effort between ARB and air district staffs. Updating the emission inventory is an on-going process.

Quality Assurance of Base Year Point and Area Source Emissions

In order to prepare the best inventory possible for use in modeling, ARB and district staff devoted considerable time and effort to conduct quality assurance (QA) of the 1997 inventory. Staff from the South Coast AQMD, San Diego County APCD, Santa Barbara County APCD, Ventura County APCD, Mojave Desert AQMD, and Imperial County APCD conducted extensive quality assurance to provide an accurate and complete inventory.

The level of detail of inventory related data is greater for modeling than for annual emission inventory estimates. Additional work is needed when preparing an inventory for use in a photochemical model. In particular, facility location, stack data, and temporal information were closely checked in the 1997 CEIDARS database. This information is critical in modeling studies but was not always of sufficient quality in the database since this information is not needed in the actual calculation of emissions. ARB ran several types of QA reports on the inventory to assist the districts in locating errors or incomplete information.

- Stack data – The report checks for missing or incorrect stack data. The report lists missing stack data and also checks the data for reasonable stack height, diameter, temperature, and stack velocity. Additionally, the report compares the reported stack flow rate with the computed theoretical flow rate (calculated using the diameter and stack velocity).
- Location data – The report checks for missing or wrong Universal Transverse Mercator (UTM) coordinates. The report lists missing UTM coordinates for both facilities and stacks. UTM coordinates are also checked to ensure that they are in the range for a given county. Another report is also run that shows the UTM coordinates for a facility grouped by the city in which the facility is located. This allows staff to look for outliers that may indicate facilities whose locations are in the county, but not in the correct location.
- Temporal data – The report checks for missing or invalid temporal information. Temporal codes used to describe the hours per day, days per week, and weeks per year are checked for completeness, accuracy and validity. The relative monthly throughput, which assigns a relative amount of activity to each month of the year, is checked to ensure the sum is 100%.

Forecasted Point and Area Source Emissions

Air pollution programs have always depended on predictive models for gaining a better understanding of what the emissions will be in the future—these predictions are based on expectations of future economic conditions, population growth, and emission controls.

ARB's system to forecast emissions is known as the California Emission Forecasting System (CEFS). The purpose of CEFS is to track the effects (forward or backward in time) of emission control rules and growth activity for stationary and other mobile sources on a district, air basin, and county level. Thus, based on a specific base year CEIDARS inventory, CEFS can forecast future year emissions or back-cast prior calendar year estimates of emissions. CEFS does this by linking rule-based emission reduction factors directly to the emission categories contained in CEIDARS. A key component of CEFS is the Rule Tracking Subsystem (RTS). The RTS was developed to link emission control rules to the emission process level. The emission process level is identified one of two ways. For facilities, the Source Classification Code (SCC) are used. For all other sources, the Standard Industrial Classification (SIC) or Emission Inventory Code (EIC) is used. In total, the emission process level comprises more than 30,000 possible emission process/industry categories statewide.

For this project, the best available district, air basin, and county level inventory in CEIDARS had a 1997 base year. Using CEFS, this 1997 inventory was forecasted to 1998 emissions (on an average day, district, air basin, and county level). The forecasted 1998 inventory was disaggregated spatially and temporally to hourly, grid-cell estimates required for regional modeling. The following sections describe components of this disaggregating process.

Spatial Allocation – Creating a Gridded Inventory

A regional modeling domain is three-dimensional and can be described as a large cube constructed of many smaller cubes. It is designed to contain all emission sources that could affect modeling results (e.g. where emissions might be re-circulated back into the domain). At ground level and from a birds-eye view it can be represented as a mesh that covers a specific region, however, it's important to keep in mind that the grid also has a vertical component.

Air quality modeling requires that hourly emissions inputs be provided for each three-dimensional grid cell within a grid-based modeling domain. For this project, two modeling domains have been established. One modeling domain is based on the Universal Transverse Mercator (UTM), for CALGRID. The other modeling domain for CMAQ is based on a Lambert Conformal projection. The following tables provide more details of the grid definitions.

Table 4.2 - Domain Definition for CALGRID (UTM Based)

Parameter	Value
Modeling Year	1998
X-Origin (UTM Zone 11)	250,000 m
Y-Origin (UTM Zone 11)	3,580,000 m
Number of cells (Easting)	87
Number of cells (Northing)	67
Grid Width	4,000 m
Domain top	3,000 m
Number of vertical layers	10

Table 4.3 - Domain Definition for CMAQ (Lambert Conformal Projection)

Parameter	Value
Modeling Year	1998
Center of grids	Latitude 30° N Longitude 118° W
Origin (from center)	(-160,000 m, +260,000 m)
Projection parameters	(30, 60, -118)
Domain top	14,600 m
Number of vertical layers	17

Once the county-wide, base year or future year point and area source inventories are forecasted by CEFS, the next step of modeling inventory development is to spatially allocate the CEFS-based countywide emission estimates to the grid cells in the modeling domain. It is important that the physical location of emissions be determined as accurately as possible. Otherwise, an emission source might be allocated to the wrong grid cell. Ideally, the true location of all emissions would be known.

The spatial allocation of *on-road motor vehicles* is based on the regional transportation network that is utilized. This is described in the following mobile sources emissions section. Biogenic (or natural source) emissions are calculated with ARB's biogenic model, the Biogenic Emission Inventory Geographic Information System (BEIGIS), and utilizes GIS data to calculate the spatial distribution of natural source emissions. The following section on biogenic emissions provides more details.

Point source emissions are allocated to grid cells using the coordinates reported for each stack. If there are no stack coordinates, the facility coordinates are used. When location data are not reported, the county centroid is used. These emissions are also distributed vertically into their proper layer in the air quality modeling grid. The vertical layer to which point source emissions are assigned is determined from the calculation of plume rise for those emissions, based on upward effluent velocity and/or buoyancy. Plume rise calculations are limited to point sources where the necessary stack parameter and required operational details are available (in some cases, default parameters must be used). Generally, within a gridded inventory, the vast majority of emissions are allocated to the first (or surface) layer.

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Spatial allocation factors are used to geographically distribute countywide area source emissions to individual grid cells in a modeling grid system. Spatial allocation factors are developed using Geographic Information System (GIS) software by normalizing spatial data like demographic or land use patterns that vary geographically and calculating grid-cell-to-county ratios of spatial data, like total population. For example, if the population of an entire county in the gridded modeling domain is 100 and a grid cell within that county has a population of 10, then a population-based, spatial allocation factor of 0.1 could be assigned to that grid cell. This might be used to allocate population-related emissions, like consumer product emissions, that are reported for the entire county to the grid cell.

In support of the SCOS97, Sonoma Technology, Inc. (STI) was contracted to develop area source spatial allocation factors. Using a GIS-based approach, STI developed gridded spatial allocation factors for a 1997 base-year and three future years (2005, 2010, and 2020) for southern California resolved to a 2-kilometer (km) grid cell. Three basic types of surrogate data were used to develop the spatial allocation factors:

- land use and land cover
- facility location
- demographic and socioeconomic

Land use and land cover data are associated with specific land uses, such as agricultural tilling, feedlots, or recreational boats. Facility locations are used for sources such as gas stations and dry cleaners. Demographic and socioeconomic data, such as population and housing, are associated with residential, industrial, and commercial activity (e.g. residential fuel combustion).

To develop spatial allocation factors of high quality and resolution, local socioeconomic and demographic data were used when available; for rural regions for which local data were not available, the Caltrans Statewide Transportation Model data were used.

Each area source category is assigned a spatial surrogate. This assignment provides a cross-reference between the spatial allocation factors and the total mass of all area source emission inventory categories. A total of nine categories of surrogates were produced containing approximately 40 unique surrogates for 10 counties. Designating the surrogate-to-emission inventory assignments was an iterative process among STI staff, ARB staff, and local air district staff.

A summary of the spatial allocation categories is listed below along with a table of data sources from which surrogates were developed. Note that the spatial allocation factors and emissions category assignments can vary by county depending on the data available for each county.

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Table 4.4 - Categories of Spatial Allocation Factors

1.	Socioeconomic and demographic
2.	Facility locations
3.	Airport and military bases
4.	Lakes, reservoirs, coastline, and forested areas
5.	Computed factors for construction activities
6.	Land use/land cover
7.	Railway and railway yards
8.	Road network and VMT
9.	Bulk plants

Table 4.5 - Sources of Surrogate Data Used to Develop Spatial Allocation Factors for Southern California Regional Domain

Data Source	Parameter	Resolution	Vintage	Coverage
South Coast Association of Governments	Population, housing, employment	Traffic Analysis Zone	1990 1994 2000 2010 2020	Los Angeles, Orange, W. Riverside, W. San Bernardino, and Ventura Counties
Kern County Counsel of Governments	Population, housing, employment	Traffic Analysis Zone	1997 2005 2010 2020	Kern County
Caltrans	Population, housing, employment	Traffic Analysis Zone	1995 2005 2015 2020	Imperial, E. Riverside, E. San Bernardino, San Luis Obispo, and Santa Barbara Counties
United States Electronic Yellow Pages	Area source facility locations	Coordinate locations	1997	Domain
MapInfo GIS StreetInfo database	Railroads, military base locations, lakes and reservoirs	Line and polygon	1995	Domain
Environmental Systems Research Institute Standard Data and Maps CD-ROM	Airport, school, park, golf course, cemetery locations	Polygons	1995	Domain
United States Geological Survey	Land cover/land use	Polygons	1995	Imperial and San Luis Obispo Counties
Department of Oil and Gas	Oil well locations	Coordinate locations	1995	Los Angeles, Ventura, and Santa Barbara Counties
MapInfo	Elevation data	Elevation contours	1995	Domain

Use of SCOS97 Day-Specific Point and Area Source Emissions

Commercial Ships

Off-road emissions from commercial ships are based on the August 3-7, 1997 ozone episode developed for SCOS97. Hourly emissions from August 3, a Sunday, and August 5 are used for weekend and weekday emissions, respectively.

To estimate emissions from commercial ships, the ports of Los Angeles, Long Beach, and San Diego were contacted for activity data. The US Navy at Point Mugu was also contacted for commercial and naval ship activity data. A substantial amount of information was also obtained from the US Navy (at Point Mugu) ship traffic study. Information on emission factors, tugboats, berthing (hotelling), and maneuvering were obtained from a Marine Vessel Study ("Air Quality Impacts from NO_x Emissions of Two Potential Marine Vessel Control Strategies in the South Coast Air Basin" – CARB and SCAQMD, November 2000). The US Navy study looked at military and large commercial shipping, but not commercial fishing. The data they provided included commercial and naval ship (in-transit) traffic information for the ports of Los Angeles and Long Beach and for the area from Long Beach to Santa Barbara. The US Navy tracked ship traffic within 125 miles from the shore; however, the Navy does not track ship traffic for the southern portion (including San Diego) of the modeling domain. San Diego APCD staff contacted the San Diego harbor and collected 1997 commercial ship activity data for the study period.

Aircraft

Day-specific aircraft emissions were estimated as part of SCOS97. It was the first ever attempt to develop a three-dimensional spatial and temporal distribution of aircraft emissions using real-time data. The ultimate goal was to create a three-dimensional hourly gridded emission inventory for commercial aircraft activity. An independent contractor used the Flight Explorer™ program to provide the aircraft activity information for the study domain. Flight Explorer™ is a PC-based graphical aircraft situation display program that receives real-time data from FAA's Traffic Management System. The program provided us information on the type of aircraft and the position of the aircraft as a function of time (latitude, longitude, elevation, time, ground speed, accelerations, and ascent/descent rate).

The flight information was then combined with emission factor information to calculate emissions. The emission factor information was extracted from version 3.2.2.3 of the Emissions and Dispersion Modeling System (EDMS). EDMS was developed by the Federal Aviation Administration (FAA), in cooperation with the United States Air Force (USAF). EDMS is a complex source microcomputer model designed to assess the air quality impacts of airport emission sources, particularly aviation sources, which consist

of aircraft, auxiliary power units, and ground support equipment. It includes emissions and dispersion calculations, the latest aircraft engine emission factors from the International Civil Aviation Organization (ICAO) Engine Exhaust Emissions Data Bank, vehicle emission factors from the Environmental Protection Agency's (EPA) MOBILE5a, and U.S. EPA-validated dispersion algorithms.

Military aircraft differ from commercial aircraft in the spatial allocation of emissions and their patterns in take-off and landing. The US Navy at Point Mugu provided the ARB staff with military aircraft activity data for 1997.

For this modeling exercise, only aircraft emissions below 1000 meters are included in the inventory. Weekend and weekday emissions are from August 3 and August 5, 1997, respectively.

3) On-Road Mobile Source Emissions

EMFAC is the ARB approved on-road motor vehicle emission inventory model and provides the foundation for mobile source emission estimates used in modeling. The version used to estimate emissions was EMFAC2000 (2.02). This model provides emission estimates for 13 classes of vehicles for exhaust, evaporation, and PM emissions from tire wear and brake wear. EMFAC also produces estimates of fuel consumption, vehicle miles traveled (VMT), and the number of vehicles in use.

EMFAC does not output a gridded emission file. However, EMFAC will produce a file of emission rates that can be used with the Direct Travel Impact Model (DTIM) or other external on-road motor vehicle emission gridding program. These same emission rates are part of the information used by EMFAC to produce emission estimates for California counties or air basins.

DTIM4 is the latest version of DTIM, and is used to estimate hourly emissions within each grid cell in the modeling domain. However, because EMFAC is the approved on-road mobile source emissions model, DTIM4 results are only used as surrogates to distribute the EMFAC countywide emissions for each category. Detailed descriptions of the procedures that are used with EMFAC and DTIM4 to produce day-specific gridded on-road motor vehicle emission estimates can be found at:

http://www.arb.ca.gov/msei/on-road/latest_version.htm for EMFAC and the DTIM4 Users guide. The procedures described are carried out separately for each county in the regional modeling domain.

EMFAC Emission Categories

DTIM4 gridded emission files have fewer categories than EMFAC outputs. Each DTIM4 output category will be used to spatially allocate emissions for several EMFAC emission categories. There are also several categories of emissions that EMFAC produces that are not estimated by DTIM4.

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EMFAC produces emission estimates for the 13 vehicle classes shown in Table 4.6.

Table 4.6 – Vehicle Classes

Vehicle Class	Gross Vehicle Weight
Light Duty Autos - LDA	
Light Duty Trucks – LDT1	< 3,750 pounds GVW
Light Duty Trucks – LDT2	>3750-5750
Medium Duty Trucks - MDV	>5750-8500
Light Heavy Duty Vehicles – LHD1	>8500-10000
Light Heavy Duty Vehicles – LHD2	>1000-14000
Medium Heavy Duty Vehicles - MHD	>14000-33000
Heavy Heavy Duty Vehicles - HHD	>33000
Line Haul Vehicles - LHV	
School Bus - SBUS	
Urban Bus - UBUS	
Motorhomes - MH	
Motorcycles - MCY	

Additionally, there are up to 3 technology groups within each vehicle type: catalyst, non-catalyst, and diesel. For each of the combinations of vehicle type and technology, there can be many emission categories, as seen in Table 4.7

Table 4.7 – Emission Categories

Emission Categories	
Start Exhaust	Running Exhaust
Idle Exhaust	Hot Soak
Running Evaporatives	Resting Evaporatives
Partial Day Resting Evaporatives	Multi-Day Resting Evaporatives
Diurnal Evaporatives	Partial Day Diurnal Evaporatives
Multi-Day Diurnal Evaporatives	Brake Wear PM
Tire Wear PM	

A DTIM4 preprocessor calculates fleet average emission factors for each EMFAC technology type for each emission category. The vehicle type distribution used to calculate fleet emission factors is an input, so it can be varied as needed.

DTIM4 Emission Categories

During DTIM4 operation, all emissions are collapsed into a total of 20 emission categories that depend only on the technology and whether the vehicle is catalyst, non-catalyst or diesel as shown in Table 4.8.

Table 4.8 - DTIM-4 Emission Categories

DTIM 4 Emission Categories			
SCC	Description	SCC	Description
1	Non TOG Exhaust Emission	11	Multi-Day Resting
2	Catalyst Start Exhaust	12	Multi-Day Diurnal
3	Catalyst Running Exhaust	13	PM Tire Wear
4	Non-catalyst Start Exhaust	14	PM Brake Wear
5	Non-catalyst Running Exhaust	15	Catalyst Buses
6	Hot Soak	16	Non-Catalyst Bus
7	Diurnal Evaporatives	17	Diesel Bus
8	Diesel Exhaust	18	Catalyst Idle
9	Running Evaporatives	19	Non-Catalyst Idle
10	Resting Evaporatives	20	Diesel Idle

Creating the Emission Rate File

EMFAC will create an emission rate file for any desired combination of vehicle speeds, ambient temperatures, and relative humidities (RH). However, DTIM4 places restrictions on the total array size. The sets of values we use to build the array are shown in Table 4.9.

Table 4.9 – Value Set for Emission Rate File

Speed	5	10	15	20	25	30	35	40	45	50	55	60	65
Temp:	30	45	60	70	75	80	85	90	100	110			
RH:	0	30	50	70	80	90	100						

Emission Gridding

The method to estimate on-road mobile emissions at the grid cell level is described briefly in the following five steps:

Step 1. Gridded, hourly temperature (T) and relative humidity (RH) fields for each episode day are prepared for input to DTIM4. The T and RH fields are derived either from meteorological model predictions, observations, or some hybrid combination of model predictions and observations.

Step 2. EMFAC is run to prepare on-road mobile source emission factors by speed, temperatures, and relative humidities for each county.

Step 3. DTIM4 is run using data from the regional transportation network and EMFAC to estimate gridded, hourly on-road mobile source emission estimates by day for DTIM4 categories.

Step 4. EMFAC is run again using season-specific T and RH data to provide countywide on-road mobile source emission estimates by day for EMFAC categories. The episode-specific meteorological inputs for EMFAC are

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generated via averaging (VMT-weighted) the gridded, hourly meteorology from Step 1 by county and hour.

Step 5. Two sub-steps are taken:

Weekend adjustments. EMFAC currently does not make weekend day estimates, so EMFAC daily emissions are scaled to represent weekend estimates based upon available data. The transportation network has activity estimates for a weekend day. In order to approximate an EMFAC weekend day inventory, we scaled each county's EMFAC pollutants, except NO_x, by the ratio of DTIM4 VMT for a weekend day divided by the DTIM4 VMT for a weekday. This ratio is 0.88 (reduction of 12%). The ratio was applied to all vehicle classes and pollutants, except for NO_x emissions from heavy-duty diesel trucks. Since heavy-duty diesel VMT is drastically reduced on weekends and their effect is largely on NO_x emissions, we multiplied the weekday NO_x emissions by a factor of 0.536 (reduction of 46.4%) to estimate the NO_x emissions on a weekend day. The factor of 0.536 represents the average reduction in NO_x for a South Coast Air Basin weekend day. This NO_x reduction was derived from Caltrans Weigh-in-Motion traffic counts that can differentiate between vehicle types.

Spatial/Temporal Distribution. EMFAC daily, countywide emissions (adjusted for weekend days, if needed), are disaggregated by category into grid-cells for each hour of the day using the DTIM4 output (Step 3) as a spatial and temporal surrogate. The disaggregation follows the equation:

$$E_{p,ij,hr,cat} = \frac{EF_{p,cat}}{DTIM_{p,daily,cat,cnty}} * DTIM_{p,ij,hr,cat}$$

where:

E=grid cell emissions	hr=hourly emissions
EF=EMFAC emissions	cat=Emission Category
DTIM=DTIM emissions	daily=daily emissions
P=pollutant	cnty=county
ij=grid cell	

The 5 steps above are used to generate sets of day-specific, gridded on-road emissions. These emissions are our best estimates at the present time. However, future work in three areas will improve the estimates. The most important may be in the allocation of heavy-duty truck emissions. At present, the only heavy-duty transportation modeling is done for Southern California counties. Second, weekend emissions should be considered an approximation since there are no transportation models to describe weekend traffic. In other words, the transportation network shows people still traveling to work; the emissions are just scaled down. Third, the on-road motor vehicle modeling emission inventories used traffic estimates for several time periods, which were

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supplied by the local regional transportation agencies (RTPAs) or Caltrans. Traffic within the time period was allocated to each hour using the hourly profiles that were developed by Dr. Debbie Niemeier of UC Davis under contract to SCOS97.

Dr. Niemeier developed two hourly profiles, one for weekdays and one for weekend days, which differ by county. However, there is no distinction by vehicle class. The same hourly profile is used for heavy-duty vehicles as for light-duty vehicles within a county. As a result, there is considerable uncertainty in the spatial and temporal distribution within each county for weekends.

Fleet Emission Factors

An important input to DTIM4 is the vehicle type weighting for emission rate. We use the vehicle type VMT for each county/air basin output from EMFAC, which is then reformatted by the CNVIRS4 computer program and composited by vehicle type distribution from BURDEN in the IRS4 computer program. For the counties that are covered by the transportation model run by the Southern California Council of Governments (SCAG), we process light/medium duty (LM) and heavy-duty vehicles (HDV) separately. The VMT for LM is the sum of EMFAC categories LDA, LDT1, LDT2, MDV, MCY, and MH. The HDV VMT is the sum of LHD1, LHD2, MHD, and HHD.

Besides the composite emission rate file, DTIM4 needs link and trip end activity files. All activity has been resolved to one-hour periods for each county. This was done for a weekday (Monday through Friday) and a weekend day (Saturday and Sunday). When we processed the weekdays and weekend days, we scaled the daily emissions for each county according to the ratio of the VMT on the transportation network to the VMT from EMFAC.

Additionally, EMFAC has different fleet mixes by county based on vehicle registrations. It is the fleet mixes in EMFAC that ultimately are the basis for the on-road mobile source emissions processing that has been done in support of SCOS97. The fleet mixes in the DTIM4 runs are based on the fleet mixes in EMFAC. The DTIM4 runs are based on the composite emissions factors that are generated by EMFAC. During the preprocessing of the EMFAC output, which occurs prior to a complete DTIM4 run that is performed by the IRS/CONVIRS programs, there is generally an adjustment applied to the EMFAC emissions factors based on vehicle counts. In most cases, the regional transportation planning agencies (RTPAs) who supplied the transportation data provided the vehicle counts that were used to adjust the EMFAC emissions factors. In the remaining cases, the vehicle count data were taken directly from EMFAC.

Evaporative Emissions

EMFAC is used to estimate evaporative emissions.

Exhaust Emissions

The exhaust emissions from EMFAC are resolved spatially and temporally by DTIM4 emission estimates. Since transportation models do not estimate VMT for buses or excess idling categories, these are added to DTIM4 emissions. The exhaust CO, NO_x, SO_x, and PM emissions that DTIM4 allocates to category 1 are reassigned to catalyst starts, non-catalyst starts, catalyst stabilized, non-catalyst stabilized, and diesel exhaust categories according to the appropriate day-specific EMFAC inventory.

Regional Transportation Network

In addition to the EMFAC emission rate file, DTIM4 uses digitized roadway segments (links) and traffic analysis zone activity centroids to allocate emissions for travel and trip ends. The regional transportation network utilized in this project covers southern California. It was developed from the transportation networks of two regional transportation planning agencies (RTPAs): the Southern California Association of Governments (SCAG) and the San Diego Association of Governments (SANDAG). The California Department of Transportation (Caltrans) Statewide Model was used to supplement the local data to cover the modeling region.

4) Biogenic Emissions

Biogenic volatile organic compounds (BVOCs), such as isoprene and monoterpenes, are another component of the emission inventory. Similar to other components of the modeling inventory for this project and due to practical considerations, the SCOS97 Study was the source of the biogenic emission estimates.

Due to the impracticality of developing daily biogenic emission estimates for an entire year, the best available data were used. Biogenic emissions were based on the July 13-19, 1998 ozone episode. Hourly biogenic emissions for the lowest biogenic emission day, July 13, were used to represent winter biogenic emissions. The day with the highest emissions, July 16, was used to represent summer conditions. July 15 with mid-range emissions was used to represent spring and fall emissions. Winter biogenic emissions were likely overestimated. Spring and fall biogenic emissions may have been overestimated, but less so than winter. Even so, these emissions were generally located in areas with high vegetation away from population centers and model sensitivity at populated areas was probably low.

Due to the heterogeneity of vegetation landcover, species composition, and leafmass distribution in California, quantifying BVOC emissions in this domain requires an emission inventory model with region-specific input databases and a high degree of spatial and temporal resolution. In response to this need, the California Air Resources Board (CARB) has developed a Geographic Information System (GIS)-based model for estimating BVOC emissions, called BEIGIS, which uses California-specific input

databases with a minimum spatial resolution of 1 square kilometer (km) and an hourly temporal resolution.

The BEIGIS isoprene emission algorithm (Guenther et al. 1991, 1993) is of the form

$$I = I_S \times C_L \times C_T$$

where I is the isoprene emission rate (grams per gram dry leafmass per hour) at temperature T and photosynthetically active radiation flux PAR . I_S is a base emission rate (grams per gram dry leafmass per hour) at a standard temperature of 30 °C and PAR flux of 1000 $\mu\text{mol m}^{-2}\text{s}^{-1}$. C_L and C_T are environmental adjustment functions for PAR and temperature, respectively. The monoterpene emission algorithm adjusts a base monoterpene emission rate by a temperature function (Guenther et al. 1993). Methylbutenol (MBO) emissions are modeled with an algorithm developed by Harley et al. (1998) similar to that for isoprene. Dry leaf mass/leaf area ratios, and base emission rates for isoprene, monoterpenes, and MBO are plant species-specific and assembled from the scientific literature. Modeled BVOC emissions for a given spatial domain therefore represent the contribution by various plant species (through their leaf mass and emission rates) to the total BVOC emissions.

The main inputs to BEIGIS are landuse and vegetation landcover maps, gridded leaf area indices (LAI) derived from AVHRR satellite data (Nikolov 1999), leaf area/dry leaf mass factors, base emission rates, and gridded hourly ambient temperature and light intensity data (from a meteorological model). For urban areas, land use/vegetation landcover databases were developed from regional planning agency data and botanical surveys (Horie et al. 1990; Nowak 1991; Sidawi and Horie 1992; Benjamin et al. 1996, 1997; McPherson et al. 1998). Natural areas are represented using the GAP vegetation database (also satellite-derived and air photo interpreted) developed by the U.S.G.S. Gap Analysis Program (Davis et al. 1995). Agricultural areas are represented using crop landcover databases developed by the California Department of Water Resources (<http://www.waterplan.water.ca.gov>). Ground surveys have been funded by CCOS to validate the vegetation landcover and LAI input databases used in BEIGIS (Winer et al. 1998; Karlik and McKay 1999; Winer and Karlik 2001, Karlik 2002). Validation using flux measurements in the field is on going.

Using BEIGIS, the ARB developed hourly-resolved emissions of isoprene, monoterpenes, and methyl butanol (MBO), gridded at a 1-km resolution. Each 4-kilometer (km) grid cell, using the statewide 4-km grid cell domain defined by the ARB, was divided into 16 1-km grid squares. After the biogenic emissions were calculated, the emissions from the 1-km cells were aggregated for each 4-km grid cell.

Biogenic OVOCs (other VOCs) are added to the BEIGIS biogenic emissions estimate for input to air quality models. Biogenic OVOCs comprise around twenty percent of some biogenic inventories and are known to affect air quality modeling predictions

(e.g. Hanna et al., 2002). Guenther et al. (1994) estimates that the OVOCs comprise 8-73% of total BVOCs. OVOCs are estimated by ARB as an added fraction of 30%, scaled to the total isoprene, monoterpene, and MBO emissions.

The estimate of OVOC emissions used by ARB is the result of an August 2001 peer review of modeling procedures by Dr. William P. C. Carter (UC Riverside). During the discussion with ARB modeling staff, it was noted that estimates of OVOC were reported by some sources to be as great as the inventoried species (isoprene, m-butenol and monoterpenes). Since OVOCs are very uncertain in both mass and species characterization, ARB had not been including them in the modeling programs. Dr. Carter suggested this omission was inappropriate. He recommended that OVOC emissions be included with the best estimates we could make. During this discussion, it was decided that doubling the known species would be like an upper limit which was felt to be too high. Collectively it was decided that an OVOC amount equal to 30% of the total known species would be a reasonable estimate.

ARB reviewed the literature to find a reasonable speciation to assign to OVOCs. Dr. Arthur M. Winer (UCLA) sent a list of the compounds that were intended at that time (2001) to be included in BEIS-3. However, no amounts were assigned to each chemical specie, so ARB could not derive an OVOC profile. Dr. Allen Goldstein (UC Berkley) had published an article 'In Situ Measurements of C2-C10 Volatile Organic Compounds Above a Sierra Nevada Ponderosa Pine Plantation' in the Journal of Geophysical Research (9-20-1999) which did allow us to create a profile to use until better information could be obtained. This profile is dominated by methanol and acetone and also contains ethene, propene, hexanal, and acetaldehyde. These compounds were some of the species proposed for BEIS-3.

ARB's intention is to use this profile for all OVOC from all vegetation types until better information becomes available. In the future, use of BEIS-3 may allow ARB to create BVOC inventories that contain enough compounds so that the additional step of adding a chosen amount of OVOCs' could be eliminated.

5) Profiles of Toxic Air Pollutant Emissions

Speciation

The emission inventory developed for SCOS97 provided estimates of organic compound emissions as Total Organic Gases (TOG). Because we are interested in the regional estimates for toxic air pollutants, we applied chemical speciation profiles to disaggregate the chemical composition of TOG emissions from each source type into discrete chemical species, including toxic air pollutants. Total particulate matter (PM) emissions are also quantified in ARB's emission inventory and are the basis for deriving PM₁₀ and PM_{2.5}.

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Speciation profiles are used to estimate the amounts of various organic compounds that make up TOG. A speciation profile contains a list of organic compounds and the weight fraction that each compound composes of the TOG emissions from a particular source type. Each process or product category is keyed to one of several hundred currently available speciation profiles. The speciation profiles are applied to TOG to develop both the photochemical model inputs and the emission inventory for ROG.

To the extent possible given available data, ARB's organic gas speciation profiles contain all emitted organic species that can be identified (ideally, detected to very low levels). This includes reactive compounds, unreactive and exempt compounds, and to the extent the data are available, low vapor pressure compounds. Research studies are conducted regularly to improve ARB's species profiles. These profiles support ozone modeling studies but are also designed to be used for aerosol and regional toxics modeling. The profiles are also used to support other health or welfare related modeling studies where the compounds of interest cannot always be anticipated. Therefore, organic gas emission profiles should be as complete and accurate as possible.

The speciation profiles used in the emission inventory are available for download from the ARB's web site at <http://www.arb.ca.gov/ei/speciate/speciate.htm>. The Organic Speciation Profiles (ORGP) file contains the weight fraction data (expressed as percent for ease of display) of each chemical in each profile. Each chemical fraction is multiplied by the Total Organic Gas (TOG) emissions for a source category to get the amount of each specific constituent chemical. In addition to the chemical name for each chemical constituent, the file also shows the chemical code (a 5-digit internal identifier) and the Chemical Abstracts Service (CAS) number, which is a unique identifying code (up to 9 digits) assigned to chemicals by the CAS Registry Service.

The Particulate Matter Speciation Profile (PMP) file contains the weight fraction data (expressed as percent for ease of display) of each chemical in the profile, within each of the specified size fractions. Another file, the PMSIZE file, shows the PM size fractions for each profile. The PM speciation profiles used in the emission inventory are available for download from the ARB's web site at <http://www.arb.ca.gov/ei/speciate/speciate.htm>.

The PM speciation profiles are applied in two steps. To get the amount of a specific chemical constituent from the total PM, each PM chemical weight fraction must be multiplied by the appropriate PM size fraction and the emissions amount.

Also available for download from ARB's web site is a cross-reference file that indicates which PM and Organic Gas profile is assigned to each source category in the inventory. The inventory source categories are represented by an 8-digit Source Classification Code (SCC) for point sources, or a 14-digit Emission Inventory Code (EIC) for area and mobile sources. This file also contains the fraction of reactive organic gas (FROG) values for organic profiles, and the PM₁₀ and PM_{2.5} size fraction data for PM profiles.

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Some of the organic gas speciation profiles related to motor vehicles and fuel evaporative sources vary by the inventory year of interest, due to changes in fuel composition and vehicle fleet composition over time. A summary of the speciated toxic air pollutant inventory for Barrio Logan can be found in Chapter 5, Table 5.25.

6) Summary of the Regional Emission Inventory

A summary of the regional emissions inventory can be found in Table 4.10.

Table 4.10 – Barrio Logan Regional Emission Inventory

	1998 Seasonal Emissions - Regional Toxics Modeling Region (Tons/day)							
	Win WD	Win WE	Spr WD	Spr WE	Sum WD	Sum WE	Fall WD	Fall WE
Fuel Combustion								
CO	117	88	75	44	77	47	117	88
NOx	156	132	157	133	158	134	159	135
SOx	23	22	30	28	30	28	30	29
ROG	16	14	14	12	15	12	17	14
TOG	84	77	81	75	82	75	84	77
PM	13	9	48	44	48	45	49	45
Waste Disposal								
CO	2	1	2	1	2	1	1	1
NOx	3	2	3	2	3	2	3	2
SOx	0	0	0	0	0	0	0	0
ROG	4	3	4	3	4	3	4	3
TOG	482	357	482	357	481	357	481	357
PM	9	0	9	0	9	0	9	0
Cleaning & Surface Coatings								
CO	9	9	9	9	9	9	9	9
NOx	1	1	1	1	1	1	1	1
SOx	4	4	4	4	4	4	4	4
ROG	207	113	207	112	208	113	208	113
TOG	308	175	308	175	309	175	310	175
PM	2	2	2	2	2	2	2	2
Petroleum Prod. & Marketing								
CO	4	4	4	4	4	4	4	4
NOx	2	2	2	2	2	2	2	2
SOx	7	7	7	7	7	7	7	7
ROG	69	68	69	68	69	68	69	68
TOG	228	227	207	206	214	213	207	206
PM	1	1	1	1	1	1	1	1
Industrial Processes								

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1998 Seasonal Emissions - Regional Toxics Modeling Region (Tons/day)								
	Win WD	Win WE	Spr WD	Spr WE	Sum WD	Sum WE	Fall WD	Fall WE
CO	91	90	91	90	91	90	91	90
NOx	37	37	37	37	37	37	37	37
SOx	10	9	10	9	10	9	10	9
ROG	67	49	67	49	67	49	67	49
TOG	88	64	88	64	88	64	88	64
PM	298	269	299	269	299	269	298	269
Solvent Evaporation								
CO	0	0	0	0	0	0	0	0
NOx	0	0	0	0	0	0	0	0
SOx	0	0	0	0	0	0	0	0
ROG	227	210	255	229	280	252	223	206
TOG	253	235	282	255	308	278	249	231
PM	0	0	0	0	0	0	0	0
Miscellaneous Processes								
CO	853	669	88	38	30	30	600	550
NOx	57	48	36	34	22	22	48	45
SOx	2	2	1	1	0	0	2	2
ROG	73	59	28	24	23	23	56	53
TOG	323	300	225	219	217	217	291	284
PM	899	652	1129	785	1142	804	1038	726
On-Road Mobile								
CO	8290	7850	8150	7674	9811	9290	8102	7641
NOx	1364	1133	1305	1070	1405	1109	1352	1110
SOx	52	47	52	47	61	55	52	47
ROG	874	837	874	838	984	944	960	924
TOG	942	900	941	900	1061	1014	1027	986
PM	28	23	28	23	33	25	28	22
Other Mobile								
CO	907	1466	1234	2811	1308	3148	909	1484
NOx	446	350	450	394	453	406	432	346
SOx	64	71	64	72	64	72	62	70
ROG	171	244	215	441	227	493	170	244
TOG	189	265	237	479	249	535	187	265
PM	26	23	28	31	28	33	25	22
Natural Sources								
CO	0	0	0	0	0	0	0	0
NOx	0	0	0	0	0	0	0	0
SOx	0	0	0	0	0	0	0	0
ROG	335	335	490	490	635	635	490	490
TOG	364	364	532	532	690	690	532	532
PM	0	0	0	0	0	0	0	0

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1998 Seasonal Emissions - Regional Toxics Modeling Region (Tons/day)								
	Win WD	Win WE	Spr WD	Spr WE	Sum WD	Sum WE	Fall WD	Fall WE
Total Regional Emissions								
CO	10155	10090	9577	10627	11253	12572	9716	9779
NOx	1909	1572	1834	1540	1922	1579	1874	1542
SOx	139	140	137	140	147	149	137	139
ROG	2027	1918	2209	2254	2496	2579	2246	2148
TOG	3176	2887	3302	3186	3617	3544	3373	3101
PM	1264	969	1496	1110	1513	1134	1401	1043

C) Micro-Scale Emission Inventory

The development of a micro-scale or neighborhood scale emission inventory requires supplementing the CEIDARS inventory with more detailed information than is typically collected to support regional air quality modeling. This is especially the case with regard to small stationary sources and mobile sources. In the regional emission inventory, small stationary sources and mobile sources are spread uniformly throughout the grid square. In the micro-scale emission inventory, more precise placement of the emission release point is necessary to determine local impacts. This is particularly important for small sources of toxic air pollutants because these facilities have the potential to create significant localized impacts that could not be identified through the regional inventory alone. Surveys or actual site visits of facilities in the area of study are necessary to collect this enhanced level of detail for the neighborhood assessment. The neighborhood-scale emissions inventory for micro-scale modeling for Barrio Logan is comprised of the following elements:

- **Point Sources**
Point sources are emission sources that are not mobile or area-wide. These stationary sources may include power plants, refineries, chrome platers, and others.
- **On-Road Sources**
The on-road mobile source activity in Barrio Logan was determined using the regional transportation model from SANDAG. DTIM4 and EMFAC2000 are used to produce gridded motor vehicle emissions.
- **Off-Road Sources**
Off-road mobile source activity near Barrio Logan includes the airports of Lindbergh Field and the North Island Naval Air Station. Additional off-road mobile sources include the railways where there are over three miles of track in Barrio Logan and commercial shipping activity of one to two ships per day.
- **Area-Wide Sources**

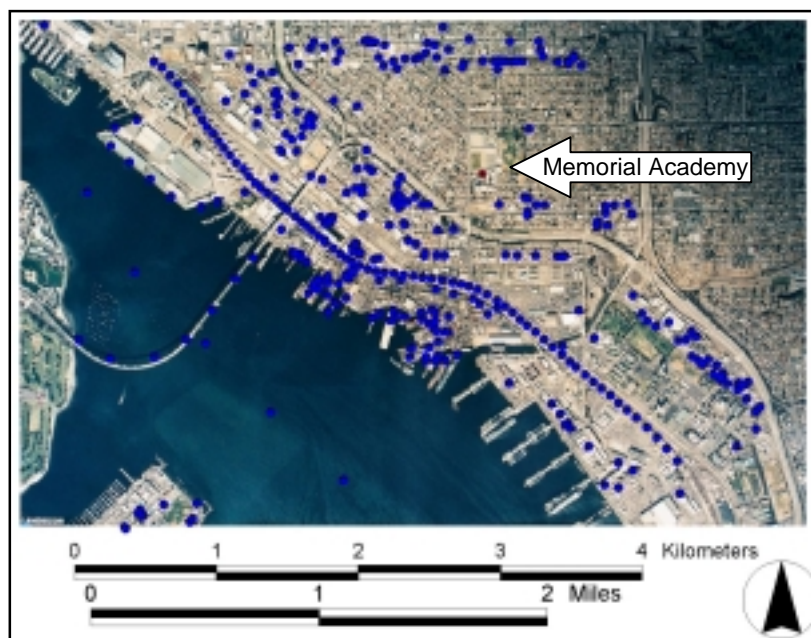
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The area-wide source category includes paints, consumer products, and natural emissions or biogenics.

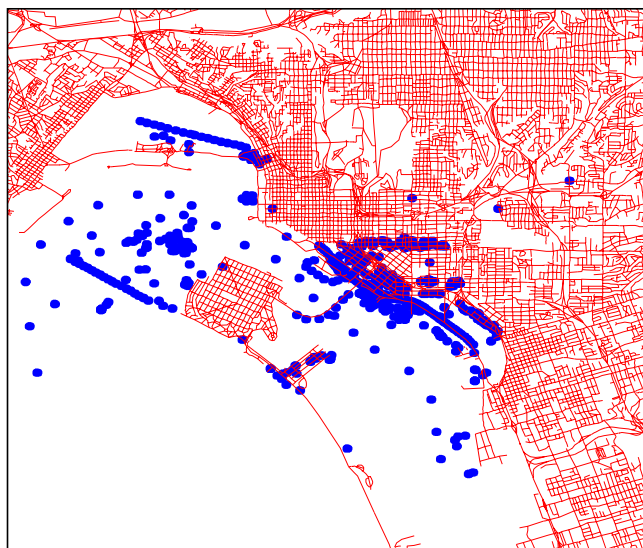
For these categories, over 100 toxic air pollutants are included in the neighborhood-scale emission inventory.

Figure 4.1 provides a birds-eye view of the Barrio Logan emission sources that are characterized for micro-scale modeling. Sources are plotted as dots on the map; a rail line is plotted as a series of volume sources and the shipping lane is plotted as a series of volume sources. Individual facilities are modeled as stationary and volume sources in the micro-scale modeling. Memorial Academy Charter School is shown by the arrow.

Figure 4.1 - Aerial View of Barrio Logan



The micro-scale modeling domain for the Barrio Logan emissions inventory data includes an area approximately 15 km by 15 km. A schematic map of the domain for the neighborhood-scale inventory is shown in Figure 4.2. In this figure, the locations of point and off-road emission sources are shown as circles.

Figure 4.2 - Micro-scale Modeling Domain for Emissions

1) Summary of Micro-Scale Emission Inventory for Selected Toxic Air Pollutants

Table 4.11 summarizes selected toxic air pollutant emissions for the micro-scale modeling in the Barrio Logan domain. Additional details on each source type are provided in the sections that follow.

Table 4.11

Pollutant	Point Sources (lbs/yr)	Off-Road Mobile (lbs/yr)	On-Road Mobile (lbs/yr)	Total (lbs/yr)
Formaldehyde	20,567	109,750	10,400	140,717
Diesel PM	17,663	106,776	8,000	132,439
Acetaldehyde	478	33,841	2,000	36,319
Benzene	1,807	15,542	14,000	31,349
Acrolein	0	16,429	-	16,429
Lead	25	1,703	-	1,728
Arsenic	15	1,640	-	1,655
Cr(VI)	14	82	-	96
- no data				

Stationary Sources

The methods used to enhance the point source inventory for Barrio Logan were presented to the 10th Annual Emission Inventory Conference (Smith, 2001) and are outlined below. This paper entitled "Community Scale Estimation of Air Toxics from Stationary Sources" can be found on the ARB website at

http://www.arb.ca.gov/ch/communities/studies/barriologan/bl_inventory.pdf

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Point Sources in Barrio Logan

Statewide emission information can be found in the ARB's California Emission Inventory Development and Reporting System (CEIDARS). To capture all relevant facilities in the Barrio Logan community, ARB staff used the CEIDARS point source database, information from the San Diego County APCD permit files, and a business license database from the Office of the Treasurer of the City of San Diego. These databases are searched by zip code and roughly 1,500 businesses were identified. This list was reduced to approximately 300 facilities by deleting businesses outside of the Barrio Logan and Logan Heights region, and by deleting businesses that are likely nonpolluting, such as service oriented businesses (accountants, health professions, law and insurance firms, certain retail operations, etc.). Cleaning/maintenance operations and contracting/construction businesses headquartered in Barrio Logan were assumed to operate outside of the study community, and thus, were also deleted. Approximately 200 facilities were visited to collect specific information on facility physical characteristics, types of on-site processes and activities, and assignment of SIC codes.

Point sources in CEIDARS include sources that emit 10 tons or more per year of criteria air pollutants. Emissions from small facilities are calculated en masse on a regional basis in the CEIDARS database. For the micro-scale analysis in Barrio Logan, some small source emissions have been identified individually and are included with the point source inventory. The remaining small sources are included in the regional model emissions inventory.

From the information collected during site visits, 38 facilities were excluded from the emission inventory because they were either out of business, outside of the study region, or were determined not to have significant on-site emissions. Also, ARB staff was unable to contact 57 of the listed facilities. Because the operation of those facilities could not be verified, they could not be further analyzed, and thus, are not included in the inventory. We believe that the exclusion of these facilities did not result in a serious underestimation of the emissions in the Barrio Logan community because these facilities are small and conducted types of activities that would not significantly impact the inventory. The final Barrio Logan point source inventory included 205 facilities.

Types of Point Sources

Of the 205 facilities in this micro-scale inventory, 38 were major source facilities, which had San Diego County APCD permits and were also in the CEIDARS point source database. Emissions data for these facilities was retrieved from the CEIDARS database and included in the inventory without further manipulation. Emissions from the thirty additional facilities that had San Diego County APCD permits, but are not reported in CEIDARS, were quantified from information contained in the San Diego County APCD permit files, such as process rates and product information. In some cases, permit information is supplemented with specific data obtained from visits of the facilities.

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Of the remaining 137 unpermitted facilities, two types are predominant: autobody and auto repair (89 facilities) and welding and metal fabrication (24 facilities). These facilities do not have permits because they either do not generate air emissions or the levels they do emit are below thresholds that would require a permit. ARB staff visited 32 auto repair shops in the community and developed emission inventory estimates for these facilities based on product usage data obtained during visits and the chemical composition of the products, which are obtained from Material Safety Data Sheets (MSDS) and ARB speciation profiles. ARB staff also visited 18 welding and metal fabrication shops in Barrio Logan and calculated inventories using a method similar to that used for auto repair shops.

Twenty-two unpermitted facilities did not fall into any of the above categories, but these facilities performed a number of emission-producing activities, such as wood finishing, engraving, and machine cleaning and repair. Emissions for these facilities were calculated using permit threshold regulatory limits, speciation profiles, and information collected during site visits.

Point Source Diesel Particulate Matter (PM) Inventory for Barrio Logan

Emission data for diesel PM from facilities in the Barrio Logan community are limited. Many of the major facilities in Barrio Logan report diesel PM emissions from stationary engines as a single total for the facility. Therefore, the diesel PM emissions from engines are divided equally among all the engines at the facility. In order to spatially allocate these emissions, the location of each stationary engine is determined by using data from health risk assessment reports submitted to the San Diego County APCD. Alternatively, if the risk assessment data are not available, all emissions from these sources are assumed to be emitted from an assumed stack located at the center of the facility. CEIDARS inventory data containing criteria emissions from diesel-powered compression ignition engines are reported in this inventory as diesel PM, while other diesel sources, such as boilers, are speciated using ARB profiles.

Comparison of the Point Source Emission Inventory to the CEIDARS Database

In this study, we found that only 38 facilities located in the Barrio Logan area are included in the CEIDARS point source database. These facilities accounted for most of the emissions of toxic air pollutants from point sources. Using the technical approach developed for this work, we were able to develop emission inventories for an additional 167 facilities within just a three square mile area. With few exceptions, these additional facilities did not greatly contribute to the emission inventory; the regional inventory derived from the CEIDARS database is sufficient to capture most air pollutants from stationary sources located in the Barrio Logan community. Still, emissions from large point sources alone may not be adequate for a neighborhood scale assessment. For example, when emissions of toxic air pollutants from small facilities are modeled, local areas of elevated exposure and associated health risk may be simulated if the facilities

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are co-located in proximity to sensitive receptors. These areas would remain undetected in the absence of a micro-scale analysis with an enhanced inventory.

Table 4.12 is a snapshot of the point source emission inventory developed for Barrio Logan. While the numbers are not based on the final modeling emission inventory presented in Table 4.11, we include it to show that the majority of emissions originated from the 38 facilities in the CEIDARS database.

Table 4.12 – Initial Micro-scale Emission Inventory for Selected Toxic Air Pollutants^b

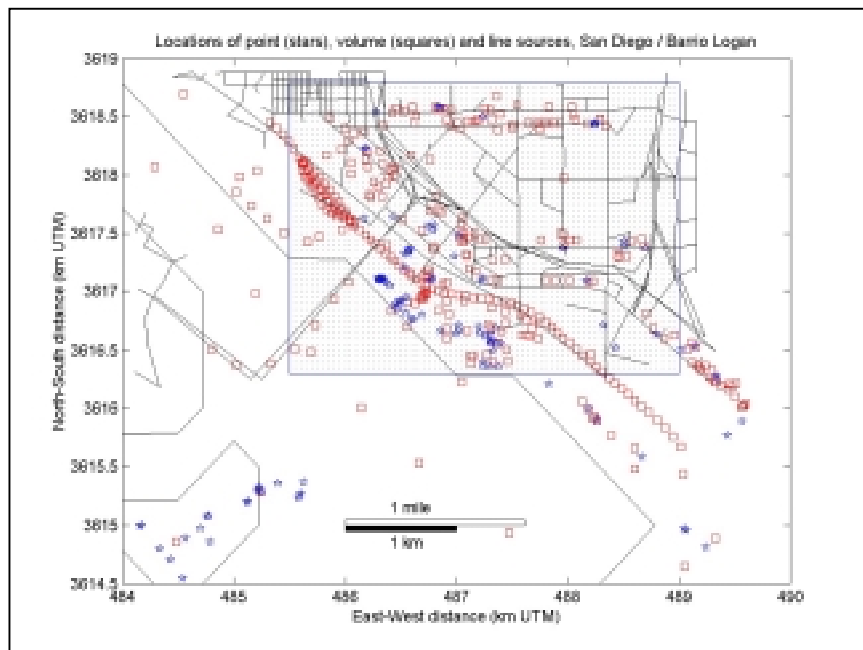
Pollutant	Emissions from Facilities in CEIDARS Database (38) ^a (lbs/yr)	Total Emissions (205) ^a (lbs/yr)	% of CEIDARS in Total
Diesel PM	16,475.0	17,675.6	93.2
Methanol	2,117.3	2,683.5	78.9
Isopropyl Alcohol	1,381,871.8	1,384,331.1	99.8
n-Butyl Alcohol	164,180.7	164,712.0	99.7
Benzene	1,677.0	1,791.1	93.6
Methylene Chloride	24,478.6	24,500.8	99.9
Propylene Oxide	22,716.4	22,716.4	100.0
Methyl Ethyl Ketone	28,250.9	35,962.8	78.6
Trichloroethylene	2,327.2	2,327.2	100.0
Naphthalene	310.2	687.2	45.1
Ethyl Benzene	6,861.7	7,226.4	95.0
Methyl Isobutyl Ketone	16,227.2	17,036.7	95.2
Toluene	7,918.0	19,073.5	41.5
Perchloroethylene	1,411.1	2,055.8	68.6
Xylenes	48,954.1	53,351.8	91.8
Lead	19.8	22.8	86.9
Manganese	1,216.6	1,234.5	98.6
Nickel	185.0	187.4	98.7
Chlorine	528.9	529.0	100.0
Cr(VI)	15.8	16.5	95.6
^a Represents the Number of Facilities			
^b Final Inventory Summary can be found in Table 4.11			

Mobile Sources

On-road mobile source emissions for micro-scale modeling in Barrio Logan are based on hourly traffic volumes and emission factors. The San Diego Association of Governments (SANDAG) provided the 1999 travel demand model results and traffic network for San Diego County. The travel demand model does not provide separate miles traveled for cars and trucks. Therefore, regional assumptions were applied to the travel demand model results to estimate diesel truck miles traveled. Total vehicle miles traveled in Barrio Logan is estimated as 898,292 VMT/day as compared to 70,036,699 VMT/day in San Diego County. San Diego County is an area of 4260 square miles and contains 48,583 roadway links. The Barrio Logan area is approximately 0.2% of the

San Diego County area (7 square miles) and includes 991 road links. The roadway links used for modeling on-road emissions are shown in Figure 4.3. In this figure, model receptors (70x50 central gridded area on the map) are shown as dots, on-road links shown within the box area are used for micro-scale modeling, and point and off-road sources are shown as stars and squares.

Figure 4.3 - Micro-Scale Roadway Links



The emission factors for diesel PM and volatile organic compounds (VOC) were obtained from EMFAC2000 (version 2.02r) for calendar year 1999.

Diesel PM Emissions

Diesel emission factors for PM₁₀ obtained from EMFAC are a function of vehicle speed alone. The default fleet in EMFAC was used for diesel exhaust emission factors for San Diego County in this study. The vehicle speed was obtained from DTIM for the morning peak (6-9 am), afternoon peak (3-6 pm), and off-peak hours. The hourly traffic volume, together with the emission factors, was used to obtain the emission rates in grams per mile. Diesel traffic was distributed hourly based on the hourly profile (Table 4.13) from a truck traffic count of the Long Beach Freeway (CARB 1998) because similar data is not available for San Diego.

Table 4.13 – Hourly Truck Traffic Profile (CARB 1998)

Hour	Profile	Hour	Profile	Hour	Profile
1 am	.10	9	.88	5	.40
2	.09	10	.85	6	.26
3	.11	11	1.0	7	.27
4	.18	noon	.80	8	.18
5	.29	1 pm	.89	9	.12
6	.39	2	.82	10	.10
7	.58	3	.82	11	.08
8	.80	4	.70	midnight	.07

The profile is for freeway truck traffic observed on the Long Beach Freeway one mile north of the San Diego Freeway interchange. The data were gathered on December 7-8, 1993. The peak one hour truck traffic count was 2280 trucks/hour.

TOG Emissions

TOG emission factors obtained from EMFAC are a function of

- vehicle class;
- relative humidity;
- temperature; and
- speed.

The composite emission factors are based on the default fleet for San Diego County. Monthly average relative humidity and ambient temperatures for each hour of the 24-hour day were used to estimate TOG emission factors from EMFAC. For convenience, only the annual average values of relative humidity and temperature are presented in Table 4.14. The vehicle speed and traffic loading were obtained from DTIM4 for the morning peak (6-9 am), afternoon peak (3-6 pm), and off-peak hours.

Table 4.14 – Annual Average Hourly Relative Humidity and Temperature (C) – San Diego

Hour	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
RH %	73	73	74	74	74	73	73	71	67	63	60	57	56	56	57	58	60	63	67	69	71	72	72	73
T (C)	16	16	16	16	16	15	15	16	17	18	19	20	21	21	21	20	20	19	18	18	18	17	17	17

TOG emissions were summarized with the Impact Rate Summary module from Caltrans' DTIM4. TOG speciation profiles for non-catalyst and catalyst gasoline fueled vehicles are used to obtain emission factors for TACs from VOCs. The speciation profiles applied to resolve individual pollutants are shown in Table 4.15. These profiles are part of ARB's organic gas speciation data. These profiles are available at the following ARB web site:

<http://www.arb.ca.gov/ei/speciate/speciate.htm>

Table 4.15 – Weight Fractions of TOG for Specified Organic Chemicals (1999)

Pollutant	Non-Cat. Stabilized (Profile ID 401)	Catalyst Stabilized (Profile ID 438)
Formaldehyde	0.0312	0.0173
Acetaldehyde	0.0075	0.0025
1,3-butadiene	0.0083	0.0056
Benzene	0.0344	0.0268
Styrene	0.0013	0.0013
Toluene	0.0679	0.0599
Xylenes	0.0600	0.0499
Acrolein	0.0018	0.0014
MTBE	0.0186	0.0198
Profiles available at: http://www.arb.ca.gov/ei/speciate/speciate.htm .		

A composite emission factor for gasoline vehicles and diesel fueled vehicles is estimated for each hour of the day and for each link for direct input to the CAL3QHCR air quality model. The CAL3QHCR model is a roadway model that accepts hourly meteorological data for a full year to estimate annual average concentrations.

Off-Road and Area-Wide Sources

Off-road emissions include sources such as:

- ships;
- trains;
- airports;
- forklifts;
- cranes;
- off-road vehicles; and
- portable engines.

For this project, only certain selected off-road sources (i.e., ships, trains, commercial aircraft, and military aircraft) are included for micro-scale modeling. The remaining sources for off-road emissions are included in the regional modeling.

The selected off-road emissions were obtained directly from CEIDARS and were spatially allocated using information obtained from the SDAPCD. The Port of San Diego marine logs were used to spatially allocate shipping emissions to each of three berthing locations and transit lines. ARB's speciation profiles were used to speciate emissions generated by each category. Diesel PM emissions were not speciated but instead quantified as total PM₁₀.

Smaller sources of diesel PM emissions such as on-road and off-road mobile sources operating at facilities were not included for the micro-scale inventory because of their portability and lack of data to spatially allocate these emissions. Rather, these emissions were included in the regional inventory. Sources of these types include:

- portable engines,
- truck idling and running emissions on-site,
- forklifts, and
- transportation refrigeration units.

2) Special Micro-Scale Model Input Preparation

In some cases, additional decisions, analyses, or processing was required in order to produce micro-scale model emission inputs. The following paragraphs provide specific details of such instances.

CEIDARS Sources

Stationary sources that are in the CEIDARS database include UTM coordinates and stack conditions of the release parameters. When available, the Health Risk Assessments on-file from the facilities were reviewed to improve the data available from CEIDARS. A few of the UTM coordinates did not represent the stack locations and were corrected.

Area Sources

ArcView GIS software is used to geo-locate area sources that are included as stationary sources based upon the street address. Data obtained from the site surveys are used to set the facility back from the street. The facility locations were verified for those facilities with higher risk estimates. Two facilities were relocated from the GIS-derived coordinates to a more representative UTM coordinate. Release parameters for the area sources were estimated based upon the site surveys.

Railroad Emissions

The San Diego County APCD indicated that the switchyard does not have switching activities. Therefore, only line haul emissions are allocated to the rail line. The diesel exhaust emissions for the rail line are 5,621 lbs/yr. Emissions are simulated as a series of volume sources.

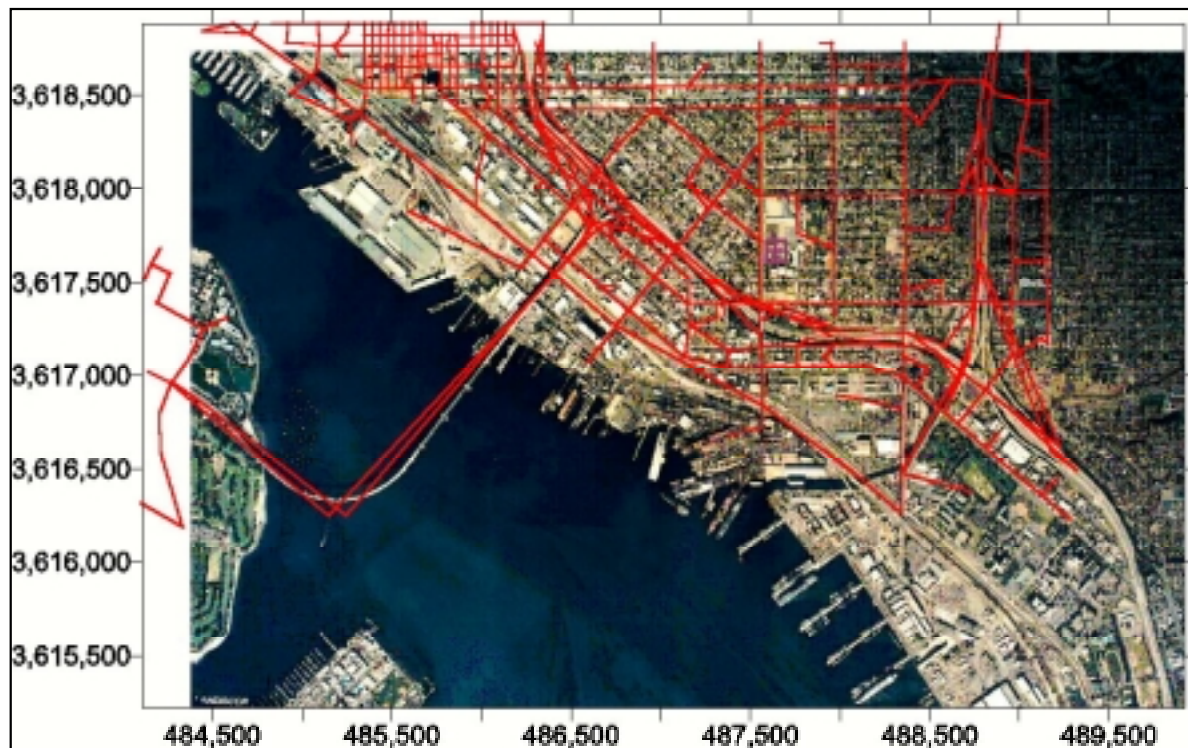
Coronado Bridge Emissions

Diesel PM emissions from Coronado Bridge initially were included with the CAL3QHCR analysis. Due to the significant impact of diesel PM impacts, the emissions from the bridge were modeled with ISCST3 instead as a series of volume sources. The bridge maximum clearance is 217 feet (66.1 meters). Diesel PM emissions from the bridge were placed at this height for the crest and gradually decreasing heights to ground level at the bridge on and off ramps for ISCST3. TOG emissions from Coronado Bridge remain in the CAL3QHCR analysis and are placed at ten meters above ground level. Ten meters is the upper limit for CAL3QHCR inputs.

Motor Vehicle Emissions

The motor vehicle emission sources were modeled as line sources. Figure 4.4 shows the modeled roadway links superimposed on an aerial photograph of Barrio Logan. These are the links used to simulate emissions from the roadways in the CAL3QHCR model.

Figure 4.4 - Roadway Links in Barrio Logan



Airport Emissions

The airport emissions from two nearby airports were included in the micro-scale inventory for Barrio Logan modeling. The two airports are Lindbergh Field (commercial airport) and North Island. Airport emissions were allocated to four emission modes: approach, climb out, takeoff, and taxi/idle. In addition, emissions from the auxiliary power units (APU) were assigned at the gate only.

The FAA defines LTO as an aircraft's landing and takeoff (LTO) cycle. One aircraft LTO is equivalent to two aircraft operations (one landing and one takeoff). The standard LTO cycle begins when the aircraft crosses into the mixing zone as it approaches the airport on its descent from cruising altitude, lands, and taxis to the gate. The cycle continues as the aircraft taxis back out to the runway for takeoff and climb out, and heads out of the mixing zone and back up to cruising altitude. The five specific

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operating modes in a standard LTO are: approach, taxi/idle-in, taxi/idle-out, takeoff, and climb out. Most aircraft go through this sequence during a complete standard operating cycle (FAA 1997a).

For the purpose of allocating aircraft emissions, we distinguish four areas where emissions are released. These locations are: approach, taxi and idle, take off, and climb out. In addition, emissions from the APU's are released from the gate only. Emissions from the taxi/idle modes are uniformly distributed along the taxiways to the gate.

Emissions from the approach and take off are treated somewhat differently. The FAA recommends the use of the Emission Dispersion Modeling System (EDMS) for modeling emissions from airports. The EDMS is based on the standard Gaussian plume equation in many of EPA air dispersion models. This is the same formulation as used in the ISCST3 and AERMOD.

The EDMS omits the emissions from the approach and climb out in the dispersion calculations. We include these emissions in our analysis. The approach is defined as the zone where the aircraft enters the mixing zone. The climb out is defined as the zone up to where the aircraft exits the mixing zone. As a default, the EDMS uses a mixing zone height of 3,000 feet when the mixing zone is unknown (FAA 1997b).

According to AirNav.com, the approach angle for Lindbergh Field in San Diego is 3.5 degrees. With this type of approach angle and a mixing zone of 3,000 feet, we can calculate the horizontal distance over which emissions from the approach can be distributed, 14.95 kilometers. We also assume the climb out angle from Lindbergh Field is 3.5 degrees for lack of data. In addition we assume the approach and climb out at North Island are similar to the approach and climb out at Lindbergh Field.

We use the approach of simulating the aircraft emissions in the various modes as a series of volume sources. This approach is an approximation to a line source, however, given the relatively large distances from the aircraft emissions to the Barrio Logan receptors, this approximation should result in negligible differences on the concentrations calculated at Barrio Logan receptors.

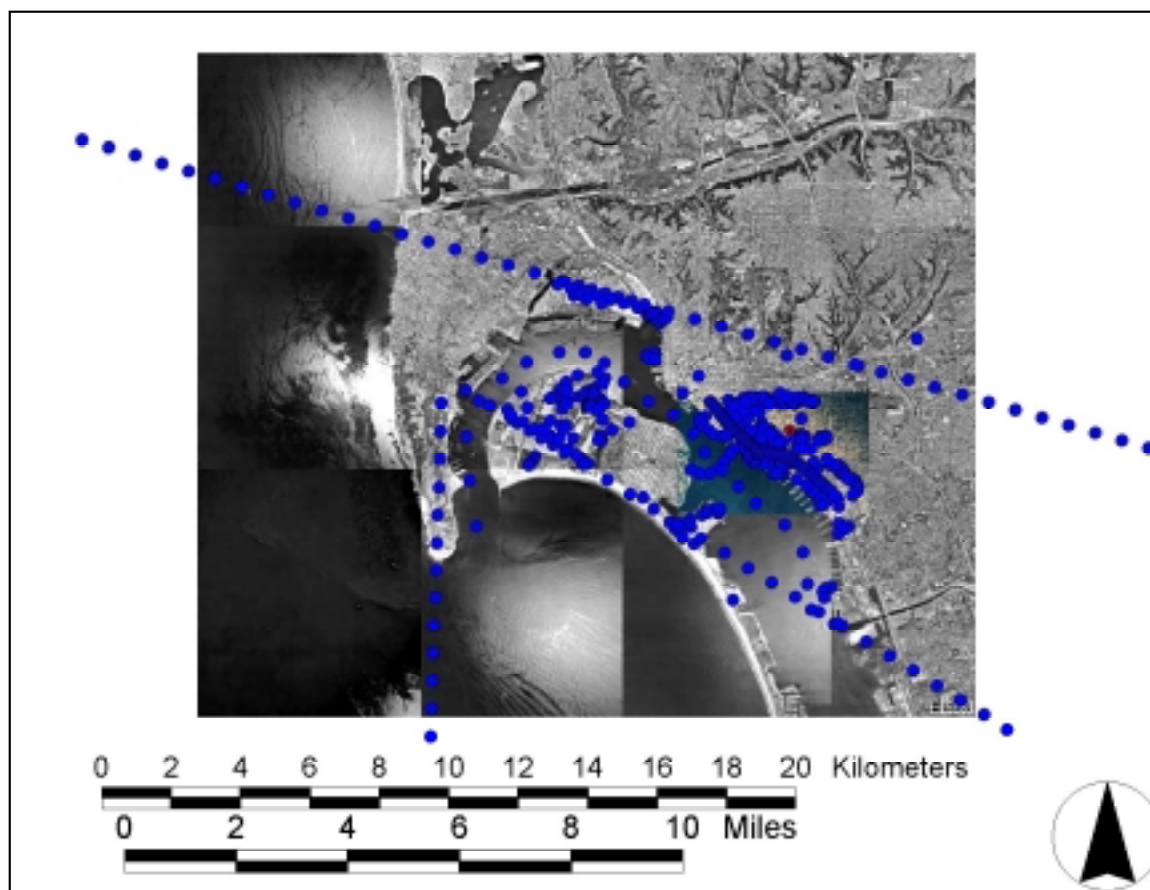
The volume source calculations from the aircraft emissions require initial dispersion for the Gaussian plume in the vertical and the horizontal. The initial dispersion in the horizontal (σ_y) is estimated as $W/2.15$ per the guidelines. For approach, taxi, and climb out modes, we assume W to be the distance between volume source releases. For idle emission modes such as at the gate, we assume W to be 30 meters.

The initial dispersion in the vertical (σ_z) is estimated as $H/2.15$ for surface modes and as $H/4.13$ for elevated release modes. We assume H is 15 meters for surface modes such as taxi and idle. For elevated modes such as approach and climb out, we assume H is 40 meters.

Normally we assume the flight path for the approach and the climb out from the airports are in line with the airstrip. However, it was pointed out to us that the climb out path of aircraft from North Island changes course to a due south direction (San Diego County APCD in a meeting at the ARB).

Figure 4.5 is a satellite view of San Diego. In this figure, the Lindbergh Field and North Island air traffic is shown as a series of dots. The approach and climb out shown in this two-dimensional figure actually have a height representing the approach and climb out paths. The shipping lane and Memorial Academy are also visible in the figure. All together, 660 point and volume sources are used to simulate all micro-scale emission sources in Barrio Logan.

Figure 4.5 - Satellite View of San Diego



3) Findings

As discussed in this chapter, both regional photochemical models and micro-scale dispersion models require inputs that properly characterize emissions and meteorology. To ensure this, the development of a complete and accurate emission inventory is

MODELING EMISSION INVENTORY DEVELOPMENT

essential. Findings from this project include the importance of source locations, the development of micro-scale inventories, and the uncertainties of emission inventories. It is important in both regional and micro-scale inventories that the physical location of emission sources are determined as accurately as possible. This is to guard against allocating emissions to the wrong grid cell.

The development of micro-scale emission inventories requires supplementing the regional inventory with more detailed information than is typically collected to support regional air quality modeling. The micro-scale inventory developed for Barrio Logan provided us with additional information that was not available in CEIDARS. With few exceptions, these additional facilities did not greatly contribute to the emission inventory; the regional inventory derived from the CEIDARS database was sufficient to capture most air pollutants from stationary sources located in the Barrio Logan community. Although, in this case the additional emissions did not make a large contribution to the overall inventory, this might not be true in other communities. Therefore, we need to keep in mind that emissions from large point sources alone may not be adequate for neighborhood local-scale assessments. An example of this is when the emissions of toxic air pollutants from small facilities are modeled, local areas of elevated exposures and associated health risks may result if the facilities are co-located in proximity to a sensitive receptor. These areas would remain undetected in the absence of a micro-scale analysis.

Emission inventories for both regional and micro-scale are based on various assumptions, specific to each category, which create various levels of uncertainty. We have based our work on the best information available and expect the methodology to change as we continue our work to develop neighborhood assessment tools.

MODELING EMISSION INVENTORY DEVELOPMENT

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CHAPTER 5 - MODELING RESULTS FOR BARRIO LOGAN

This chapter describes how specific micro-scale and regional models in Barrio Logan perform. Two types of air quality models were exercised to simulate the concentrations measured during the air monitoring studies described in Chapter 2. Micro-scale dispersion models were used to simulate the proportion of pollutant concentrations dispersed within the neighborhood from sources located inside the neighborhood. Regional models were used to simulate the general background portion of pollutant concentrations transported from sources outside of the neighborhood or produced through photochemical reactions.

An essential part of this analysis is an assessment of the adequacy of inputs, input data collection methods, and model performance metrics. This includes emission estimates and meteorological inputs to the models as well as the collection and use of representative, neighborhood scale ambient air quality measurements, against which the models' simulated concentrations, will be compared. Initially, for practical reasons, some inputs and input collection methods will come from readily available sources while other inputs will come from special data collection efforts. As a result, the input data often represents different years of record. However, we have assumed that the year of record variability has a minimal impact on annual modeling estimates, due in part to the long averaging time.

Table 5.1 provides a summary of the input data and year of record utilized for the Barrio Logan modeling analysis.

Table 5.1– Summary of Data and Year of Record Used for Barrio Logan Modeling Analysis

Data	Regional Model	Micro-scale Model
Meteorological Data	1998	11/99 – 10/00
Emissions Inventory Data	1997 (SCOS)	1999 motor vehicle ^a , 2000 other
Ambient Data ^b	1999-2000	1999-2000
Tracer Studies	2001	2001
a. EMFAC 2000 (2.02)		
b. Regular network and Memorial Academy ambient air data used		

We begin with a description of the micro-scale modeling because it is specific to Barrio Logan, and we wanted to first understand the impact of sources within the community. As we found out in the course of this study, the regional contribution turned out to be

significant. The details of the Barrio Logan micro-scale and regional modeling analyses are presented in subsequent sections of this chapter.

A) Micro-Scale Dispersion Modeling

This section presents the results from the application of the ISCST3 and CAL3QHCR micro-scale models in Barrio Logan. ISCST3 is used for the point sources and CAL3QHCR is used for the motor vehicle line sources. The motor vehicle inventory is for 1999 base year emissions. The point source inventory is based on the latest available data as discussed in Chapter 4. The meteorological data are obtained at Memorial Academy for November 1999 through October 2000.

1) Modeling Domain

The micro-scale modeling domain extent spans a 15 km x 15 km area as shown by the box in Figure 5.1. The domain includes most of the San Diego area with the downtown area near the center. A nested domain of receptors (70 x 50 grids) with 50 m grid spacing is 3.5 km x 2.5 km and is shown in Figure 5.2.

Figure 5.1 - Micro-scale Modeling Domain and Receptor Field

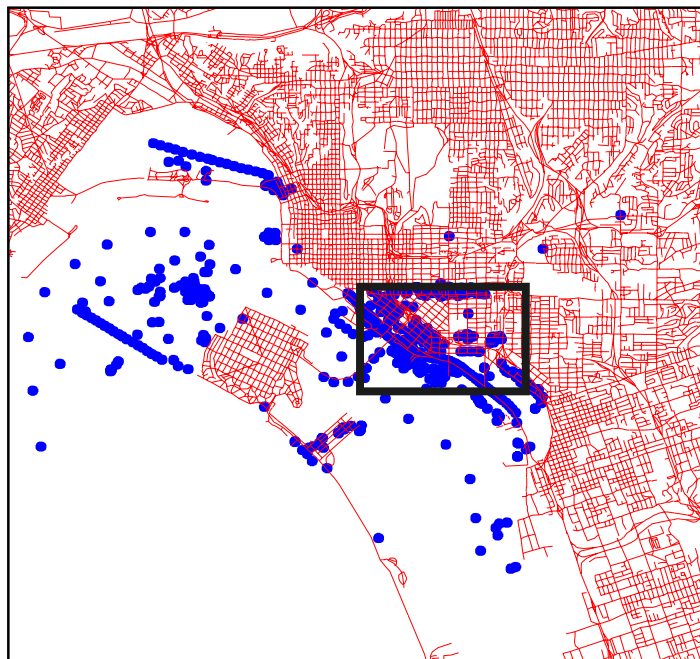
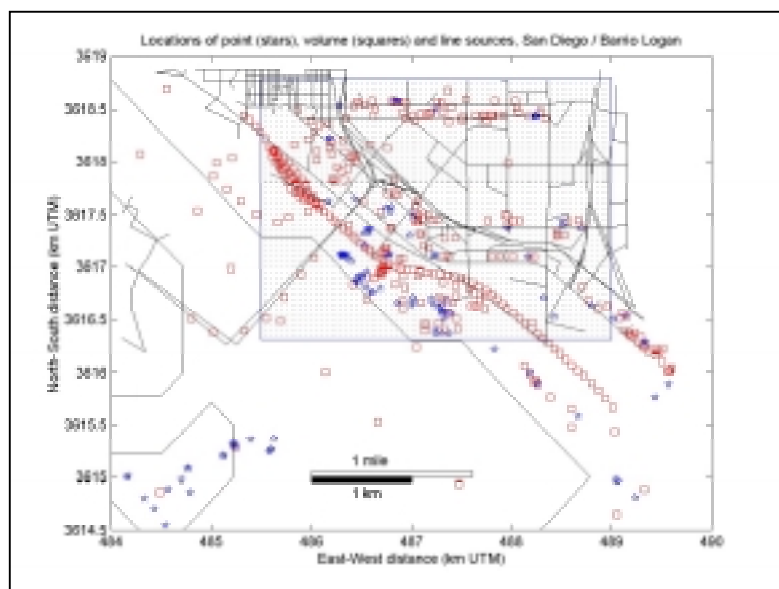


Figure 5.2 - Micro-scale Nested Modeling Domain – Receptor Field

2) Micro-Scale Modeling Input Data

Meteorology

Micro-scale models require hourly meteorological observations, and representative on-site observations are preferred. For this project, meteorological data for ISCST3 dispersion modeling were constructed from both on-site and nearby representative meteorological observational data from the nearest National Weather Service (NWS) stations.

Figure 5.3 shows the location of Memorial Academy Charter School where on-site surface meteorological measurements were collected. This was the primary site for meteorological data in this study. Hourly wind speed, wind direction, temperature, and relative humidity collected at this location were processed for the period of November 1, 1999 - October 31, 2000. These on-site surface meteorological observations were supplemented with meteorological data obtained from the NWS stations at Lindbergh Field International Airport and Miramar Naval Air Station. These data were processed in accordance with U.S. EPA recommendations to estimate atmospheric stability (US-EPA, 1996). A constant value of 500 m was used as default for urban and rural mixing heights in the ISCST3 meteorological input file.

Figure 5.3– Locations of Surface Observations

Figure 5.4 shows a wind rose for the meteorological conditions at Memorial Academy Charter School. Wind roses are used to summarize a period of meteorological data using bars plotted on a compass. The direction of each bar represents the direction from which wind is measured during a time period, while the size of the bar represents the frequency that wind blows from the associated direction. The onshore breezes at Memorial Academy Charter School are evident from the west and southwest, and the drainage flows are from the northeast.

Wind directions at the other stations used in this study differ from those at Memorial Academy Charter School. At Lindbergh and Miramar, the onshore breezes are from the northwest and drainage from the east.

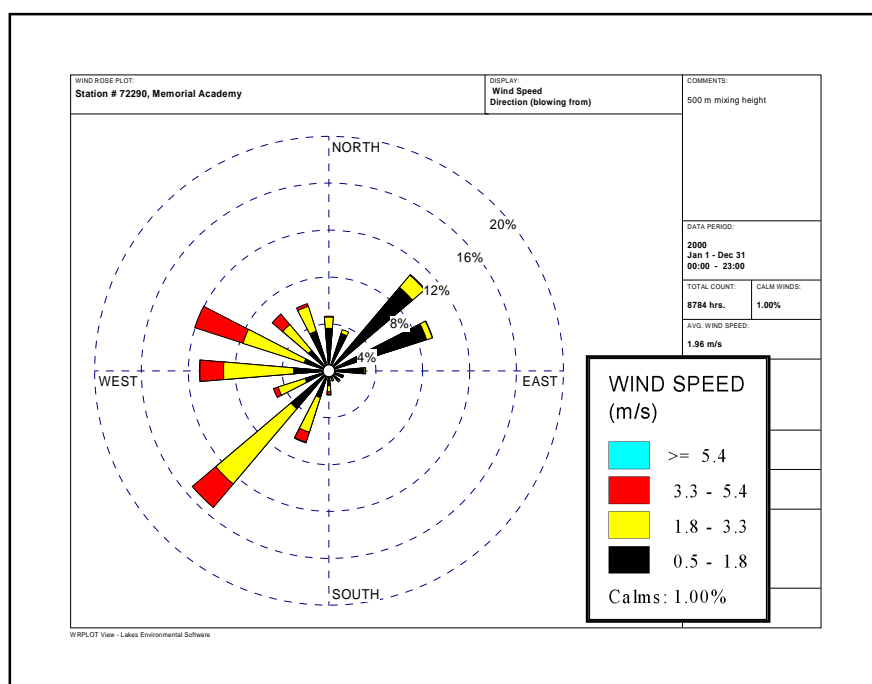
Figure 5.4 – Memorial Academy Wind Rose

Table 5.2 shows a summary of the surface station observations used in this study. Although the mean wind speed is lower at Memorial Academy Charter School than at Lindbergh or Miramar, there could be multiple reasons for this difference such as site elevation, anemometer height, upwind fetch of anemometer, and general surface roughness differences.

Table 5.2 - Meteorological Surface Station Summary

Station	Latitude	Longitude	Elevation (ft)	Anemometer Height (m)	Period of Observations	Mean Wind Speed (m/s)	% of Calms
Memorial Academy	32.6983	-117.1322	26	7.3	2000 ^b	1.96	1.00%
Lindbergh Field	32.7335	-117.1896	14	10 ^a	1984-1988	3.59	7.25%
Miramar Naval Air Station	32.8683	-117.1425	478	10 ^a	1967-1971	2.80	16.90%

a) 10 m sensor height assumed.
b) The actual period of observation is November 1, 1999 through October 31, 2000.

Ideally five years of consecutive meteorological data are desired when evaluating the downwind dispersion of pollutants with models such as ISCST3 (U.S. EPA 2003). The purpose of this is to minimize year-to-year variability in model predictions. At Memorial Academy Charter School, we only have data for one year and cannot ascertain whether this year is more or less dispersive than an average year.

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Of note is that there are a higher percentage of nighttime stable conditions for Memorial Academy Charter School data compared to Lindbergh and Miramar. This may be a minor issue, since the diurnal emission patterns in Barrio Logan show that most emissions are released during daytime conditions¹.

The San Diego County APCD commissioned a special report to evaluate the influence of the marine layer on the use of rural and urban dispersion coefficients (Wagner, 1996). This is relevant because the ISCST3 air dispersion model simulates the magnitude of dispersion based on whether rural or urban dispersion coefficients are selected. The report recommends one of two options to best simulate dispersion in San Diego coastal environments with the ISCST3 air dispersion model. The first option is to reclassify the urban dispersion coefficients two steps more stable than would be estimated using standard U.S. EPA practices. This method would reclassify C stability to E stability, for example. The second option is to use rural dispersion coefficients in urban areas of San Diego along the coast. Additionally, the report supports the use of dispersion models that do not require the use of rural and urban dispersion coefficients. AERMOD is a model that does this. However, we only performed some preliminary testing of AERMOD in Barrio Logan.

For our evaluation, we chose to use ISCST3 with urban dispersion coefficients. The meteorological data processed for Memorial Academy Charter School resulted in higher stability conditions than what would be normally used from Lindbergh Field. Memorial Academy Charter School shows twice as many hours of F stability as Lindbergh. In addition, Memorial Academy Charter School shows less than half the hours of neutral D stability than Lindbergh Field. This tendency of higher stability conditions for the Memorial Academy Charter School data compared to the Lindbergh data show that using ISCST3 with urban dispersion coefficients and Memorial Academy Charter School data is similar to the recommendations of the Wagner report.

Emissions

Chapter 4, titled "Modeling Emission Inventory Development," provides a detailed account of the modeling emissions inventory development for both regional and micro-scale modeling.

3) Approaches to Assessing Model Performance

The performance of the micro-scale models was evaluated using tracer gas studies performed in Barrio Logan and UC Riverside. Tracer gas data were obtained when a

¹ Stability is a measure of the degree to which the atmosphere resists turbulence and vertical motion and it changes throughout the day. Micro-scale models use classifications of stability as an input to calculating pollutant dispersion, where stability category A represents the least stable hourly conditions and E the most stable conditions.

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known amount of SF₆ was released from the NASSCO facility in Barrio Logan and at the UC Riverside location for very near field applications. The models' ability to simulate the observed distribution of tracer gas concentrations was assessed (i.e., model performance) using the meteorological data and tracer gas emission release parameters collected at the same time as the field observations.

Our understanding of dispersion in urban areas is limited because of the relative paucity of experimental tracer data that has been collected in urban environments. One of the first urban experiments, the St. Louis Dispersion Study (McElroy et. al., 1968) was carried out from 1963 to 1965. The data from this experiment was used to construct the urban dispersion curves incorporated in regulatory models such as ISC. However, the St. Louis experiment did not include the turbulence measurements needed in the new generation of dispersion models. In 1978 and 1979, an experiment was conducted in Copenhagen, Denmark (Gryning and Lyck, 1984) to study dispersion of elevated releases over urban areas. However, because these experiments were limited by the lack of instrumentation to measure vertical profiles of micrometeorology and concentrations, the associated data sets cannot be readily used to evaluate models that reflect current understanding of the relationship between dispersion and urban meteorology. Several recent experiments conducted in Europe and the United States (Allwine et. al, 2002; Britter and Hanna, 2003) have attempted to overcome these problems with past experiments, but the associated data were not available at the time of this study.

Given the lack of urban datasets at the time, several special tracer studies were conducted under ARB guidance that specifically support the urban, neighborhood-scale NAP analyses. These studies are detailed below. In general, the findings of these studies are that regulatory dispersion models tend to over predict concentrations in the near field and under predict concentrations far away from emission sources. Credible near-source concentration estimates depend on accurate characterization of emissions, on-site micrometeorology, and a method to account for lateral meandering in the near-field.

Barrio Logan Tracer Experiment

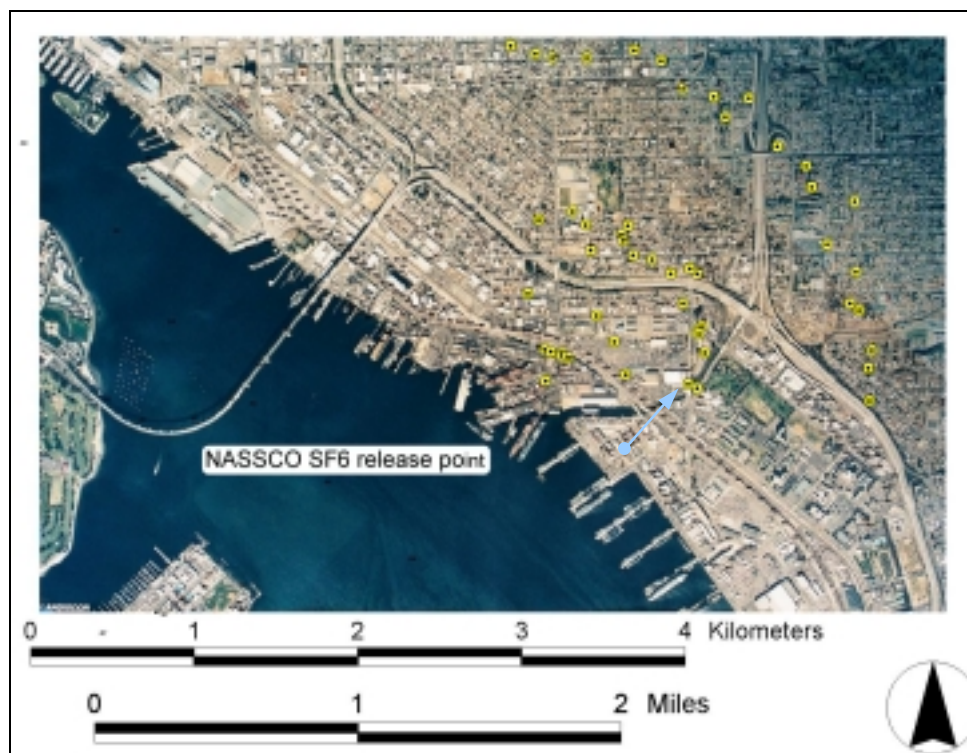
In 2001, we conducted two tracer studies – one in the summer and a second during the winter months. The experiment was conducted in 2001 by researchers from University of California, Riverside (Venkatram, 2004). In both studies, community members participated by allowing monitors in their yards.

The Barrio Logan field experiment is similar to the St. Louis study in that it focuses on near surface releases. It was designed to examine the impact of near surface releases on receptors within 5 km from the source. While some of the results from the St. Louis study are applicable to Barrio Logan, they are not compatible with currently used dispersion models, such as AERMOD, which are based on understanding developed after the 1960s time period of the St. Louis experiment.

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The experiment conducted in Barrio Logan included both surface and upper level time resolved measurements to characterize the mean and turbulent structure of the atmospheric boundary layer up to a height of 200 m. The study site, Barrio Logan, is located on the San Diego shoreline, where most of the industry is located. The predominant wind direction is SW, which brings emissions from the industrial area into the residential area located downwind to the NW. The summer experiment involved releasing the tracer gas for five days in August of 2001 and the winter experiment released the tracer gas for four days in December of 2001. The tracer, SF₆, was released at a height of 5 m from the NASSCO shipyard on the shoreline, and the concentrations of the tracer were sampled on 4 arcs at 200 m, 500 m, 1000 m, and 2000 m from the source during ten hours of the day starting at 10 am. The sampler network was designed to delineate the major features of the plume at the 1000 m and 2000 m arcs, each of which contained 21 samplers; 4 samplers were placed on the 200 m and 500 m arcs. High-resolution measurements from mobile monitoring were used to supplement the measurements from the stationary samplers. Figure 5.5 shows the locations of the bag samplers for the summer experiment.

Figure 5.5 - Barrio Logan Tracer Study Sampling Sites



The tracer study evaluated the performance of three models: a simplified dispersion model designed for the data analysis that was developed under the tracer study contract (UCR Model), a specialized U.S. EPA version of AERMOD that is designed for near-source application (AERMOD-PRIME), and ISCST3. The summer tracer study is more conclusive than the winter study.

The wind fields during the winter tracer study were complex. The winter tracer study had some limitations because of the direction the mean wind flow and the source-receptor configuration made it difficult to sample the tracer release concentrations. In general, for the winter tracer study, all three models did not perform well and there was a general bias towards under-prediction. However this under-prediction may be due to the complex wind field and inability to represent the wind fields with the simple models.

The database for the summer tracer experiment was better suited for model performance evaluations than the database for the winter experiment. The summer model simulations resulted in over-prediction of maximum observations, while the winter simulations were essentially inconclusive. Therefore, we cannot be certain whether there was a bias in the annual average calculations. In addition, the AERMOD results may be an improvement over the ISCST3 results provided that additional site-specific turbulence parameters are collected.

The summer Barrio Logan experiment resulted in about 50 hours of data. These were initially analyzed using a simplified dispersion model designed for this analysis. A similar approach was used in the analysis of data from field data collected in Salt Lake City and Los Angeles (Hanna, 2003). The ability of the model to explain the spatial distribution of the observed concentration was measured through the conventional r^2 and the ratio of the means of the highest 10 modeled values to the highest 10 observed values. Focusing on the highest values helped to avoid averaging uncertain modeled and observed values in the lower tail of the distribution; the low values were likely to be affected by small uncertainties in the plume position relative to the receptors. The model overestimated the maximum concentrations by close to a factor of 2. The model captured the spatial distribution of the observed concentrations during most of the day, but overestimated the ground-level concentrations by a factor of 2.5. This tendency to overestimate the concentrations suggests that the modeled vertical plume spread might be too small. This simple model (UCR Model) provided maximum concentration estimates that on an average were within a factor of two of the observed values during all the field study days.

The results obtained in this study imply that measurements of turbulence and mean flow in the boundary layer above the roughness sub-layer are essential to estimating ground-level concentrations in an urban area. This poses problems for the development of a practical dispersion model, because the meteorology of the boundary layer is not readily available.

It might be possible to adjust measurements made in the roughness sub-layer (in our case 0 – 5 m) to obtain average boundary layer parameters relevant to dispersion. If velocity ratios between the boundary layer and roughness sub-layer do not vary substantially in the horizontal, it might be possible to use appropriately adjusted roughness sub-layer parameters in a practical model for dispersion in the urban boundary layer. However, measurements made within the roughness sub-layer require careful siting to minimize local building effects.

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The analysis of data from the Barrio Logan experiment indicates that it is possible to obtain "average" relationships for the plume spread: $\sigma_y = \sigma_z = 0.2x$. These equations are tentative because more definitive conclusions require a careful examination of the relationships among meteorological variables. Even if they are proven to be valid, they only summarize the observations made during the 5 days of the experiment. We need to be cautious about recommending their application to other sites and meteorological conditions different from those of this field study. However, such relationships are valuable even if they are site specific because they allow useful estimates of concentrations at the site of concern using a minimum number of meteorological inputs. These inputs, in turn, could be either measured or obtained from a model that relates rural boundary layer variables to corresponding urban values using morphology as inputs.

The following is a summary of findings from the Barrio Logan tracer experiment:

- For the summer study, the UCR model outperforms both AERMOD and ISCST3. AERMOD shows better performance than ISCST3. Of particular note is that AERMOD requires additional meteorological inputs above those traditionally available (i.e., on-site turbulence). There is a need to develop a method to obtain AERMOD data using existing measurements. It may be possible to estimate these from prognostic meteorological model results. The AERMIC Committee, the developers of AERMOD, is aware of this and is working on it.
- For the summer study, the models perform well for two days of the experiment. On the other three days, the models overestimate the maximum values of concentrations by more than a factor of two.
- For the winter study, none of the models provided an adequate description of the spatial patterns of observed concentrations because of the complex meteorology during the winter experiments.
- For the winter study, however, the models were able to estimate the magnitude of observed concentrations by using site-specific observations of turbulence and mean winds.

Near Field Tracer Studies

Dispersion models are not designed for estimating concentrations very near a source of toxic air pollutants (e.g., within ten meters). However, this scale is especially important for assessing the risk posed by sources in urban areas such as gasoline stations and dry cleaners, where human receptors may be located within meters from the sources.

In principle, several models, such as AERMOD-PRIME, are applicable to such sources because they are designed to treat the effects of buildings on near source dispersion.

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The near source dispersion component of these models, PRIME (Plume Rise Model Enhancement, Schulman et al., 2000), has been evaluated primarily with data from experiments involving isolated buildings. These models have not been tested with data relevant to dispersion from small sources located in the midst of buildings. Although the models allow a user to simulate dispersion as close as one meter from a source, the dispersion in this near field is an extrapolation of the original data obtained 50 meters away and beyond.

To study the effects of near field impacts, the ARB and UC Riverside CE-CERT conducted a near-field dispersion modeling study using two case studies:

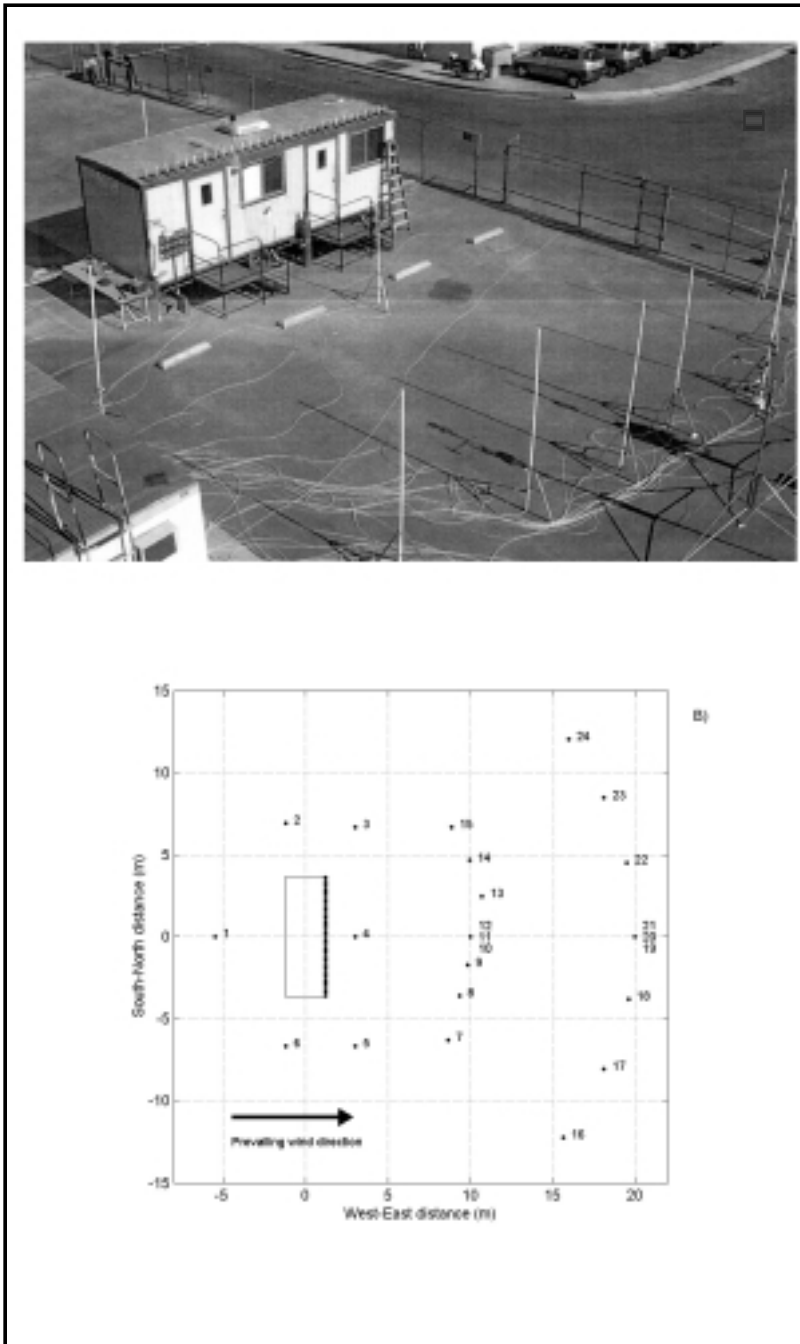
1. Near-field tracer study conducted at UCR CE-CERT. The results from the CE-CERT tracer study suggest that dispersion models commonly used for regulatory applications generally underestimate the lower range of pollutant concentrations and overestimate high pollutant concentrations in the near-field. This problem can be corrected by accounting for wind direction meandering in the vicinity of a source.
2. Barrio Logan Special Hexavalent Chromium Monitoring Study. This study indicates that credible near-source concentration estimates using ISC depend on accurate characterization of emissions, on-site micrometeorology, and a method to account for lateral meandering in the near-field.

Detailed summaries of these two studies are below.

Near-Field Tracer Study at UCR CE-CERT

This tracer experiment was conducted at a parking lot of the University of California, Riverside, CE-CERT facility (Isakov, 2004). During the experiment, SF₆ was released at ambient temperature from the top of a trailer situated in a parking lot surrounded by buildings. The height of release was 3.2 m. Figure 5.6 shows the experimental design (upper panel) and locations of sources and receptors (lower panel).

The results from the CE-CERT tracer study suggest that dispersion models commonly used for regulatory applications generally underestimate the lower range of pollutant concentrations and overestimate high pollutant concentrations in the near-field. This problem can be corrected by accounting for wind direction meandering in the vicinity of a source. Formulating the dispersion model using a polar coordinate system, as suggested by Hanna (2003), facilitates the use of large direction fluctuations that can transport material to receptors that would be considered upwind in a Cartesian coordinate system. This formulation is important because low winds and hence large wind direction meandering are common in the urban canopy. Estimating near source concentrations requires modeling dispersion when the vertical plume spread is smaller than the average building height.

Figure 5.6 - CE-CERT Tracer Experiment: 06/11/01 – 06/28/01

An algorithm that accounts for upwind meandering has already been integrated into AERMOD. However, our analysis indicates that the PRIME algorithm, which is used to calculate dispersion in the wake cavity, neglects upwind meandering and overestimates pollutant concentrations in the near-field. These concentration estimates might be improved by combining upwind meandering with the PRIME algorithm in AERMOD.

These conclusions apply to non-buoyant releases such as that used in the tracer study. Because PRIME was designed for buoyant power plant releases, it might not overestimate concentrations when buoyancy allows the plume to “escape” dispersion in the near field. However, small sources in urban areas are likely to be non-buoyant. For such sources, the model improvements suggested here are clearly applicable.

Although AERMOD has undergone extensive evaluation with close to 20 datasets (Paine et al, 1998), the CE-CERT tracer study is the first in which the meandering component of the model has been tested. This study demonstrates that AERMOD can provide reliable near-field concentration estimates from urban emission sources if turbulent velocity estimates close to a source are used to estimate plume dispersion. Turbulent velocity estimates may be obtained using sonic anemometers, which can be operated at relatively low cost. However, detailed on-site meteorological estimates may not be available in all cases. Future research should examine the relationship between urban morphology and meteorological parameters within the urban canopy.

Special Hexavalent Chromium Field Study – Micro-scale Modeling

Another example of the application of dispersion models to estimate near-field pollutant concentrations was a modeling assessment during the Barrio Logan Special Hexavalent Chromium Monitoring Study. The ISCST3 model was evaluated with hexavalent chromium measurements collected within 100 meters of two hexavalent chromium plating facilities in Barrio Logan, San Diego (Isakov, 2003).

Results of the modeling and the ambient air quality study (discussed in Chapter 2) indicated that the dominant contributor of hexavalent chromium to pollutant concentrations was a decorative hexavalent chromium-plater in the community. The initial analysis consisted of running ISCST3 with emission estimates calculated from emission factors and activity data. The results were not in agreement with observed values. This indicates one or all of the following: a) uncertainties in the model’s formulation; b) inaccuracy of the emission factor and/or activity levels; c) presence of an unaccounted source; and d) uncertainties in the ambient measurements.

ISCST3 was run again using measured indoor concentrations as they exit the chrome plating facility as an estimate of emissions and the results were within a factor of two of the observed downwind concentrations at the upper end of the observed values. Because CARB staff conducted on-site surveys of all surrounding potential emissions sources during the period of high ambient hexavalent chromium measurements and identified no other sources that had significant contribution during the study period, we felt confident that the decorative chrome plater was the source of the hexavalent chromium emissions. The performance of the ISCST3 model in explaining observations suggests that the model’s treatment of dispersion is reasonable

when the plume is moving directly from the source to the receptor, and the emissions inputs accurately represent both the magnitude and the conditions of the release. However, ISCST3, like other plume models, cannot model transport associated with the complex flows next to buildings. These complex flows can transport plume material to receptors that are upwind in relation to the time averaged wind direction. For convenience, we will refer to this phenomenon as meandering.

ISCST3 model results have been compared with and without application of the “meandering” dispersion mechanism using the Barrio Logan Special Hexavalent Chromium Monitoring Study as a test case. Because turbulence measurements were not taken during this study, turbulent velocities were estimated using the empirical relationship between the turbulent velocities and the wind speed measured during the CE-CERT tracer experiment. Statistical analysis of these results demonstrated the application of the “meandering” mechanism reduced mean bias from 0.09 [ng/m³] to 0.02 [ng/m³], even when using an empirical relationship to estimate turbulent velocities.

This study found that incorporating lateral “meandering” for non-buoyant urban plumes in Gaussian dispersion models could improve concentration estimates even when downwash is not considered. Incorporating a meandering component in ISCST3 resulted in improvements in estimating hexavalent chromium concentrations in Barrio Logan. Credible near-source concentration estimates depend on accurate characterization of emissions, on-site micrometeorology, and a method to account for lateral meandering in the near-field.

NASSCO Uncertainty Analysis

To evaluate the impact of the uncertainty in emissions on micro-scale model performance, we conducted uncertainty analyses on hexavalent chromium emissions generated by welding operations at National Steel Shipbuilding Company (NASSCO). This involves analyzing sources of variability and uncertainty in the models and determining how those various sources affect confidence in the simulation results. Variability refers to the temporal, spatial, or inter-individual differences in the value of an input (Cullen and Frey, 1999). Uncertainty refers to the lack of knowledge or information about an unknown quantity whose true value could be established if a perfect measurement device were available (Cullen and Frey, 1999).

Both variability and uncertainty affect Gaussian modeling results. Variability in Gaussian model results is present primarily through meteorology and emission rates, because weather conditions and processing rates vary over time. Uncertainty in Gaussian models can be categorized into three components: input uncertainty, parameter uncertainty, and conceptual uncertainty (Sax and Isakov, 2003). Model input uncertainty arises where inputs to an air quality model, such as meteorological data or emissions, are themselves uncertain due to measurement error, estimation error, and inherent variability. Parameter uncertainty is present because a single model parameter value can never completely characterize a modeling domain. Conceptual uncertainty

occurs because simple mathematical and numerical programming code used to predict dispersion cannot completely characterize complex physical processes and associated inherent naturally occurring variability (Hanna, 1998). Because data are limited, further research is necessary to characterize conceptual uncertainty in Gaussian model results.

We believe quantitative analysis of model uncertainty is best accomplished through a three step process that can be applied regardless of model application types (Sax and Isakov, 2003):

Step 1. The first step in this process is defining the purpose and scope of the problem. This problem statement should clearly define the spatial and temporal parameters of the model result to be analyzed. For health risk assessment applications, the model result may be average annual concentration for chronic exposures or peak one-hour concentrations for acute exposures at a specified receptor or modeling domain. For chemical grid modeling, peak or daily average ozone concentrations may be analyzed in a predefined area or within specific grid cells.

Step 2. The second step in our methodology requires separating air dispersion modeling applications into discrete modeling components and analyzing uncertainty in each component individually. Fundamentally, air dispersion models are a complex system of inputs and parameters that are mathematically integrated to develop modeling results. Dispersion modeling inputs and parameters may be estimated through the use of related models such as emissions models or meteorological processing programs, which have their own underlying model inputs and parameters. A model component can be defined as a group of related dispersion modeling inputs, parameters or underlying models (with their own associated inputs and parameters) which are themselves uncertain and can be considered independently of other model components. Modeling components include the emissions inventory, spatial and temporal allocation of emissions, meteorology, pollutant transformation, model options, and model formulation, including deposition/removal processes. In order to understand uncertainty in air dispersion modeling results, one must develop a complete understanding of the sources of uncertainty in each modeling component. To evaluate uncertainty in modeling components, a review of data sources used to develop input data or model parameters in each component can be conducted. Provided enough data are available for meaningful examination, detailed evaluation or sensitivity analysis can be used to assess the structure of input variables, model options, and/or the performance of models used to develop inputs or parameters within each modeling component.

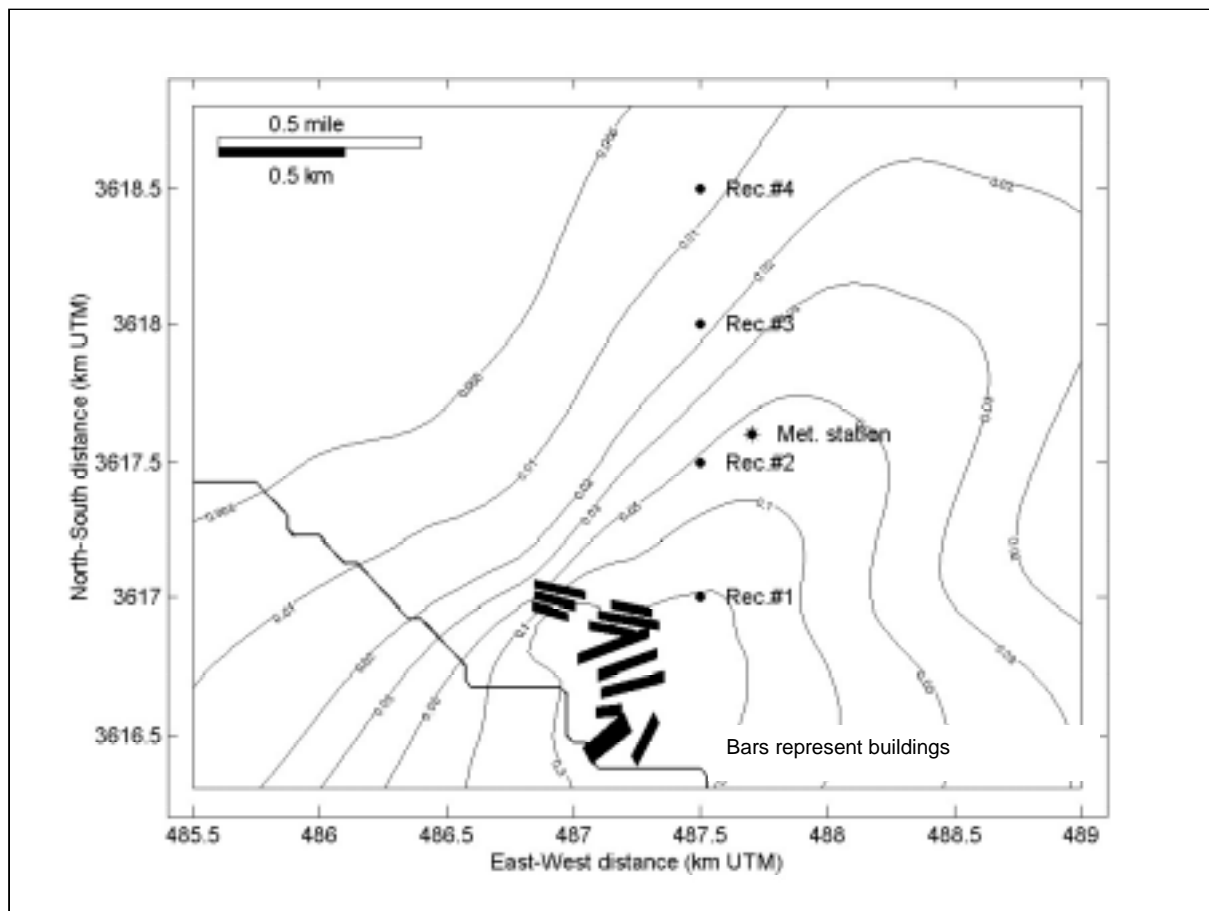
Step 3. The final step in our methodology requires applying Monte Carlo methods to distributions developed for each model component in order to estimate uncertainty in the entire modeling system. Over the past two decades, Monte Carlo techniques have been used for assessing uncertainty in emissions,

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variability in meteorology and its effect on dispersion model results, and uncertainty in air quality modeling results.

To demonstrate this methodology, ARB staff conducted an uncertainty analysis on hexavalent chromium emissions generated by welding operations at the NASSCO shipbuilding facility in Barrio Logan (Sax and Isakov, 2003). Annual average modeled hexavalent chromium concentrations are shown in Figure 5.7. As can be seen from the figure, concentrations are highest near the source, decreasing rapidly with distance from the source. The magnitude of concentrations drops off by almost a factor of 100 when receptors are about a kilometer away from the source.

Figure 5.7 - Modeled Annual Average Hexavalent Chromium Concentrations from Welding Operations



For the uncertainty analysis, two Gaussian dispersion models were selected as appropriate: ISCST3, the traditional regulatory model approved by U.S. EPA for near-field dispersion modeling, and AERMOD, a new advanced dispersion model with improved model physics. The models were separated into four components: emissions, spatial and temporal allocation of emissions, model options and release

parameters, and meteorology. Then, variability and/or uncertainty were assessed in each component, and Monte Carlo techniques were applied to propagate results and estimate a range of possible annual average hexavalent chromium concentrations.

The results indicated the 95% confidence interval of predicted pollutant concentrations spanned roughly an order of magnitude at each receptor. For Gaussian model results involving low-level releases, uncertainty is a more important factor at receptors located close to emission release points. Gaussian models are also sensitive to location of emission releases, meteorology, and model parameters. While emissions were the dominant source of uncertainty in this case study, the spatial allocation of emissions may be a dominant factor when release locations are not well characterized. Simplified modeling approaches, when emission release parameters are taken from the statewide emission database, may lead to errors in pollutant concentration estimates, especially in close proximity to emissions sources where predicted concentrations are highest. To minimize air quality modeling uncertainty, the scale of model inputs and parameters must be at least as refined as the modeling scale to be analyzed.

In this case study, AERMOD predicted a greater range of pollutant concentrations than ISCST3. This range increased as source-receptor distance decreased. If AERMOD is to be applied on a regulatory basis in the future, it will be important to minimize uncertainty in model options by using consistently applied modeling approaches. Additional guidance may be necessary to ensure AERMOD applications are sufficiently credible to ensure consistent risk management decisions.

4) Facility-Specific Health Risk Assessments (HRAs)

In order to have the most complete and up-to-date emission and source configuration data for use in Barrio Logan micro-scale modeling, we obtained facility-specific health risk assessments (HRAs), where available. The updated database was for the Barrio Logan modeling analysis only. The CEIDARS emissions inventory was not updated.

Near source impacts due to emissions from individual facilities were simulated with ISCST3 in order to compare our model results with those from the health risk assessment (HRA) completed by the facility for the AB2588 Hot Spots Program. The two facilities that were selected for this comparison are Southwest Marine and NASSCO. The comparison was made only for non-diesel TAC emissions since diesel PM was not identified as a TAC when the facilities conducted their risk assessments.

A cursory review of the risk estimated with the model simulations and the risk estimated by the facility HRA show that the estimated risks are similar between the two analyses for both facilities. This was expected, since both analyses used the same emission inputs. There are minor differences, which are likely due to differences in parameters such as meteorological data. For example, meteorological data for the HRAs completed for AB2588 are from Lindbergh Field, whereas we used data from Memorial Academy Charter School. Figures showing the estimated risk from Southwest Marine

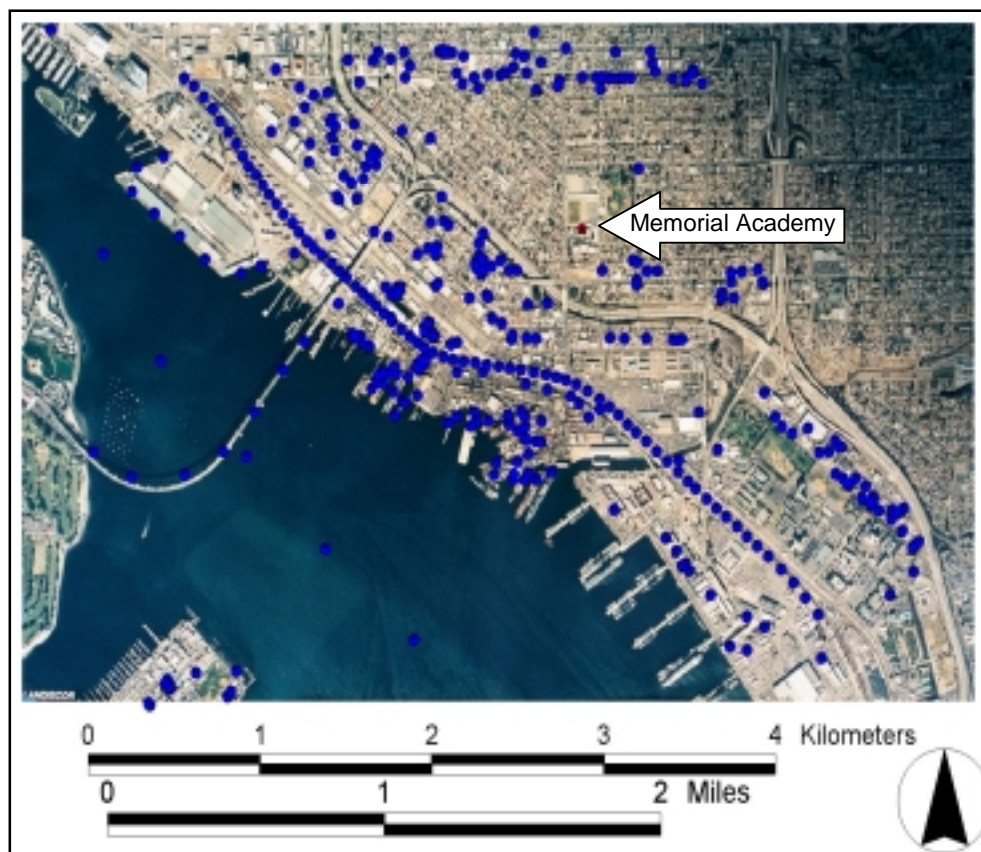
and NASSCO estimated with the ISCST3 simulation are available in the section titled, “Hexavalent Chromium.”

5) Micro-Scale Modeling Results for Toxic Air Pollutants

The following section presents the results of this analysis for eight pollutants from local emissions that originate in the micro-scale modeling domain. Regional background emissions are estimated separately with the regional grid model. To illustrate this further, Figure 5.8 shows an aerial view of Barrio Logan. Local sources are plotted as dots on the map. Individual facilities are modeled as point and volume sources in the micro-scale modeling. The rail line is plotted as a series of volume sources. The shipping lane is also plotted as a series of volume sources. Memorial Academy Charter School is shown on the maps as a pentagon. In addition,

- the results of the micro-scale models are from primary emissions only (secondary reactions are not part of the simulation);
- deposition of pollutants in the micro-scale analysis is not considered; and
- risk is estimated through inhalation only (multi-pathway risk is not part of the analysis; however, CR-VI is the only pollutant in this analysis that has a multi-pathway component).

Figure 5.8 – Aerial View of Barrio Logan



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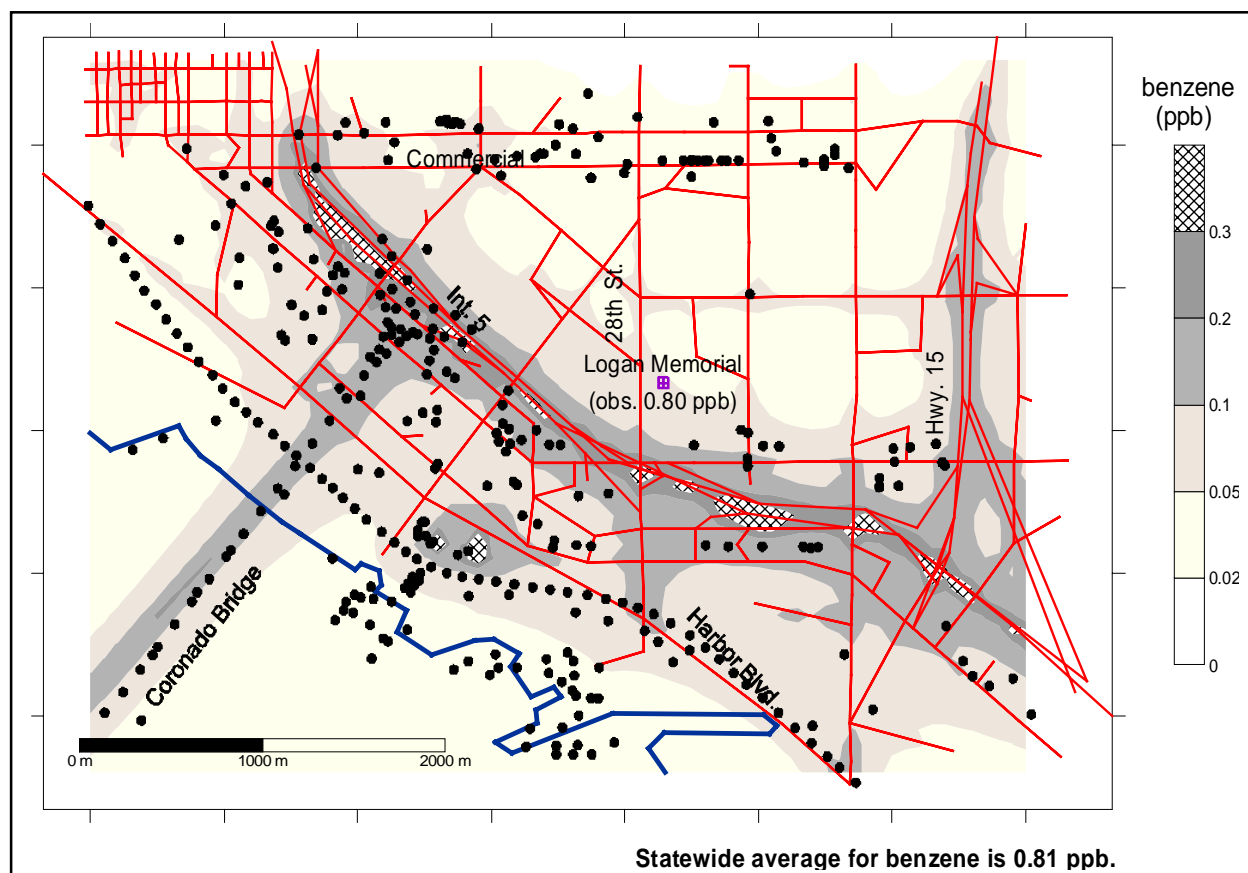
Benzene

Table 5.3 lists the major sources of benzene in Barrio Logan, with motor vehicles as the largest single category. This emission inventory was modeled using CAL3QHCR for roadways and ISCST3 for point sources. The results of the two model simulations were superimposed and the results are shown in Figure 5.9. The highest estimated local benzene concentrations, > 0.3 ppb can be seen along Interstate 5 and the refinery tank farms. The statewide average concentration of benzene is 0.81 ppb, which is similar to the observed benzene concentrations measured at Memorial Academy.

These benzene concentrations can be multiplied by a pollutant specific risk factor to estimate inhalation cancer risk. Cancer risk estimates represent the chances of developing cancer assuming a person is continuously exposed to these concentrations over a 70-year lifetime. Micro-scale modeled benzene risk is 5 in a million for the concentrations at Memorial Academy. The cancer risk estimate based on ambient measurements at Memorial Academy for benzene is 74 in a million. These results suggest that the regional benzene concentrations may drive the benzene risk at Memorial Academy. Additionally, we may have underestimated the emissions in the micro-scale inventory.

Table 5.3 - Summary of Benzene Sources Near Barrio Logan

Source	Inventory (lbs/yr)
Motor Vehicles	14,000
North Island Naval Air Station, Taxi/Idle ^(a)	9,160
Lindbergh Field, Taxi/Idle ^(a)	3,440
Lindbergh Field, Ground Support Equipment ^(a)	1,330
Others	3,070
Total	31,000
a) These sources are located outside of the receptor field but are included in the micro-scale analysis.	

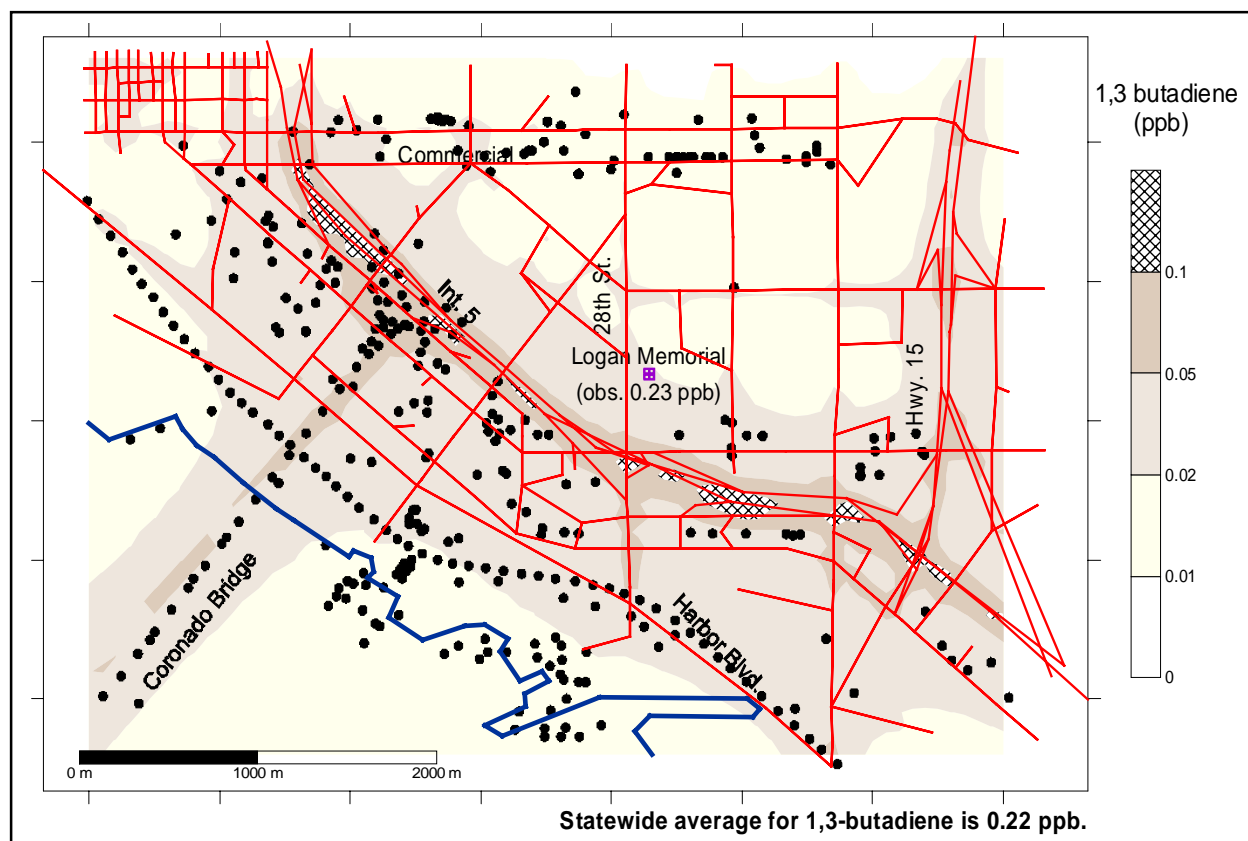
Figure 5.9 - Benzene Concentration - Local Emissions

1,3-Butadiene

The sources of 1,3-butadiene in Barrio Logan are shown in Table 5.4. The regional and micro-scale modeling results were superimposed and are shown in Figure 5.10. The highest estimated local 1,3-butadiene concentrations, > 0.1 ppb, can be seen along Interstate 5. The statewide average concentration of 1,3-butadiene is 0.22 ppb and is similar to the concentration measured at Memorial Academy. The micro-scale modeled 1,3-butadiene cancer risk is 8 in a million at Memorial Academy. The cancer risk estimate based on ambient measurements at Memorial Academy for 1,3-butadiene is 88 in a million. Similar to benzene, the risk due to 1,3-butadiene seems to be dominated by regional air.

Table 5.4 - Summary of 1,3-Butadiene Sources Near Barrio Logan

Source	Inventory (lbs/yr)
Motor Vehicle	3,100
North Island Aircraft ^(a)	9,080
Lindbergh Field ^(a)	4,260
Others	68
Total	16,500
a) These sources are located outside of the receptor field but are included in the micro-scale analysis.	

Figure 5.10 - 1,3-Butadiene Concentration, Local Emissions

Formaldehyde

Table 5.5 summarizes the formaldehyde emissions in Barrio Logan. The dispersion of formaldehyde emissions was simulated with the CAL3QHCR and ISCST3 models, superimposed, and the results are shown in Figure 5.11. The highest estimated formaldehyde concentrations, > 0.7 ppb, can be seen along Interstate 5. The statewide

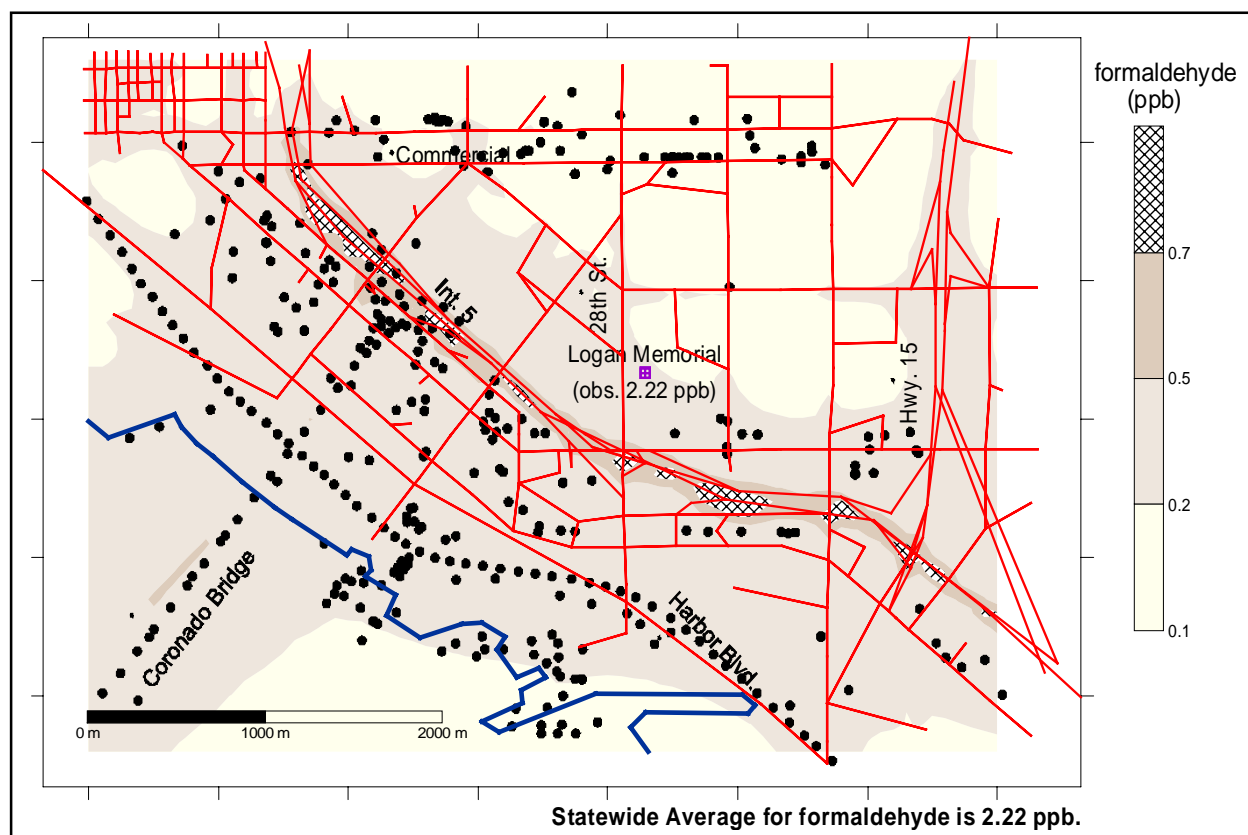
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average concentration for formaldehyde is 2.22 ppb, which is similar to the concentration observed at Memorial Academy. The micro-scale modeled formaldehyde cancer risk estimate is 2 in a million at Memorial Academy. The cancer risk estimate based on ambient measurements from Memorial Academy for formaldehyde is 16 in a million.

Table 5.5 – Summary of Formaldehyde Sources Near Barrio Logan

Source	Inventory (lbs/yr)
Motor Vehicles	10,400
North Island Aircraft ^(a)	77,100
Lindbergh Field ^(a)	34,600
Applied Energy ^(a)	14,200
ISP Alginates	3,500
Others	1,200
Total	141,000
a) These sources are located outside of the receptor field but are included in the micro-scale analysis.	

Figure 5.11 - Formaldehyde Concentration, Local Emissions



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Hexavalent Chromium

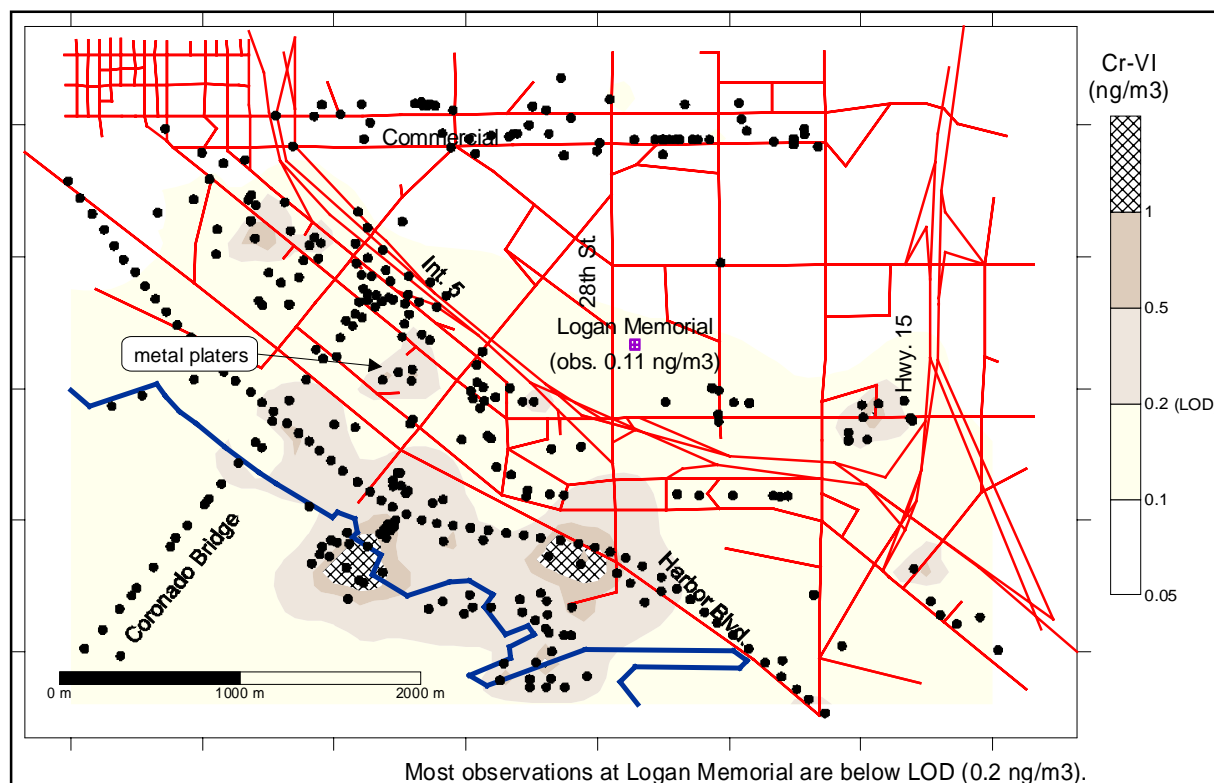
Table 5.6 summarizes local hexavalent chromium emissions in Barrio Logan, with North Island Aircraft, accounting for the largest single category of sources. Figure 5.12 shows the concentrations from local chromium emissions. The emissions from North Island Aircraft are broken down into various categories as shown in Table 5.7 and may require further refinement. The highest estimated concentrations of hexavalent chromium, $> 1 \text{ ng/m}^3$, are highly localized near the shipyard facilities of NASSCO and Southwest Marine. Observations at Memorial Academy, 0.11 ng/m^3 , are based on observations above and below the level-of-detection, 0.2 ng/m^3 . The micro-scale modeled cancer risk estimate is 16 in a million for the micro-scale local hexavalent chromium emissions at Memorial Academy.

Table 5.6 – Summary of Hexavalent Chromium Sources in Barrio Logan

Source	Inventory (lbs/yr)
North Island Aircraft ^(a)	74.3
Lindbergh Field ^(a)	7.8
NASSCO	6.2
North Island, Ground Equipment ^(a)	1.8
Southwest Marine	1.6
US Navy ^(a)	1.3
Continental Maritime	0.8
Southern California Plating	0.3
Fraiser's Boiler Service	0.2
Pacific Ship Repair	0.1
Others	1.6
Total	96
a) These sources are located outside of the receptor field but are included in the micro-scale analysis.	

Table 5.7 - Detail of Hexavalent Chromium Emissions for North Island Aircraft

Source	Inventory (lbs/yr)
Approach	16.7
Climb Out	8.9
Landing / Takeoff	6.9
Idle / Taxi	41.5
APU/GSE/Idle	0.3
Total	74.3

Figure 5.12 - Hexavalent Chromium Concentration, Local Emissions

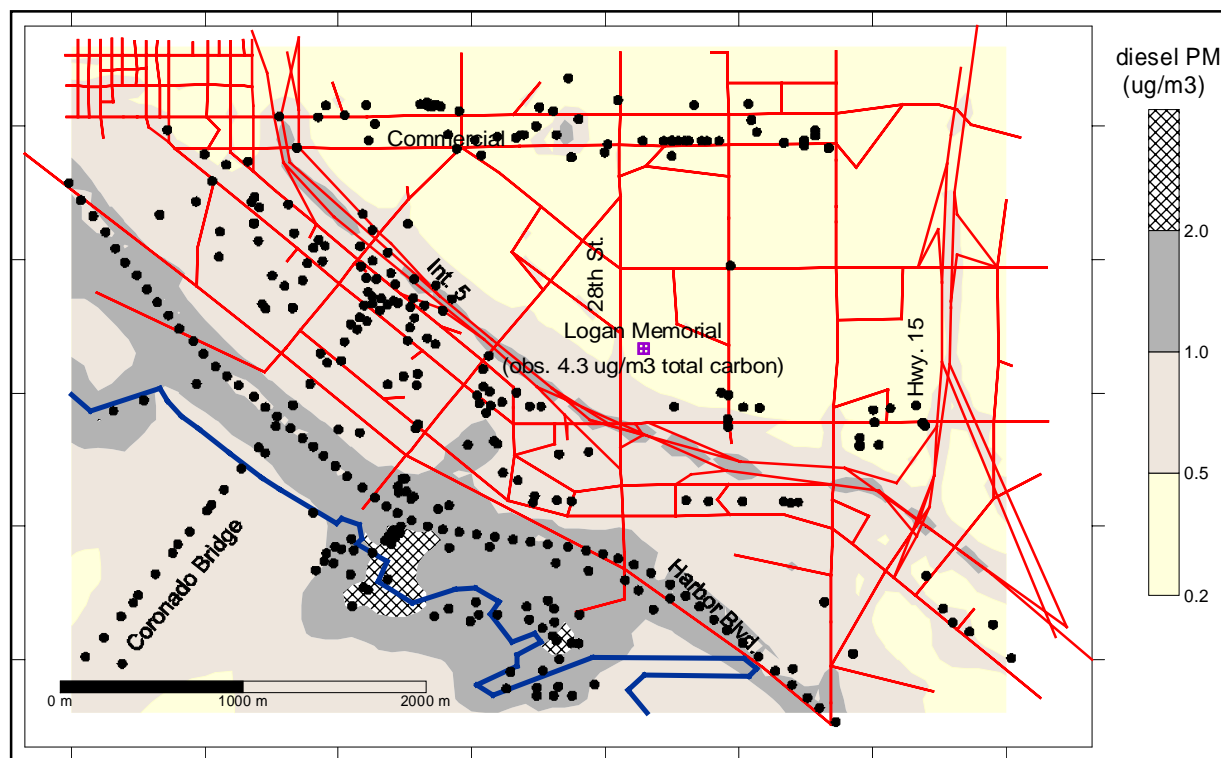
As discussed previously, a special monitoring study for hexavalent chromium was conducted for about five months in 2001-2002 near two metal plating facilities. This intense focus on hexavalent chromium within a small portion of the domain is discussed in Chapters 2 and 5. These hot spots may not appear in the micro-scale estimates if the localized emission inventory is not representative of actual emissions as we found in the special study. The observed hexavalent chromium for the five month average at the highest impacted monitor is 0.76 ng/m^3 . Nearfield impacts of inert or low reactive pollutants, such as hexavalent chromium, are generally higher in the winter, due to lower wind speeds and higher atmospheric stability. The observed five-month average includes winter months and is higher than the predicted annual average, as we would normally expect. The modeled annual average concentration from ISCST3 at this same location is 0.6 ng/m^3 (90 per million inhalation risk). This comparison is strictly for the sake of corroborating, in a relative sense, model-simulated annual concentrations (i.e. with regard to whether the modeling results generally meet expectations). For model performance evaluations, whereby observations are compared more formally with predictions, such comparisons must be conducted on datasets spanning the same span of time. As discussed previously, enhanced modeling (Isakov, 2003) of emissions from the two nearby hexavalent chromium sources show that additional data on activity can improve modeling estimates on shorter time scales.

Diesel PM

As previously mentioned, there is no peer-reviewed method to specifically measure the contribution of diesel exhaust to total measured particulate matter. As such, there is no observation-based means to characterize the relative risk posed by diesel PM versus other toxic air pollutants. However, the modeling tools and inputs described in this report allow diesel PM to be tracked independently in model simulations. Table 5.8 summarizes local diesel PM emissions in Barrio Logan. Figure 5.13 shows the estimated diesel PM concentrations from local diesel PM emissions, with the highest concentrations located near a shipyard facility. Observations at Memorial Academy are not available for diesel PM or elemental carbon. Rather, total carbon is measured at 4.3 ug/m³ at Memorial Academy. The micro-scale modeled cancer risk at Memorial Academy is 130 in a million for local sources of diesel PM.

Table 5.8 Summary of Diesel PM Sources near Barrio Logan

Source	Inventory (lbs/yr)
HD Trucks	8,000
Railroad	5,600
Shipping ^(a)	84,000
Southwest Marine	4,700
Northstar Propellers	380
NASSCO	3,400
Others	26,920
Total	133,000
a) These sources are located outside of the receptor field but are included in the micro-scale analysis.	
<i>Emissions from shipping and railroads are first order estimates and may need to be refined.</i>	

Figure 5.13 - Concentration from Diesel PM, Local Emissions Only

Perchloroethylene

Table 5.9 summarizes the local perchloroethylene emissions in Barrio Logan. The results of the model simulations were superimposed and are shown in Figure 5.14. The highest estimated local concentrations, > 0.04 ppb, are highly localized and can be seen near Carlos Cleaners. The concentration measured at Memorial Academy was 0.08 ppb, while the average statewide concentration of perchloroethylene is 0.11 ppb. The micro-scale modeled cancer risk estimate at Memorial Academy is 0.01 in a million. Cancer risk estimates based on ambient measurements at Memorial Academy are 3 in a million.

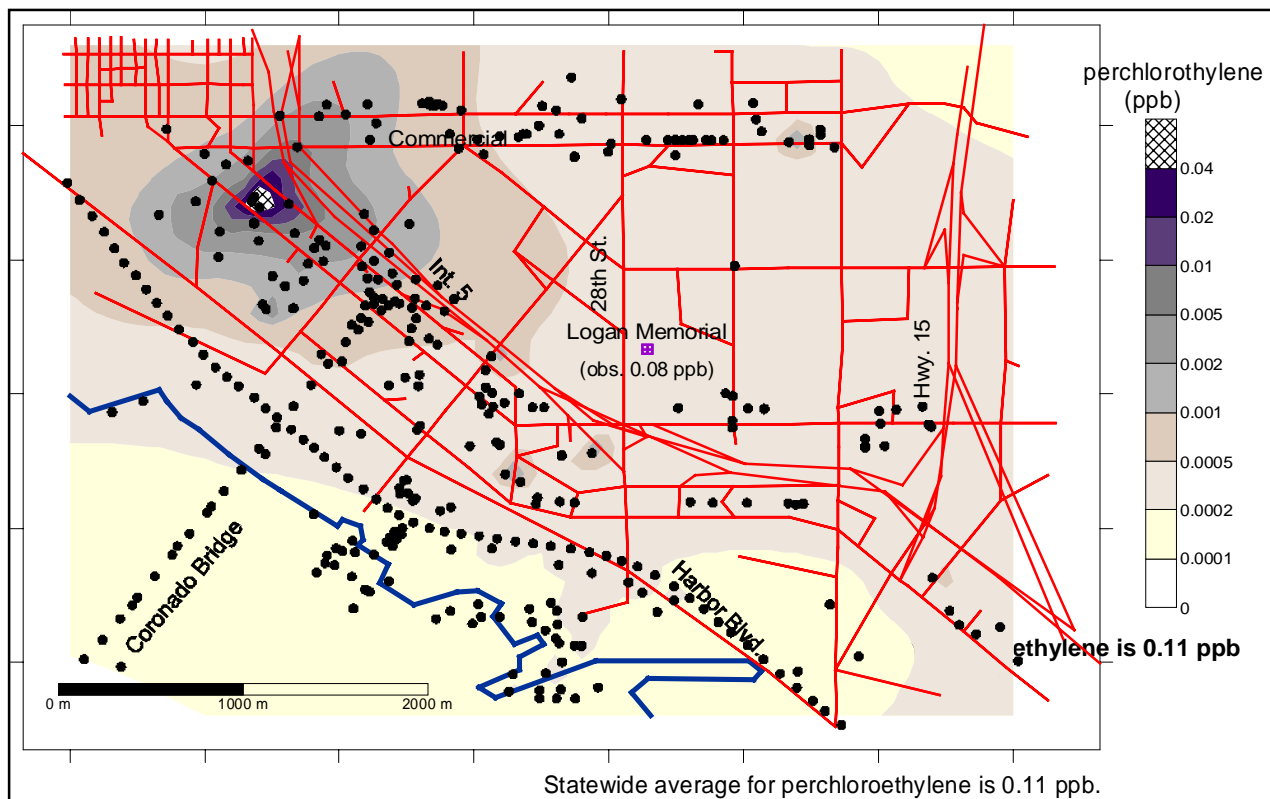
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Table 5.9 – Summary of Perchloroethylene Sources near Barrio Logan

Source	Inventory (lbs/yr)
Speedy Clean ^(a)	440
San Diego Marriot Hotel ^(a)	404
Carlos Cleaners	180
North Island ^(a)	87
US Navy ^(a)	11
Others	28
Total	1,150

a) These sources are located outside of the receptor field but are included in the micro-scale analysis.

Figure 5.14 – Concentration from Perchloroethylene, Local Emissions Only



Manganese

Table 5.10 summarizes local manganese emissions in Barrio Logan. The modeling results are provided in Figure 5.15. The highest concentrations, $> 50 \text{ ng/m}^3$, are highly localized and are located near the shipyard facilities. The concentration of manganese measured at Memorial Academy was 31 ng/m^3 and is slightly higher than the statewide

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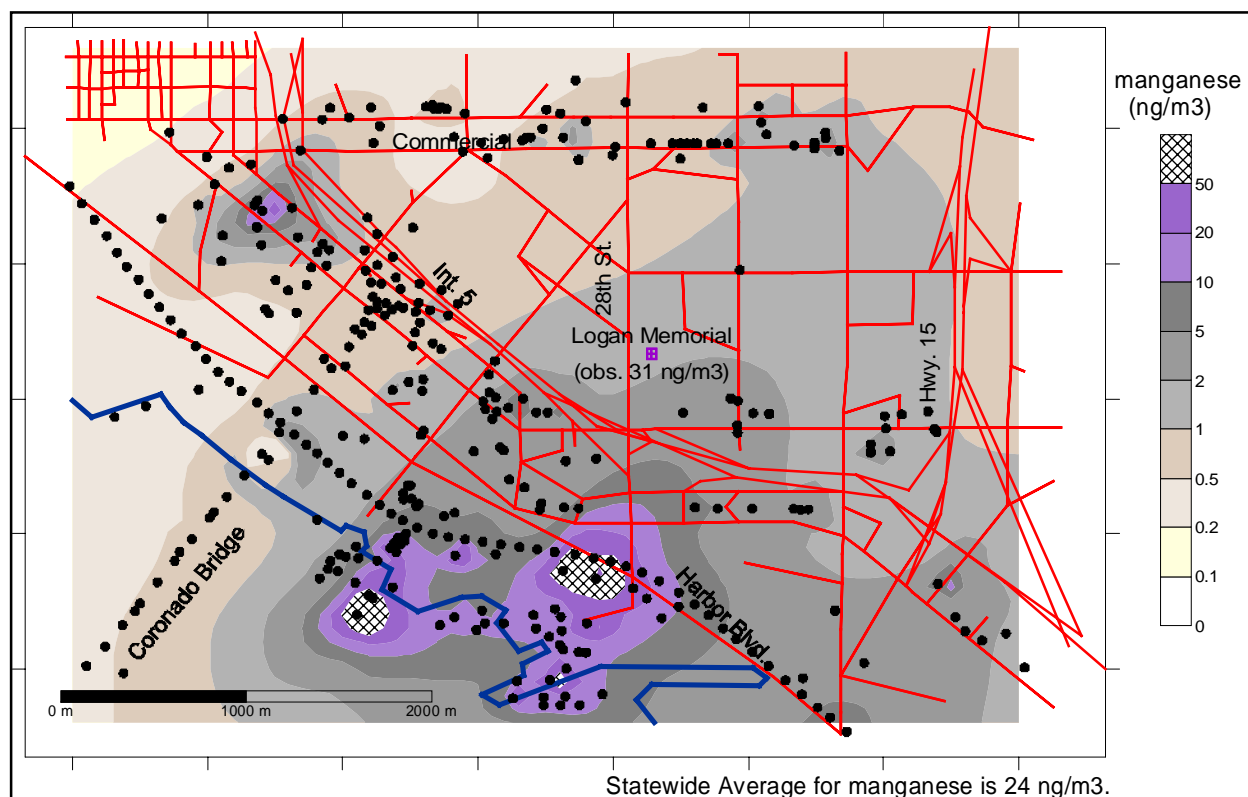
average of 24 ng/m³. The micro-scale modeled concentration at Memorial Academy is 1.8 ng/m³. Although the average concentration of manganese from Memorial Academy is slightly higher than the statewide average, the levels are below the manganese chronic reference exposure level of 200 ng/m³. Manganese is not listed as a toxic air pollutant.

Table 5.10 – Summary of Manganese Sources near Barrio Logan

Source	Inventory (lbs/yr)
NASSCO	418
US Navy ^(a)	60
Southwest Marine	57
North Island ^(a)	22
Superior Welding of Southern California	8
Others	24
Total	589

a) These sources are located outside of the receptor field but are included in the micro-scale analysis.

Figure 5.15 – Manganese Concentration, Local Emissions Only



6) Summary of Findings for the Micro-Scale Modeling

U.S. EPA approved models were applied to estimate annual average concentrations of toxics from hundreds of sources over the Barrio Logan region, which spans several kilometers. More specifically, the ISCST3 air dispersion model was applied to point sources and CAL3QHCR for motor vehicle line sources. Testing of the AERMOD and CALPUFF models was also conducted and indicates that the use of these models is also feasible. To our knowledge, this is the first time micro-scale modeling of hundreds of sources over several kilometers has been conducted.

Qualitatively, the micro-scale modeling results show an expected, non-uniform spatial distribution of concentrations with strong spatial gradients; simulated concentrations are much higher near the source and rapidly decrease with distance away from the source. However, quantitatively, levels of simulated concentrations are low compared to observations. Possible explanations for this are:

- Uncertainties in the emissions inventory;
- Uncertainties in the micro-scale model formulations; and
- Regional source influences (i.e. sources outside of the micro-scale modeling domain) that may dominate the concentrations observed at the monitoring stations used for model performance purposes.

Roadway emissions tend to dominate concentrations near major throughfares such as Interstate 5. These emissions include diesel PM and benzene. Impacts from individual facility emissions are similar to impacts reported in risk assessments available in the San Diego APCD files.

The summer tracer study shows the micro-scale model performs well for two days of the experiment. On the other three days, the model overestimates the maximum observed hourly values by about a factor of two and underpredicts the lower observed concentrations. AERMOD outperformed ISCST3 and a new dispersion model, developed under contract to the University of California at Riverside, outperforms AERMOD. The winter tracer study showed more inconclusive model performance; suggesting that winter meteorological conditions have added complexity for which model improvements could be made.

Although AERMOD has undergone extensive evaluation, the CE-CERT tracer study is the first in which the meandering component of the model has been tested. This study demonstrates that AERMOD can provide reliable near-field concentration estimates from urban sources if turbulent velocity estimates close to a source are used to estimate plume direction. Future research should examine the relationship between urban morphology and meteorological parameters within the urban canopy.

B) Regional Photochemical Modeling

The CALGRID and CMAQ photochemical models were applied to simulate regional hourly and annual average pollutant concentrations in southern California over a region that includes the Barrio Logan and Wilmington neighborhoods. The two models use the same emissions, initial conditions, and boundary conditions. However, the models are driven by different meteorological inputs. CALGRID uses the output from the CALMET meteorological model and CMAQ uses the output from MM5. It should be noted that CALMET could run independently for each month, since no initial conditions are needed. However, MM5 was run as a continuous simulation for all of 1998. The meteorological models were applied for the period January 1 through December 31, 1998. The following five regional modeling simulations were conducted.

Baseline runs to test model performance:

- January 1 through December 31, 1998 using CALGRID (*Baseline*)
- January, April, August, and November of 1998 using CMAQ (*Baseline*)

Double-counting assessment:

- January 1 through December 31, 1998 using CALGRID and omitting the emissions in the domain cell where *Barrio Logan* is located
- January 1 through December 31, 1998 using CALGRID and omitting the emissions in the domain cell where the *Wilmington* neighborhood is located

Sensitivity to boundary conditions:

- Investigated the impact of changing boundary conditions during February and August 1998 using CALGRID

1) Modeling Domain

The regional modeling domain covers a large portion of the population in the State and includes the counties of Ventura, Los Angeles, Orange, and San Diego as well as parts of Riverside, San Bernardino, and Imperial counties. The domain consists of 87x67 horizontal cells and is slightly smaller than the SCOS97 domain, but approximately 3.7 times larger than the MATES II domain (Figure 5.16). Each horizontal grid cell is 4x4 km². CALGRID uses 10 vertical layers with a domain height of 3 km, and CMAQ uses 17 vertical layers with a domain height of 14.6 km. Table 5.11 lists domain specifications for CALGRID and Table 5.12 lists domain definitions for CMAQ.

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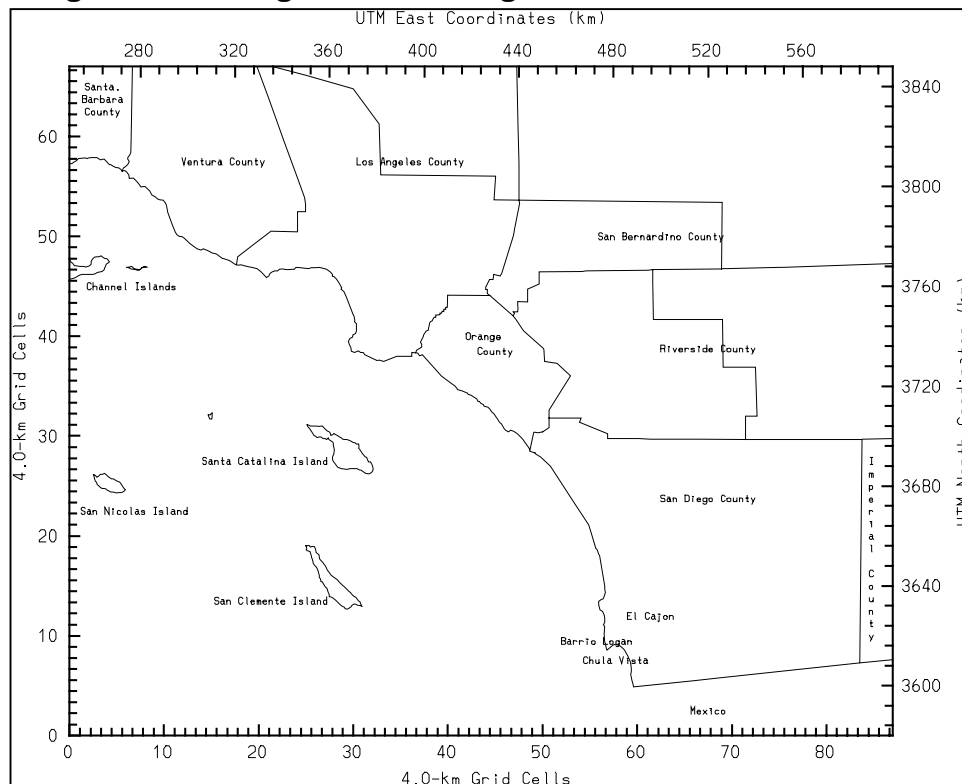
Table 5.11 - Regional modeling domain Definition for CALGRID

Parameter	Value
x-Origin (UTM Zone 11)	250,000 m
Y-Origin (UTM Zone 11)	3,580,000 m
Number of cells (Easting)	87
Number of cells (Northing)	67
Grid width	4,000 m
Domain top	3,000 m
Number of vertical layers	10

Table 5.12 - Regional modeling domain Definition for CMAQ

Parameter	Value
Center of grids	Latitude 30° N Longitude 118° W
Number of cells (Easting)	90
Number of cells (Northing)	68
Origin (from center)	(-160,000 m, +260,000 m)
Projection parameters	(30, 60, -118)
Domain top	14,600 m
Number of vertical layers	17

Figure 5.16 - Regional Modeling Domain



2) Regional Modeling Input Data

This section describes the input data used for regional modeling. As mentioned previously, both air quality models use the same initial/boundary conditions and emissions, but each model is driven by different meteorological inputs. CALGRID uses the output from the CALMET meteorological model and CMAQ uses the output from MM5.

Emissions

Chapter 4, titled “Modeling Emission Inventory Development”, provides a detailed account of the modeling emissions inventory development for both regional and micro-scale modeling.

Chemical Mechanism

This modeling utilized the SAPRC99 chemical mechanism as described by Carter (2000). Explicit reactions were added to represent the reactive toxic air pollutants. Because of limitations in the models’ code, pseudo reactions are used to incorporate the inert species. For the case of CMAQ, an artificial decay rate is used to represent deposition effects on the inert PM species and hexavalent chromium. Table 5.13 summarizes the toxic air pollutants that were modeled.

Table 5.13- Toxic Air Pollutants and Abbreviations

Name	Symbol	Inert or Reactive	Name	Symbol	Inert or Reactive
1,3-Butadiene	BUTD	R	Lead	LEAD	I
Acetaldehyde	CCHO	R	Manganese	MANG	I
Acrolein	ACRO	R	Mercury	MERC	I
Arsenic	ARSE	I	Methylene chloride	DICM	R
Benzene	C6H6	R	MTBE	MTBE	R
Beryllium	BERY	I	Nickel	NICK	I
Cadmium	CADM	I	<i>o</i> -Dichlorobenzene	ODCB	R
Carbon Tetrachloride	CCL4	R	<i>p</i> -Dichlorobenzene	PDCB	R
Chloroform	CHLO	R	Perchloroethylene	PERC	R
Diesel PM	DIES	I	Styrene	STYR	R
Ethylene dichloride	TEDC	R	Toluene	C7H8	R
Ethylene oxide	ETOX	R	Trichloroethylene	TCE	R
Formaldehyde	HCHO	R	Vinyl chloride	VCHL	R
Hexavalent chromium	CRVI	I	Xylenes	OXYL	R
Iron	IRON	I	Zinc	ZINC	I

The SAPRC99 atmospheric chemical reaction mechanism also includes a default set of reactive species that are used to represent how the emissions of hydrocarbons and

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oxides of nitrogen react in the ambient air (Carter, 2000). These species are listed in Table 5.14.

Table 5.14. Default Reactive Model Species Included in SAPRC99 (Carter, 2000)

Species	Description	Species	Description
O3	Ozone	ALK1	Alkanes and other non-aromatic compounds that only react with the hydroxyl radical (OH) and have an OH reaction rate constant (KOH) between 2×10^2 and 5×10^2 ppm-1min-1 (primarily ethane)
CO	Carbon monoxide	ALK2	Alkanes and other non-aromatic compounds that only react with OH and have a KOH between 5×10^2 and 2.55×10^3 ppm-1min-1
ACET	Acetone	ALK3	Alkanes and other non-aromatic compounds that only react with OH and have a KOH between 2.5×10^3 and 5×10^3 ppm-1min-1
MEK	Ketones with a KOH less than 5×10^{-12} cm ³ molec ⁻² sec ⁻¹	ALK4	Alkanes and other non-aromatic compounds that only react with OH and have a KOH between 5×10^3 and 1×10^4 ppm-1min-1
ETHE	Ethene	ALK5	Alkanes and other non-aromatic compounds that only react with OH and have a KOH greater than 1×10^4 ppm-1min-1
CH4	Methane	ARO1	Aromatics with KOH less than 2×10^4 ppm-1min-1 (primarily benzene, toluene and monoalkyl benzenes). For this study benzene and toluene were not lumped with ARO1.
ISOP	Isoprene	ARO2	Aromatics with KOH greater than 2×10^4 ppm-1min-1 (primarily xylenes and polyalkyl benzenes). Note that for this study xylens were not lumped with ARO2.
MEOH	Methanol	OLE1	Alkenes (other than ethene) with KOH less than 7×10^4 ppm-1min-1
RCHO	Lumped aldehydes with more than 3 carbons	OLE2	Alkenes (other than ethene) with KOH greater than 7×10^4 ppm-1min-1
CRES	Cresols	TRP1	Biogenic alkenes other than isoprene (primarily terpenes)
PHEN	Phenols		
BALD	Aromatic aldehydes		
NO, NO2	Nitrogen oxides		
HO2H	Hydrogen peroxide		
PAN	Peroxyacetyl nitrate		
PROD2	Ketones with a KOH greater than 5×10^{-12} cm ³ molec ⁻² sec		

Meteorological Inputs

As mentioned in Chapter 3, two different meteorological models were used: CALMET and MM5. A brief description of each model is provided in Chapter 3.

CALMET requires hourly surface observations of several variables. Meteorological variables required by CALMET are routinely measured at National Weather Service (NWS) surface stations. Supplemental data from the Aerometric Information Retrieval System (AIRS) and California Irrigation Management Information System (CIMIS) datasets were also used. For this study, data were obtained from the 10 NWS stations, 154 AIRS stations, and 38 CIMIS stations.

The upper air data required by CALMET are twice-daily observations of vertical profiles of upper air data obtained from Miramar Naval Air Station. In addition, buoy data at two stations along the coast were used to provide meteorological conditions at sea level.

The non-hydrostatic version of the MM5 model (which is used by CMAQ) is applied with one coarse and one fine nested domain. The MM5 numerical model is initialized from the analysis files created by the National Climate and Environmental Prediction (NCEP) center using analysis nudging only. Atmospheric circulation patterns that are prevalent over the region during the study period are numerically simulated using the coarse and fine nested grids with a two-way nested grid approach. With this approach, the fine nested grid captures the effects of small-scale terrain on the evolution of the atmospheric circulation patterns.

Due to the volume of data involved in producing annual meteorological data sets as well as the absence of an established protocol to evaluate hourly wind fields on an annual basis, the wind fields were not formally evaluated for a complete year of data. However, qualitative assessments were made. For example, wind roses for five observational sites for the months of January and August 1998 were compared to the CALMET and MM5 outputs (January and August were randomly selected to represent winter and summer). In addition, hourly wind fields were plotted and reviewed, which revealed that, in general, the model outputs capture some of the features of the observed wind speeds and wind directions. Comparisons between the CALMET and MM5 outputs did show some differences between the two meteorological models, which could be the cause, at least in part, of differences in model results between CMAQ and CALGRID. In the future, a more formal evaluation of the annual wind fields would be desirable, pending development of a formal protocol, to assess how representative the annual meteorological model outputs are to drive annual air quality model simulations.

Initial and Boundary Conditions

The utilized boundary conditions are based on updated SCOS97 Regional Modeling and are the same for each month. Tables 5.15 and 5.16 show the initial conditions and

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the boundary conditions used for the top of the domain as well as the lateral boundary conditions used for the rest of the domain.

Table 5.15 - Upper-Level, Vertical Boundary Conditions (Concentrations)

Species	Concentration (ppb)	Species	Concentration (ppb)	Species	Concentration (ppb)
O ₃	30.	ALK1	2.656	FORM	2.02
CO	180.	ALK2	0.023	ALD	2.02
HCHO	0.67	ALK3	1.082	Acetone	0.178
CCHO	0.001	ALK4	1.352	Toluene	0.478
Ethene	0.495	ALK5	2.732	Styrene	0.292
Methane	1,660.	ARO1	0.301	Xylenes	0.637
		ARO2	1.726	PDCB	0.521
		OLE1	0.556	Terpenes	0.079
		OLE2	0.558	All other species	0.001

Note: FORM represents that formaldehyde concentration produced by direct emissions from sources, while HCHO corresponds to formaldehyde formed through photochemical reactions. Similarly, ALD and CCHO correspond to primary emitted and secondary acetaldehyde. Organic alkanes are lumped according to their reactivity into five lumped model species (ALK1, ALK2, ALK3, ALK4 and ALK5), Alkene species are lumped, according to their reactivity, into two lump model species (OLE1 and OLE2). Aromatics are lumped into two model species (ARO1 and ARO2). See Table 5.15.

Table 5.16 - Lateral Boundary Conditions (Concentrations)

Species	Over Ocean (ppb)	Over Land (ppb)	Species	Over Ocean (ppb)	Over Land (ppb)
O ₃	40.	40.	ALK1	0.2	0.6
NO	0.001	0.001	ALK2	0.76	2.28
NO ₂	0.001	2.	ALK3	0.19	0.57
CO	350.0	350.0	ALK4	0.001	0.001
HCHO	0.03	2.79	ALK5	0.74	2.22
CCHO	0.67	2.01	ARO1	0.42	1.26
Ethene	0.18	0.57	ARO2	0.14	0.42
Methane	1660.	1660.	OLE1	0.36	1.98
			OLE2	0.001	0.001
			Acetone	0.178	0.178
			All other species	0.001	0.001

Note: FORM represents that formaldehyde concentration produced by direct emissions from sources, while HCHO corresponds to formaldehyde formed through photochemical reactions. Similarly, ALD and CCHO correspond to primary emitted and secondary acetaldehyde. Organic alkanes are lumped according to their reactivity into five lumped model species (ALK1, ALK2, ALK3, ALK4 and ALK5), Alkene species are lumped, according to their reactivity, into two lump model species (OLE1 and OLE2). Aromatics are lumped into two model species (ARO1 and ARO2). See Table 5.15.

Dry Deposition

Deposition onto surfaces is a process where pollutants can be removed from the atmosphere. Deposition can be an important removal process for the pollutants treated in the toxic air pollution simulation. This is particularly relevant when simulating very long periods of time, such as annual simulations. Many factors affect deposition (Sehmel, 1980; Hicks 1982). They include surface roughness and composition, vegetation, atmospheric variables (stability, turbulence, etc.), and properties of the pollutant (such as diffusivity, solubility, and reactivity).

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Typically, a resistance model is used to approximate the deposition process. The deposition velocity is expressed as a sum of inverse resistances. Each resistance represents an opposition to the movement of the particle through the atmosphere to the surface. The CMAQ model has default deposition parameters that are hardwired for selected species, which prevented us from assigning deposition parameters for most toxic air pollutants, except for particulate species where deposition was represented as a first order decay. The CALGRID model allows the user to input pollutant specific properties that are used to estimate the net removal rate due to dry deposition (Yamartino et al., 1989). Table 5.17 summarizes the parameters used in CALGRID to represent dry deposition for a large number of simulated species. For particulate species, including hexavalent chromium, we assumed (for CALGRID) a geometric mass mean diameter of 10 microns, with a geometric standard deviation of 2 microns.

Table 5.17 - Pollutant specific parameters used in CALGRID to simulate dry deposition

Species	Diffusivity ^a (cm ² /2)	Alpha Star ^b	Reactivity ^b	Mesophyl Resistance ^d (s/cm)	Henry's law Coefficient ^{b,c} (dimensionless)
HO2H	0.2402	1	12	0	4.00E-07
O3	0.1594	10	15	4	2
NO2	0.1656	1	8	5	3.5
NO3	0.1656	1	8	5	1.00E-06
HONO	0.11	1	4	2	4.30E-04
HNO4	0.15	1	4	2	1.00E-05
HO2	0.2402	1	12	0	1.00E-06
PAN	0.105	1	4	1	1.00E-02
RNO3	0.11	1	4	1	1.00E-06
HCHO	0.2336	1	4	0	4.00E-06
NO ^d	0.1802	1	8	5	7.70E-05
BUTD	0.1013	1	4	1	5.70E-04
C6H6	0.0896	1	4	1	7.30E-03
C7H8	0.0805	1	4	1	6.50E-03
OXYL	0.0737	1	4	1	6.50E-03
CHLO	0.0894	1	4	1	9.40E-03
TCE	0.0823	1	4	1	5.30E-03
ODCB	0.0723	1	4	1	2.20E-02
PDCB	0.0723	1	4	1	1.30E-02
STYR	0.075	1	4	1	1.50E-02
VCHL	0.1099	1	4	1	1.80E-03
ACRO	0.1094	1	4	1	3.30E-01
CCL4	0.0802	1	4	1	1.30E-03
MTBE	0.0804	1	4	1	6.50E-02
DICM	0.1033	1	4	1	1.50E-02
TEDC	0.0904	1	4	1	1.50E-03
PERC	0.0749	1	4	1	2.60E-03
ETOX	0.1534	1	4	1	2.20E-01

a) Used to calculate the deposition layer resistance ;b) used to calculate ground resistance; c) taken from R, Sander (1999); d) Massman, 1998)

3) Sensitivity Studies

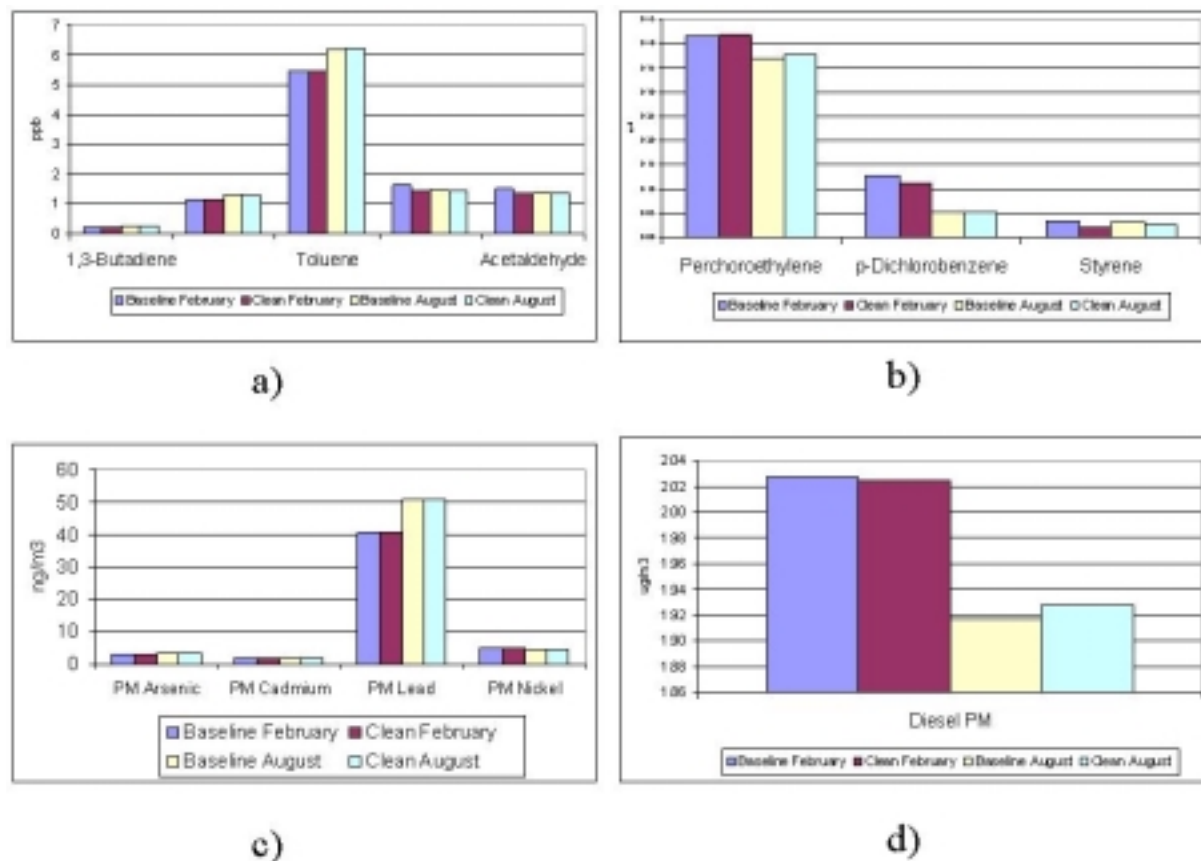
Two regional modeling baseline sensitivity studies were conducted: 1) assess the impact of changing the boundary conditions to understand the importance of boundary conditions and 2) assess the effect of estimating annual concentrations using less than a year of input data to investigate the feasibility of decreasing annual model run times. More details are provided below.

Boundary Conditions

Barrio Logan is located in the southern part of the San Diego County, as close as about 40-km from the nearest modeling domain boundary. Hence, the model-predicted long-term average concentrations for criteria and toxic air pollutants could be affected by the choice of boundary conditions.

In the baseline simulation two types of boundary conditions were used: “Over Ocean” and “Over Land”. “Over Ocean” represents pristine air quality conditions and “Over Land” represents dirtier conditions. The impact of using “Over Ocean” boundary conditions on all Barrio Logan boundaries was investigated using the CALGRID model. Attention was focused on selected toxics, including low reactivity species (like benzene and toluene), reactive species (1,3-butadiene), secondary species (formaldehyde and acetaldehyde), and inert species (like Diesel PM). Two months were simulated during 1998 with these cleaner boundary conditions (February and August were selected to represent winter and summer sensitivity). As shown in Figure 5.17, the predicted monthly concentrations (in what follows formaldehyde and acetaldehyde are the sum of primary and secondary contributions) show a small impact at Barrio Logan. The estimated concentrations of pollutants using the clean “Over Ocean” boundary conditions were slightly lower than the estimates using the “Over Land” conditions.

Figure 5.17 - Impact of boundary conditions on the monthly average concentrations at Barrio Logan during February and August 1998 for selected toxic air pollutants



The impact of the revised boundary conditions was insignificant (less than 1%) for the PM species for both months. However, the impact on the gaseous air pollutants depends on the month. For example, formaldehyde and acetaldehyde both decrease by about 10% in February and decrease about 2% in August when using cleaner boundaries. Styrene showed the largest dependency (a decrease of 34% in February and 21% in August). Other species such as perchloroethylene and 1,3-butadiene decrease by 2% in August but the effect was less than 1% in February.

Although only two months were simulated, the results suggest that the effect of the choice of boundary conditions on long-term averages can be important for some toxic air pollutants. The boundary conditions contribute to the overall chemistry of the atmosphere that specifies how species react. The very small change in the PM species is probably due to the way these species are represented in the air quality model (as pseudo first order reactions).

Temporal Resolution of Inputs and Modeling

Because of the significant computational resources and time required to simulate a complete year, it is desirable to investigate utilizing less than one full year of input data when making annual model simulations. Of particular interest is whether such ‘short-cuts’ might affect predictions of those species that account for most of the lifetime cancer risk from inhalation. This is especially true for diesel PM, which presently accounts for about 70% of the lifetime cancer risk from inhalation from all toxic air pollutants. Hence, CALGRID was used to investigate the impact of using different periods throughout the year to represent annual average concentrations, especially for Diesel PM. Specifically, the following periods were investigated:

- One month each quarter
- Two weeks each quarter
- Every other month
- Two weeks of each month

Table 5.18 summarizes the 15 averaging scenarios studied, including the baseline scenario. Other options, such as modeling episodes and adjusting for the frequency of such episodes, were not investigated.

A simple metric was developed to compare each scenario. The annual average concentration of each toxic air pollutant was calculated for each of the scenarios utilized, and then the results were compared to the baseline results. The number of surface grid-cells in the domain that differ from baseline concentrations by 10%, 30%, and 50% were calculated for selected species. This method provides a means to compare the changes in concentration associated with each scenario, both spatially and in magnitude. Table 5.19 summarizes the results for a few of the scenarios

It is expected that the difference from the baseline scenario will be related to the percentage of annual data that is omitted. Table 5.19 shows that as the proportion of the year that is simulated is reduced, the magnitude and spatial extent of the differences introduced in the model results increases. The scenarios for which data is omitted more uniformly throughout the year, such as those using two week-episodes in each month or using every other month, appear to result in fewer differences.

Although further research in this area is needed, these results illustrate that errors can be introduced by modeling a reduced number of days in a year. Of particular note is that, for this study, we ran CALGRID for 365 days and CMAQ for one month in each season. The CALGRID sensitivity results in Table 5.19 indicate that, for this study, the annual average results produced using CMAQ for one month per quarter are not comparable to the CALGRID runs, which were made for every day of the year.

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Table 5.18 - Averaging Periods Considered to Represent Annual Average Concentrations

SCENARIO	DESCRIPTION	WEEK	MONTH											
			1	2	3	4	5	6	7	8	9	10	11	12
	Baseline	1 2 3 4												
A1	1st Month of Each QTR	1 2 3 4												
A2	2nd Month of Each QTR	1 2 3 4												
A3	3rd Month of Each QTR	1 2 3 4												
B1	1st Two Weeks of 1st Month of QTR	1 2 3 4												
B2	1st Two Weeks of 2nd Month of QTR	1 2 3 4												
B3	1st Two Weeks of 3rd Month of QTR	1 2 3 4												
B4	Last Two Weeks of 1st Month in QTR	1 2 3 4												
B5	Last Two Weeks of 2nd Month in QTR	1 2 3 4												
B6	Last Two Weeks of 3rd Month in QTR	1 2 3 4												
C1	Odd Months	1 2 3 4												
C2	Even Months	1 2 3 4												
D1	First Two Weeks of Each Month	1 2 3 4												
D2	Last Two Weeks of Each Month	1 2 3 4												
D3	Weeks Two and Three of Each Month	1 2 3 4												

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Table 5.19 - Number of grid cells that differ by more than 10%, 30%, and 50% from baseline annual average concentrations for selected species and scenarios

First or Last Two Weeks Per Month

Scenario	D1				D2		
Species	>10%	>30%	>50%		>10%	>30%	>50%
BUTD	501	183	49		475	182	45
C6H6	668	84	0		639	86	0
PERC	747	176	39		738	178	0
HCHO	0	0	0		0	0	0
CCHO	0	0	0		0	0	0
DIES	568	12	0		537	0	0
CRVII	12	0	0		8	0	0

Every Other Month

Scenario	C1				C2		
Species	>10%	>30%	>50%		>10%	>30%	>50%
BUTD	877	365	186		766	260	85
C6H6	973	514	158		986	534	188
PERC	1107	504	32		1090	490	102
HCHO	267	0	0		313	0	0
CCHO	0	0	0		0	0	0
DIES	771	343	73		804	361	85
CRVII	2	0	0		3	0	0

One Month Per Quarter

Scenario	A2				A3		
Species	>10%	>30%	>50%		>10%	>30%	>50%
BUTD	1097	496	191		1430	582	283
C6H6	1588	685	107		1794	1091	871
PERC	1898	696	66		2136	1117	686
HCHO	557	0	0		1341	324	0
CCHO	9	0	0		867	0	0
DIES	1312	568	59		1553	895	666
CRVII	190	0	0		60	1	0

Two Weeks Per Quarter

Scenario	6mo_odd_2w				6mo_even_2w		
Species	>10%	>30%	>50%		>10%	>30%	>50%
BUTD	1157	478	234		1136	350	126
C6H6	1633	599	346		1514	527	292
PERC	1713	709	225		1713	628	223
HCHO	341	0	0		508	0	0
CCHO	73	0	0		90	0	0
DIES	1292	423	261		1103	374	186
CRVII	407	0	0		963	1	0

4) Model Performance

This section presents regional modeling performance results for annual simulations of ozone and toxic air pollutants. Descriptions are provided for relevant modeling studies from which experience can be gleaned, as are reviews of current regional modeling performance metrics. This is necessary, since metrics for annual simulations are not yet established (per the discussion in Chapter 3). Based on our experience and the limited information available we propose initial performance metrics and set broad expectations, and present model performance results for this study.

Generally, regional model performance for this initial application was similar to the performance experienced by other researchers that have conducted annual regional modeling simulations. Model performance metrics for 1-hour ozone were applied to assess annual ozone model performance, using 60 ppb ozone thresholds for the high ozone season and 30 ppb thresholds for wintertime periods. Simulated ozone and toxic air pollutants are generally within a factor of 2-3 of observations. Results for toxics hydrocarbons compare well with observations and with the results of previous studies. The PM species do not compare well with observations, which suggests potential deficiencies in the model inputs.

Previous Studies

In contrast to regional modeling for multi-day ozone episodes, there is relatively little experience with annual regional modeling. This section summarizes some relevant projects from which lessons might be learned, particularly with regard to making comparisons, setting expectations, and investigating reasonable model performance metrics for annual regional modeling simulations.

MATES-II Program

The Multiple Air Toxics Exposure Study (MATES II) was a monitoring and modeling program conducted by the South Coast Air Quality Management District (SCAQMD) in 1998-99. The study was initiated as part of the Environmental Justice Initiatives adopted by the South Coast Air Quality Management District Governing Board in October 1997. During MATES-II, approximately 30 air pollutants were monitored from April 1, 1998 to March 31, 1999 on 10 sites located in the South Coast Air Basin.

In addition to the monitoring, air quality modeling was performed using the Urban Airshed Model (UAM) and a newer version named UAM-TOX (Ligocki et al., 1992). The chemical mechanism used was the TOX mechanism, which is a version of the Carbon Bond IV (CB4), for UAM.

The MATES-II modeling domain was relatively small, 210 km by 120 km, however it used a fine grid (2x2 km²) and five vertical layers. Meteorological winds were prepared

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with CALMET. The MATES II domain is about 3.7 times smaller than the domain utilized in this project and described in a prior section of this Chapter.

EMFAC7G for calendar year 1998 was used for mobile sources, while area and point sources emissions were forecasted from a 1993 base year to 1998. The MATES-II program also included micro-scale monitoring and dispersion modeling using the ISCST3 model. Overall, both UAM and UAM-TOX model performance was within 50 to 80% of measured annual values (SCAQMD, 1999).

CRC/DOENREL Studies

The Coordinating Research Council (CRC) and the U.S Department of Energy (DOE) funded, through the National Renewable Energy Laboratory (NREL), two studies; one conducted by ENVIRON (CRC, 2002) using the photochemical model CAMx, and the other conducted by Seigneur et al. (Seigneur et al., 2003) using CMAQ,

The study conducted by ENVIRON (CRC, 2002) had as a primary objective to study the capabilities of photochemical models to simulate toxic air pollutants. This study is an update to the modeling performed during the MATES-II program (same time period and domain) using the Comprehensive Air Quality Model with Extensions (CAMx) and a reactive tracer module (RTRAC) versus UAM. CAMx/RTRAC is a state-of-the-science air quality model, with a special model to track reactive and inert toxic species using the Carbon Bond IV as a host chemical reaction mechanism. This study utilizes an updated emissions inventory with meteorological fields generated by CALMET (CRC, 2002). In general, the predicted and observed toxics annual average concentrations were within a factor of 2 from observations.

CAMx/RTRAC also contains provisions to interface with a sub-grid scale dispersion model (CRC, 2002). In this particular application, the ISC3 (Industrial Source Complex dispersion) model was used with hourly decay rates obtained from CAMx/RTRAC for sub-grid, near-source, modeling for a limited number of point sources (CRC, 2002).

CAMx/RTRAC was also applied by ENVIRON to the August 3-7, 1997 episode to compare the TOX mechanism with the SAPRC99 mechanism (Carter, 2000) for selected toxic air pollutants (CRC, 2002). For this episode, the MM5 meteorological model was used to generate meteorological variables using analysis nudging to the NCEP Eta analysis fields and observation nudging to the SCOS observed upper-air meteorological data. EMFAC2000 was used in generating mobile source emissions (CRC, 2002). For this limited model application, both mechanisms showed very similar performance for predicted benzene, however better performance was obtained with CBIV for acetaldehyde and formaldehyde (CRC, 2002).

A study, by Seigneur et. al. (2003), used the CMAQ air quality model to simulate benzene and diesel PM during the July 11-15 1995, episode in the northeastern United States. The modeling domain consisted of two nested grids. The outer grid had a horizontal resolution of 12-km and the inner grid had a resolution of 4-km. The results

of the coarse grid were used as boundary and initial conditions for the finer grid. Only the results of the last 3 simulation days were analyzed. Model results for benzene were compared to observations. For diesel PM, it was assumed that predicted diesel particulate concentrations contained 50% elemental carbon in their composition. Hence, predicted diesel particulate concentrations were compared to observed elemental carbon. The modeled predicted benzene with an error of 60%. Overall the general magnitudes of elemental carbon were well reproduced by the model (Seigneur et al., 2003).

ASPEN

Although the Assessment System for Population Exposure Nationwide (ASPEN) model is not a regional, photochemical model, two related projects are included for discussion here, since they have been used to estimate toxic air pollution on a regional basis.

ASPEN is a peer-reviewed, modified version of U.S. EPA's Human Exposure Model (HEM), which models long-term concentrations for simple terrain over large areas. The ASPEN model incorporates improvements to the HEM, including improved reactive decay, secondary compound formation, and particulate matter deposition. It uses a Gaussian formulation and meteorological frequency distributions to estimate long-term concentrations. For each emission source, the model calculates ground-level concentrations as a function of distance (from 0.1 km to 50 km).

The Office of Policy of the U.S. EPA funded an air toxics modeling study for 148 pollutants identified as hazardous air pollutants (HAPS). This study was completed in 1999. The ASPEN modeling domain included the continental United States and the spatial resolution was at the census-tract level. For this modeling the national, 1990 base-year emissions inventory was stratified into 10 categories. Reactive species were modeled with first-order decay, low-reactive species were modeled as inert, and the formation of secondary pollutants was parameterized. The ASPEN model consistently underestimated concentrations (Rosembaum *et al.*, 1999).

ARB has independently exercised the ASPEN model, also at the census tract level, on the State of California. Emissions for years 1990, 2000, and 2010 have been extrapolated from a 2000 base year (Francis, ARB, 2000). Risk maps have been produced for each year modeled and are available at ARB's web page (<http://www.arb.ca.gov/toxics/cti/hlthrisk/hlthrisk.htm>). Consistent with the above study, the ASPEN model tended to underestimate observed concentrations.

Ozone Performance Metrics and Expectations

Historically, regional air quality models have been used to predict 1-hour ozone for the purpose of evaluating emissions control strategies to support ozone State Implementation Plans (SIPs). Most of this modeling has been geared to the high ozone season on an episodic basis. Thus, regulatory agencies and the scientific community

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have extensive experience applying photochemical models to simulate 1-hour episodic ozone and, as a result, 1-hour model performance metrics are well established (ARB, 1992).

There are a number of reasons to evaluate annual model performance for ozone as part of toxic modeling. The primary reason is that ozone formation is well understood and model performance metrics for 1-hour ozone are readily available. Another reason is that good ozone performance may provide a level of comfort that the air quality model is generating the appropriate ambient conditions for the degradation or formation of reactive toxic air pollutants. For example, some of the toxic air pollutants considered can be highly reactive (1,3-butadiene) while others are formed mainly through atmospheric reactions (like formaldehyde).

A condensed description of the 1-hour ozone metrics is provided below (ARB, 1992). These performance standards have been exclusively used in conjunction with episodic simulations, and there is very little experience on annual performance metrics. In short, ARB recommends 1-hour ozone peak accuracy of $\pm 20\%$, 1-hour ozone bias of $\pm 15\%$, and 1-hour ozone gross error of $\pm 35\%$ (For a more detailed description of these metrics, see ARB, 1992).

Peak Ratio. The peak ratio compares the highest daily ozone measurement with the corresponding highest value predicted by the model. In an ideal situation the ratio should be one, implying an exact correspondence of model and observations; however, in practical applications, model predictions of peak ozone that are $\pm 20\%$ from measurements are considered acceptable.

Bias. Bias provides an indication of the degree to which modeled hourly concentrations are over or under-predicted. Bias is calculated for each day simulated. A bias close to zero implies good agreement between model predictions and observations. Practically, a bias of $\pm 15\%$ is acceptable (ARB, 1992).

Gross Error. The gross error is an indication of how model predictions differ in an absolute sense from observations over time (for the annual ozone performance analysis, gross error is calculated daily). As gross error approaches zero, it implies better agreement among predictions and observations. Practically, a gross error value of $\pm 35\%$ is acceptable.

Historically, 1-hour ozone performance is evaluated only when predicted and observed concentrations pairs are above a threshold of 60 ppb (ARB, 1992). This has the effect of evaluating the model's ability to reproduce ozone above that threshold, and has been typically deemed adequate for high ozone episodes. This value also assures that there will not be a division by a very low observed value that could negatively impact the performance assessment.

Winner and Cass (1999) applied the CIT regional model to simulate ozone concentrations for the entire 1987 calendar year, and also analyzed their results in terms of the frequency distribution of observed and predicted ozone concentrations. Their global results are within the typical performance range for episodic simulations. More specifically, annual ozone simulations with the CIT model over predicted the daily peak ozone by 14% and had a gross error of 35%, and a bias of 15% over the entire year. However, a 60 ppb threshold was used for the entire year. This effectively limits the performance evaluation to only those seasons of the year where ozone is above that threshold. This may be appropriate for the high ozone season but not for a winter season, where most of the prediction/observation pairs are below this threshold.

Per the discussion above and to assess annual ozone model performance for this project, 1-hour performance metrics will use a threshold of 60 ppb for the months of March–October, and 30 ppb for January–February and November–December.

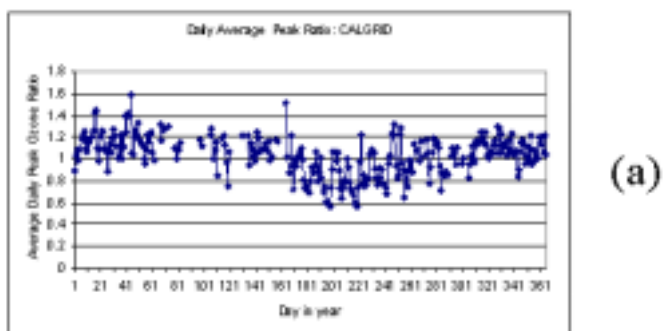
Ozone Performance

The ozone predictions from the two air quality models were compared against ozone measurements from 72 air quality monitoring sites in the modeling domain for the period January 1 through December 31, 1998. As discussed above, performance statistics were calculated for each day simulated. An acceptable comparison between ozone predictions and observations provides a level of assurance that the model results can be trusted. Assessing ozone performance also provides a level of assurance that the air quality model is generating the appropriate ambient conditions for the degradation/formation of reactive species.

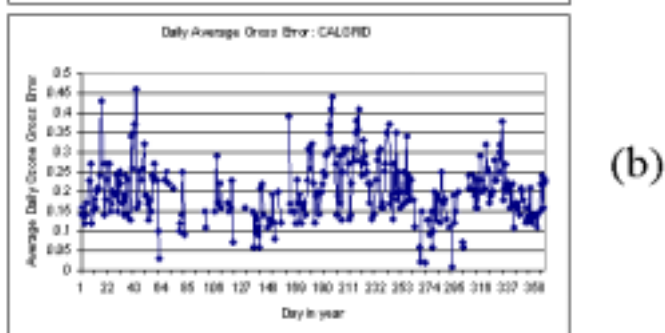
Figure 5.18 shows the domain wide peak ratio, gross error, and bias for CALGRID. Table 5.20 summarizes the ozone performance statistics for each month in 1998 for both CALGRID and CMAQ (recall that CMAQ was only run for one month each season). On average, CALGRID shows an over prediction of peak 1-hr ozone of 5%, with a normalized error of 21% and a normalized bias of 3% over the entire 1998 calendar year. For the 4 months simulated, CMAQ shows, on average, a 13% under prediction of peak ozone, an 18% normalized gross error and a –8% bias. These values agree with the Winner and Cass results (1999) and are in the range of values that are deemed acceptable (ARB, 1992). Also, these results indicate that the overall model performance of CALGRID is similar to that of CMAQ.

Based on the recommendations from Winner and Cass (1999), an additional assessment of ozone model performance is provided by comparing the model-predicted and observed ozone frequency distribution for 1998. Both models tend to over-predict or under-predict the frequency of low ozone concentrations in the winter months (Figure 5.19a). In addition, both models tend to over predict the frequency of ozone concentrations during the warmer months (Figure 5-19b).

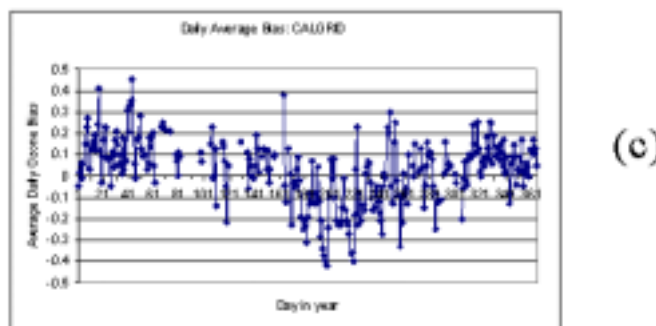
Figure 5.18 - Daily domain averaged statistics for 1-hr ozone, (a) peak ratio, (b) gross error, and (c) bias using results from CALGRID for 1998.



(a)



(b)



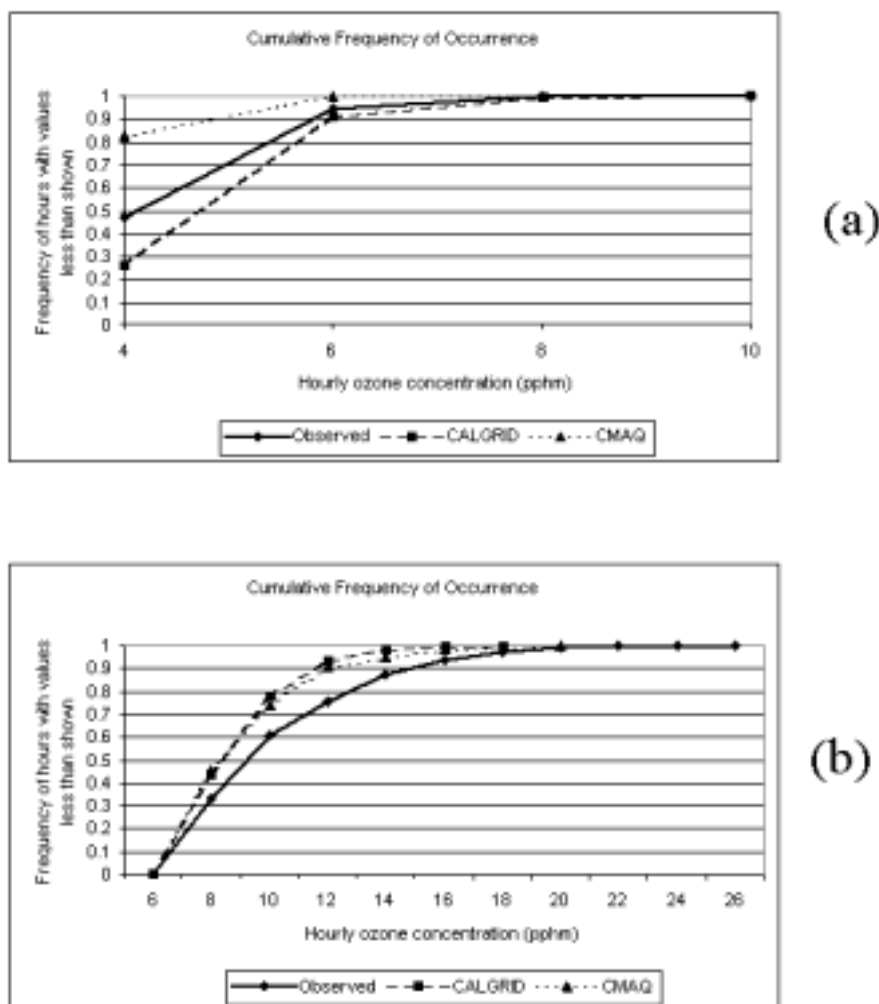
(c)

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Table 5.20 - Monthly ozone performance statistics for 1998

Period	Peak Ratio		Gross error %		Bias %	
	CALGRID	CAMQ	CALGRID	CAMQ	CALGRID	CAMQ
January	1.12	0.97	0.19	0.15	0.10	-0.02
February	1.18	--	0.22	--	0.14	--
March	1.13	--	0.18	--	0.11	--
April	1.10	0.92	0.18	0.13	0.06	-0.07
May	1.11	--	0.14	--	0.07	--
June	0.94	--	0.20	--	-0.07	--
July	0.81	--	0.26	--	-0.17	--
August	0.82	0.87	0.27	0.24	-0.14	-0.07
September	0.96	--	0.21	--	-0.04	--
October	0.98	--	0.16	--	-0.02	--
November	1.10	0.81	0.23	0.18	0.07	-0.12
December	1.06	--	0.16	--	0.05	--
Annual	1.05	0.87	0.21	0.18	0.03	-0.08

Figure 5.19 - Cumulative frequency of occurrence of predicted and observed 1-hr ozone concentration from 72 sites in domain for 1998: a) January, February, November and December, and b) March through October. In (a) all observation-prediction pairs are plotted where observed ozone is 30 ppb or higher, and in (b) includes observation-prediction pairs with observed ozone equal or higher than 60 ppb.



Toxic Air Pollutant Performance Metrics and Expectations

Use of regional air quality models to simulate annual average toxic air pollutant concentrations is a relatively new field. In typical ozone air quality applications, almost all the reactive hydrocarbons are lumped together. In toxic air pollutant modeling simulations, the toxics are explicitly represented in the models and their inputs. Therefore, for toxics simulations, model performance must be evaluated independently for each toxic air pollutant. Previous studies have extended the metrics used for ozone

performance to also evaluate toxic air pollutant model performance. Comparison of predicted and observed annual averages under previous studies suggests that air quality models can predict annual average concentrations that are within a factor of 2-3 for *most* toxic air pollutant simulated (SCAQMD, 1999; CRC, 2002; Seigneur et al. 2002). For example, these studies suggest that predicted-observed pairs for air pollutant such as benzene, 1,3-butadiene, formaldehyde and acetaldehyde are, overall, within a factor of 2-3 (or better) of observations. However, several species have observations that are very close or below the detection limit and, as a result, cannot be easily compared with predictions.

As an initial step, and based on the limited experience available, it is assumed that model predictions for most toxic species will fall within a factor of 2-3 of observations. In addition, previous toxics simulations have not used a threshold for any toxic species. The same approach will be used here. The use of detection limits as thresholds will be investigated during the Wilmington study. Basing regional performance metrics upon such little experience must be qualified. There currently isn't enough information to judge whether the factor of 2-3 found in previous studies constitutes a measure of good model performance for toxics, or if smaller factors are more appropriate. In addition, there isn't agreement on what constitutes an acceptable error or bias for each toxic.

Toxic Air Pollutant Performance

As mentioned above, there are no accepted air quality model performance standards for toxic air pollutants. Nevertheless, towards the goal of establishing metrics, it is important to compare model predictions with observations and also assess how well new model performance results compare with previous studies. This section presents comparisons of model predictions for each toxic against measurements collected at stations in ARB's regional toxic network. Comparisons with the results of other studies will also be made, such as MATES-II (SCAQMD, 1999; CRC, 2002).

Comparison with Monitoring Results

We compared the air quality model predictions from CALGRID and CMAQ against the measured toxic concentrations obtained from ARB's toxics monitoring network during the period January 1- through December 31, 1998. Recall that CALGRID was run for 365 days and CMAQ for only one month in each season. This was done to compare the results of both models, as well as to see the impact of modeling a coarser time period. The selection of months to model CMAQ was established before the start of this study. Table 5.19 clearly shows that large errors can potentially be introduced when modeling a coarser time period such as that used with CMAQ. Therefore, the CMAQ results in all the following figures and tables are only shown for comparison purposes.

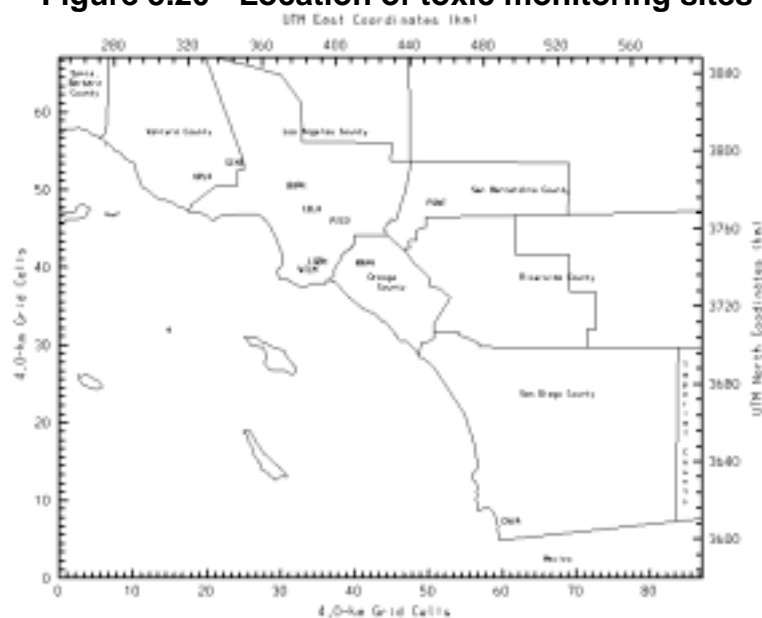
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The sampling schedule at the monitoring stations is 1 sample every 12 days. 24-hr samples are collected for each target toxic air pollutants. A total of 11 toxic monitoring sites are located in the modeling domain. Table 5.21 lists the 11 toxics sites and Figure 5.20 shows their location in the domain. Except for stations in Chula Vista and Simi Valley, all sites are in the South Coast Air Basin.

Table 5.21 - Sites Used in Toxics Model Performance Evaluation

ID	Site Name
ANAH	Anaheim-Harbor Blvd
BURK	Burbank
CELA	Los Angeles-North Main Street
CHVA	Chula Vista
FONT	Fontana-Arrow Highway
LGBH	North Long Beach
PICO	Pico Rivera
RIVR	Riverside-Rubidoux
SIMI	Simi Valley – Cochran Street
UPLA	Upland
WILM	Wilmington

Figure 5.20 - Location of toxic monitoring sites in modeling domain



Annual summary statistics for each organic toxic specie (averaged over all sites) are given in Table 5.22 for CALGRID. Note that we added acetone (ACET), methyl t-butyl ether (MTBE), and methyl ethyl ketone (MEK) for model evaluation. Note that when comparing against monitoring results formaldehyde and acetaldehyde are the sum of primary (i.e., those resulting from direct emissions) and secondary (i.e., those formed by photochemical reactions) contributions. No thresholds were used in this toxics performance evaluation. If a species was not detected at a monitoring site, its concentration is reported as the instrument detection limit, which was compared to the

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model predictions. We recognize that this will introduce an error and bias for some species. Most annual concentrations of the toxic gases were predicted within a factor 2-3 of observations, which is in agreement with previous studies. Maximum predicted concentrations over the domain are of the same order of magnitude as the measurements during 1998. Bias and error are significant for most gaseous species. Similar results were obtained from CMAQ (not shown).

Table 5-23 shows summary performance statistics for hexavalent chromium and particulate matter species. Note that we included iron in our evaluation. Diesel PM is not measured directly. We compared our model predictions against observed elemental carbon measurements. Other studies (Seigneur, 2002) have assumed that 50% of the diesel PM is elemental carbon. Note that performance statistics for PM mercury are not included in our evaluation, since our models did not capture its complex environmental reactions. No thresholds were used in this toxics performance evaluation. If an air pollutant (such as hexavalent chromium) was not detected at a monitoring site, its concentration is reported as the instrument detection limit which was compared to the model predictions. This will introduce an error and bias for some air pollutants.

Table 5-23 shows that CALGRID significantly underpredicted almost each toxic PM air pollutant, with the exception of PM arsenic and PM iron. For some species, such as hexavalent chromium, it could be due to a large number of observations below the detection limit. Similar results were obtained with CMAQ (not shown), which suggests a potential deficiency in the inventory for hexavalent chromium or other PM species.

Table 5.22 - Domain-averaged Annual Model Performance for CALGRID during 1998 for Selected VOCs

Key	Predicted Annual Average (ppb)	Observed Annual Average (ppb)	Maximum Predicted (ppb)	Maximum Observed (ppb)	Average Norm. Bias	Average Norm. Error
Acetone	4.93	2.06	16.59	10.00	3.75	3.82
Methyl ethyl ketone	1.16	0.29	5.13	2.20	7.51	7.53
Methyl t-butyl ether	2.50	2.46	7.65	10.00	0.40	0.67
1,3-Butadiene	0.20	0.28	0.72	1.41	0.32	0.86
Benzene	1.22	0.96	4.73	5.20	1.20	1.41
Toluene	4.03	2.67	15.96	11.40	2.51	2.65
Acetaldehyde	3.01	1.60	9.81	10.30	2.56	2.61
Chloroform	0.002	0.05	0.011	0.11	-0.95	0.95
Dichloromethane	0.66	0.70	4.22	7.20	0.72	1.38
Formaldehyde	2.36	3.53	6.95	13.60	0.17	0.77
Xylenes	2.38	1.23	9.92	8.10	7.81	7.90
PDCB	0.21	0.14	0.43	0.80	1.45	1.79
Perchloroethylene	0.27	0.23	0.80	2.60	2.34	2.58
Styrene	0.07	0.25	0.33	8.00	-0.29	0.65
Ethylene dichloride	0.013	0.07	0.03	0.05	-0.74	0.74
Vinyl Chloride	0.008	0.100	0.06	0.10	-0.92	0.92

a) 9-month average

Table 5.23 - Domain-averaged Model Performance for CALGRID during 1998 for Selected Particulate Matter Species

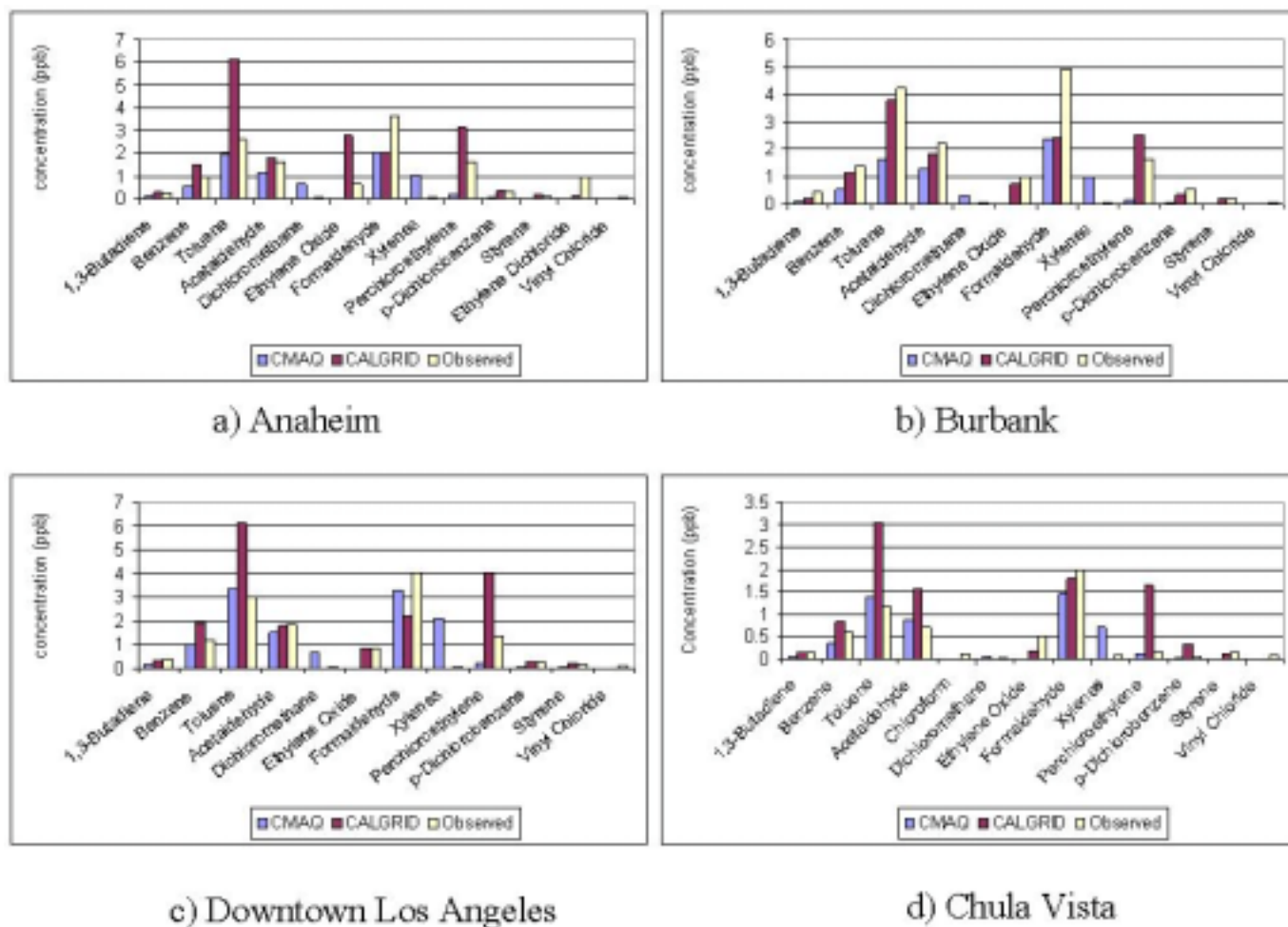
Spec.	Predicted Annual Average (ng/m ³)	Observed Annual Average (ng/m ³)	Maximum Predicted (ng/m ³)	Maximum Observed (ng/m ³)	Annual Average Norm. Bias	Annual Average Norm. Error
Hexavalent Chromium	0.05	0.13	0.18	0.90	-0.57	0.68
Elemental Carbon ^a	1,750	8,140	5,560	9,829	-0.26	0.53
PM Arsenic	1.31	1.71	5.89	4.00	-0.23	0.60
PM Cadmium	1.39	6.46	3.99	192.70	-0.72	0.72
PM Iron	1087.16	1555.56	3577.09	5874.30	4.03	4.58
PM Lead	26.74	147.05	80.69	2123.00	2.23	2.79
PM Manganese	21.81	331.96	69.03	9101.00	1.29	2.08
PM Nickel	1.68	4.90	8.03	95.00	-0.10	1.00
PM Zinc	29.91	106.33	81.90	5137.43	0.21	1.23

a) Predicted is Diesel PM and observed is elemental carbon

Significant discrepancies between model predictions and observations at particular monitoring sites may indicate potential deficiencies in model inputs. Figure 5.21(a)-(i) compares the predicted annual average concentrations for toxic hydrocarbons against the observed annual average concentrations at each toxic site in the domain. This figure demonstrates that model predictions are between a factor of 2-3 of observations for most toxic hydrocarbons. Figure 5.22 (a)-(l) compares hexavalent chromium, and PM species against observations at selected sites. Although both CALGRID and CMAQ results are shown, the reader should recall that CMAQ was only run for one month of each season while CALGRID was applied for all 365-days in the year. As mentioned before, large errors can be introduced when modeling one month of each season (see Table 5.19). Most measurements of hexavalent chromium are below the detection limit of 0.1 ng/m³; however, model predictions are also below this detection limit. For most PM species, the models did not perform well.

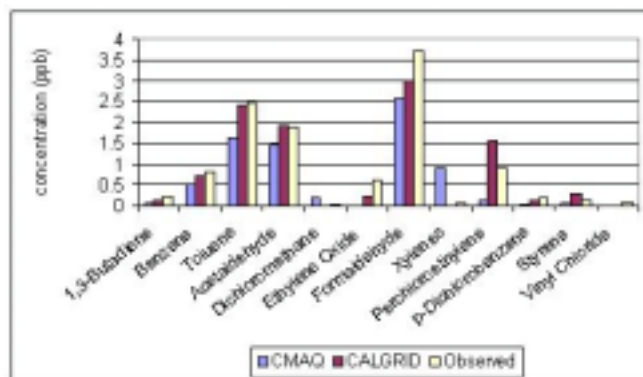
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Figure 5.21 - Predicted and observed annual average concentrations at Anaheim, Burbank, Downtown Los Angeles and Chula Vista (January 1-December 31, 1998)

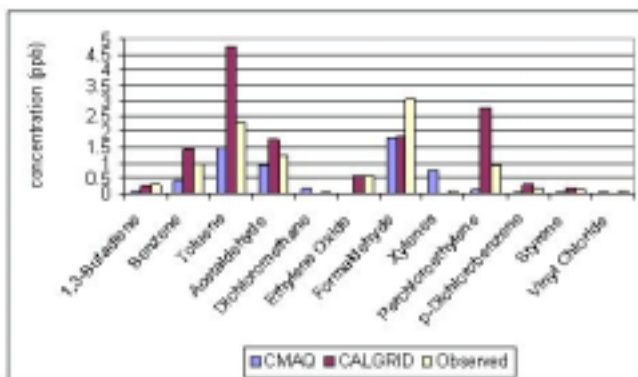


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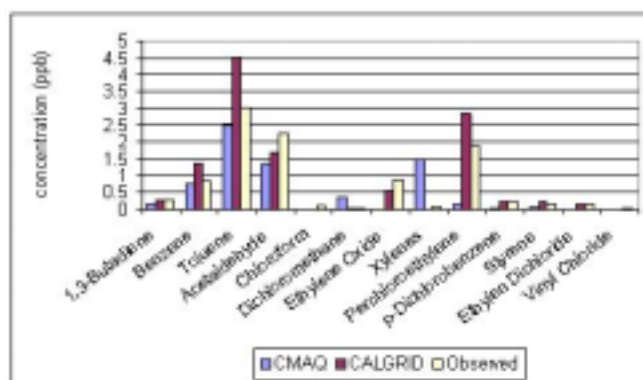
Figure 5.21 (continued) - Predicted and observed annual average concentrations at Fontana, Long Beach, Pico Rivera and Riverside (January 1-December 31, 1998)



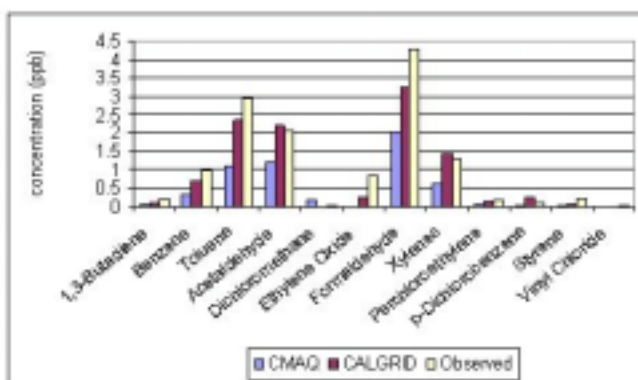
e) Fontana



f) Long Beach

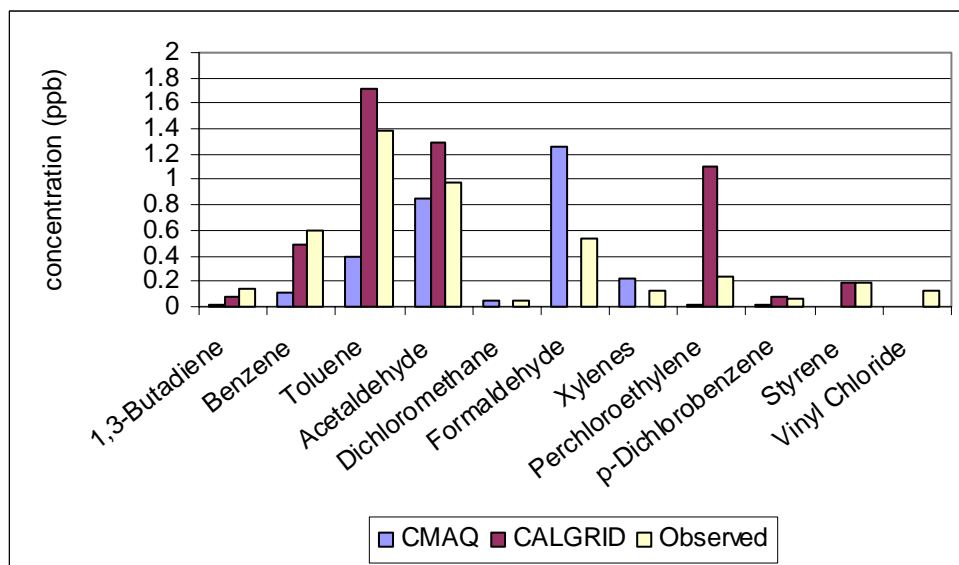


g) Pico Rivera



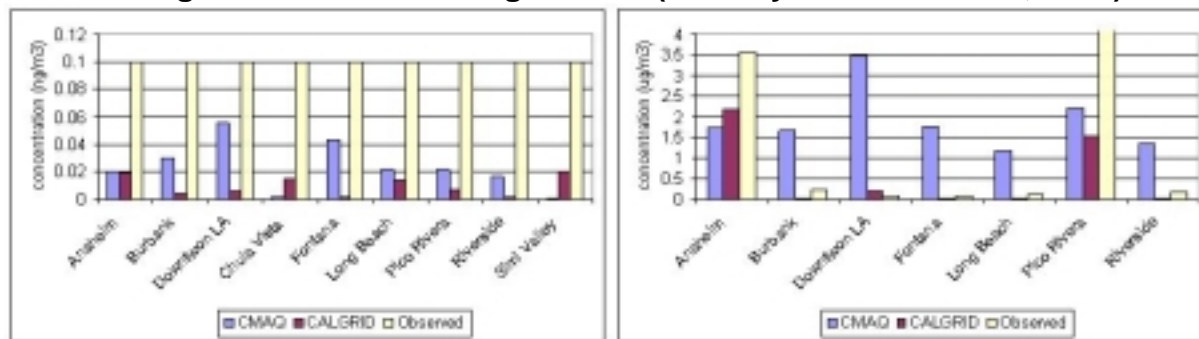
h) Riverside

Figure 5.21 (continued) - Predicted and observed annual average concentrations at Simi Valley (January 1-December 31, 1998)



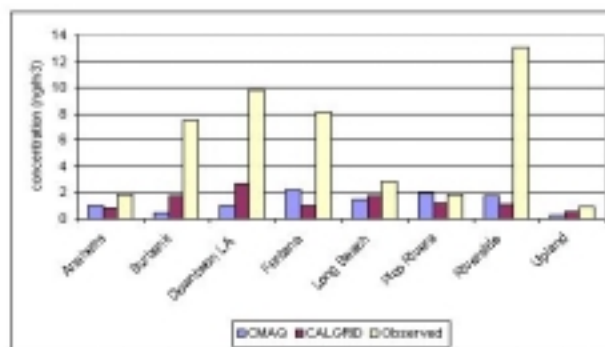
i) Simi Valley

Figure 5.22 - Predicted and observed annual average concentrations at toxic monitoring sites in the modeling domain (January 1-December 31, 1998)



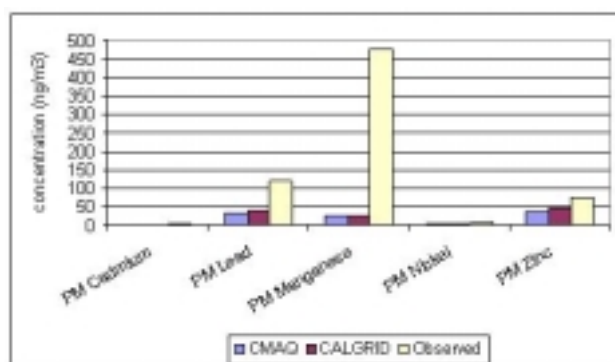
a) Hexavalent chromium

b) Diesel PM10 vs Elemental Carbon

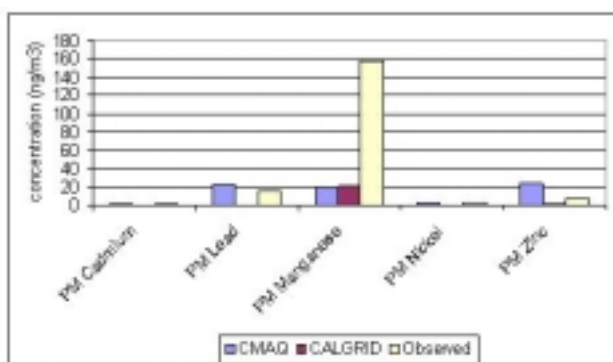


c) PM Arsenic

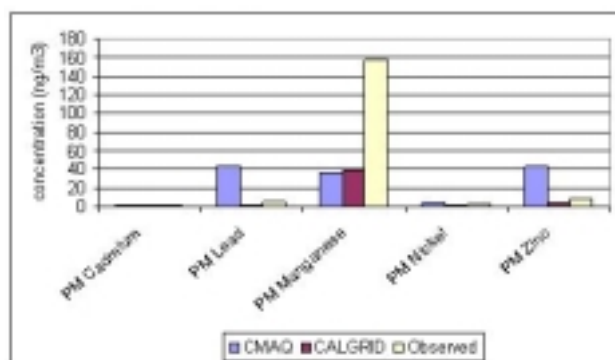
Figure 5.22 (continued) - Predicted and observed annual average concentrations at toxic monitoring sites in the modeling domain (January 1-December 31, 1998)



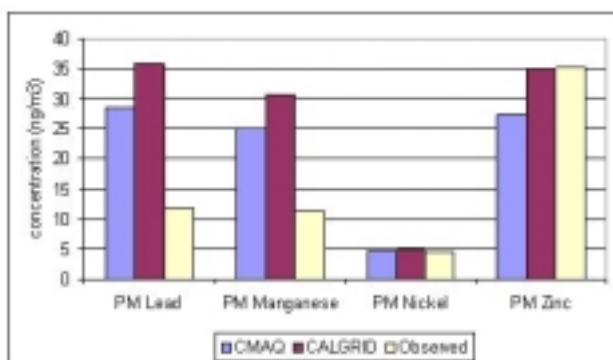
d) Anaheim



e) Burbank



f) Downtown Los Angeles



g) Chula Vista

Figure 5.22 (continued) - Predicted and observed annual average concentrations at toxic monitoring sites in the modeling domain (January 1-December 31, 1998)

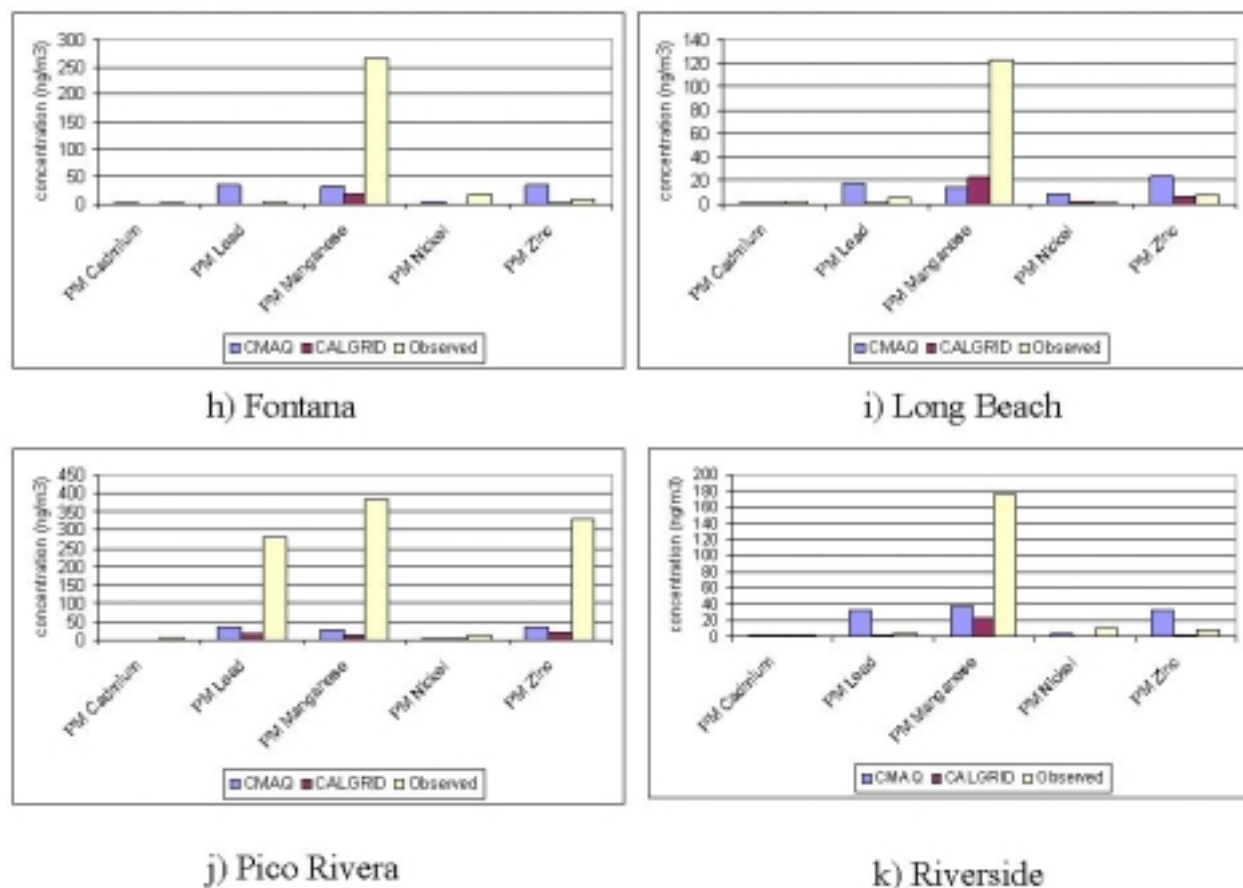
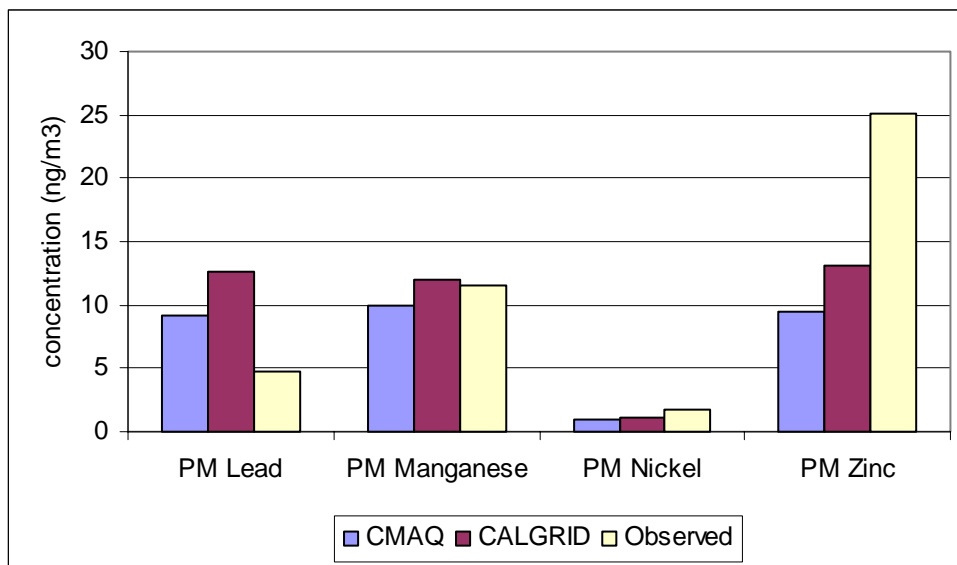


Figure 5.22 (continued) - Predicted and observed annual average concentrations at toxic monitoring sites in the modeling domain (January 1-December 31, 1998)



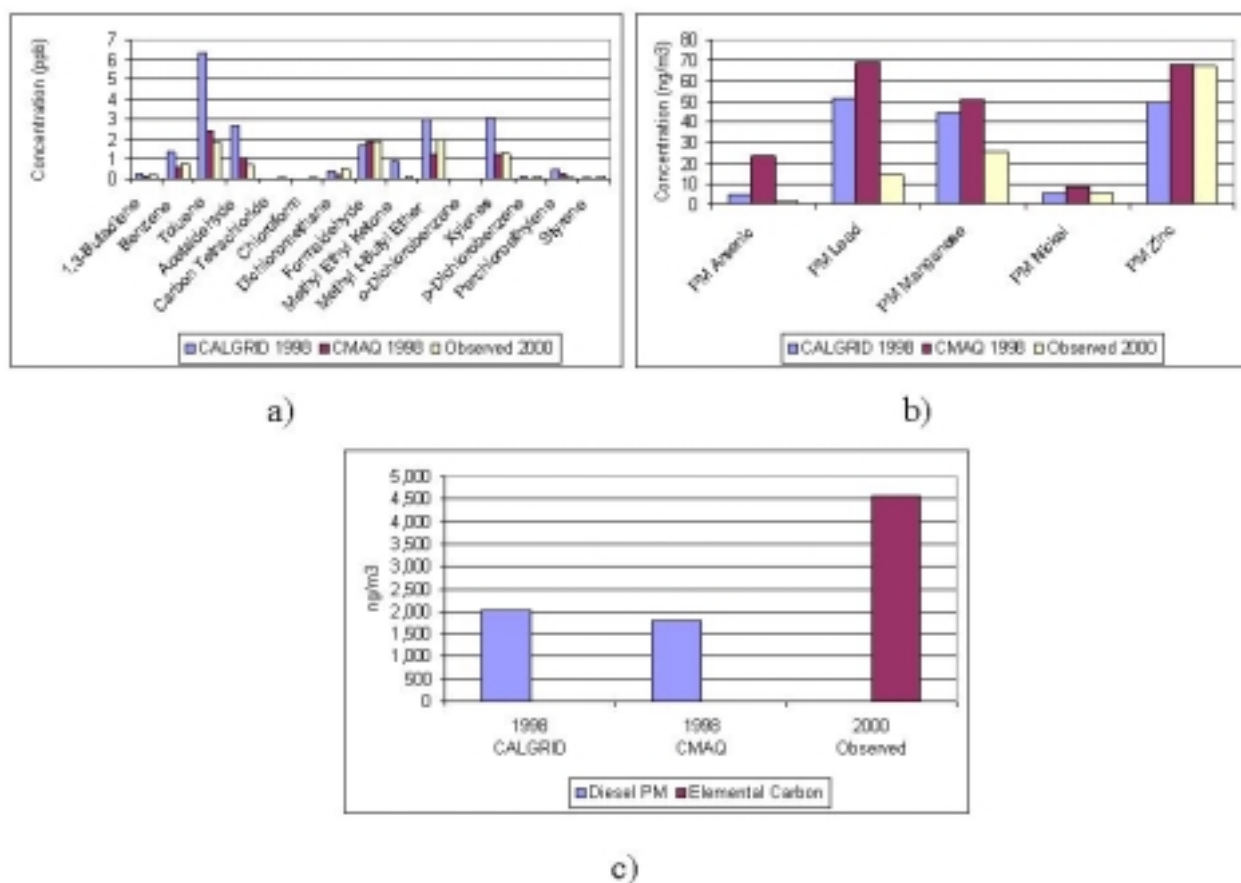
l) Simi Valley

Comparison At Memorial Academy

As described in Chapter 2, a special air quality monitoring study was conducted at Memorial Academy, Chula Vista and El Cajon sites from October 1999 through February 2001. Figure 5.23 presents the annual average concentrations for selected VOCs and PM toxics as predicted for 1998 with both CALGRID and CMAQ, together with concentrations measured at Memorial Academy in 2000. Although both CALGRID and CMAQ results are shown, the reader should recall that CMAQ was only run for one month of each season while CALGRID was applied for all 365-days in the year. As mentioned before, large errors can be introduced when modeling one month of each season (see Table 5.19).

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Figure 5.23 - Comparison of annual average toxic air pollutant concentrations at Memorial Academy as predicted for 1998 by CALGRID and CMAQ, with those measured in 2000: a) selected VOCs, b) PM species and c) diesel PM (compared to observed elemental carbon) and PM Iron. The limit of detection was used in calculating the observed annual averages. Note that observed PM concentrations correspond to the PM10 size fraction.



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Comparison with MATES-II (UAM)

The MATES-II monitoring and modeling study covered the period April 1, 1998 through March 31, 1999. Results from CALGRID and CMAQ (SAPRC-99, a 4-km x 4-km grid cell, and 10 to 17 layers) are in general agreement with those obtained during the MATES-II study (UAM using the Carbon-Bond IV mechanism, a 2-km x 2-km cell grid size, and 5-layers).

Comparison with the CRC/DOE/NRL study (CAMx/RTRAC)

As discussed previously, the CRC/DOE/NRL study conducted by ENVIRON used the Comprehensive Air Quality Model with Extensions (CAMx) with a reactive tracer module (RTRAC) to update the MATES-II modeling. This study utilizes an updated emissions inventory (using both EMFAC7G and EMFAC2000), with meteorological fields generated by CALMET (CRC, 2002).

Table 5.24 shows the domain annual average concentration for four toxic VOCs, as predicted by the CALGRID and CMAQ air quality models during 1998, together with those predicted by the CAMx/RTRAC model (with EMFAC2000 motor vehicle emissions) and the observed values. Except for formaldehyde, the CAMx/RTRAC and CALGRID predictions are within a factor of two of observations.

Table 5.24 - Comparison with MATES-II Update by ENVIRON (CRC, 2002)

Species	CAMx/RTRAC ^a (EMFAC2000) ($\mu\text{g}/\text{m}^3$)	CALGRID ^b ($\mu\text{g}/\text{m}^3$)	Observed ^b ($\mu\text{g}/\text{m}^3$)
Benzene	5.55	3.96	3.13
1,3-Butadiene	0.61	0.44	0.64
Acetaldehyde	3.04	5.44	2.99
Formaldehyde	9.10	2.93	4.46

a) Average from April 1998 through March 1999

b) Averages for 1998

In summary, regional simulation results for toxic hydrocarbon concentrations compare relatively well with observations and with the results of previous studies. The PM species do not compare well with observations and suggest potential deficiencies in the model inputs.

5) Regional Modeling Results for Toxic Air Pollutants

In this section, we will show the types of concentration gradients that the models predict across the domain, and around the Barrio Logan neighborhood in particular. Background concentrations caused by sources outside Barrio Logan are also presented.

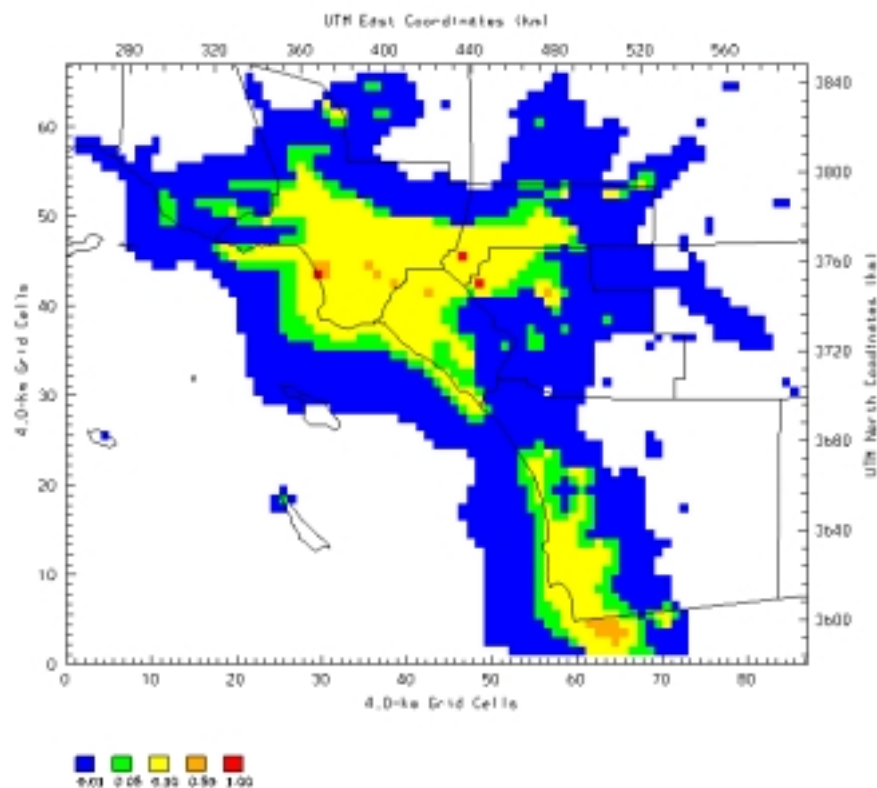
Concentration Gradients Across the Domain

Plots of simulated concentration gradients are used to qualitatively assess whether the concentration gradients predicted by the model follow expected patterns, given our knowledge of emissions, meteorology, and air quality in a modeling domain.

Figures 5.24– 5.29 display annual average concentration gradients for selected toxics derived from CALGRID. 1-3-butadiene (Figure 5.24) is emitted mainly from motor vehicles and the model predicts higher concentrations in the urban area, as expected. Perchloroethylene (Figure 5.25) is used in the dry cleaning industry and its distribution also follows the population distribution. Formaldehyde (Figure 5.26) is mostly formed as a secondary pollutant product in ambient air from photochemical reactions involving emitted hydrocarbons. As a result, high formaldehyde concentrations are predicted downwind of urban areas. Hexavalent chromium (Figure 5.27) is emitted from operations like chrome plating and the model predicts high concentrations close to the emission sources and a low concentration plume indicating the transport taking place in the domain together with the dilution and deposition effects downwind of the sources.

The boundary conditions used for hexavalent chromium were high, but don't appear to affect the model results. Figure 5.28 shows the spatial distribution of annual benzene concentrations, where higher concentrations are predicted in the urban areas and on the highways. The model also shows that benzene is transported to a large area of the domain, although its concentration drops fast outside of urban areas. Figure 5.29 displays the spatial distribution of the annual concentrations of Diesel PM as predicted by CALGRID. The model predicts high concentrations over the urban area, which rapidly declines as one moves away from urban areas.

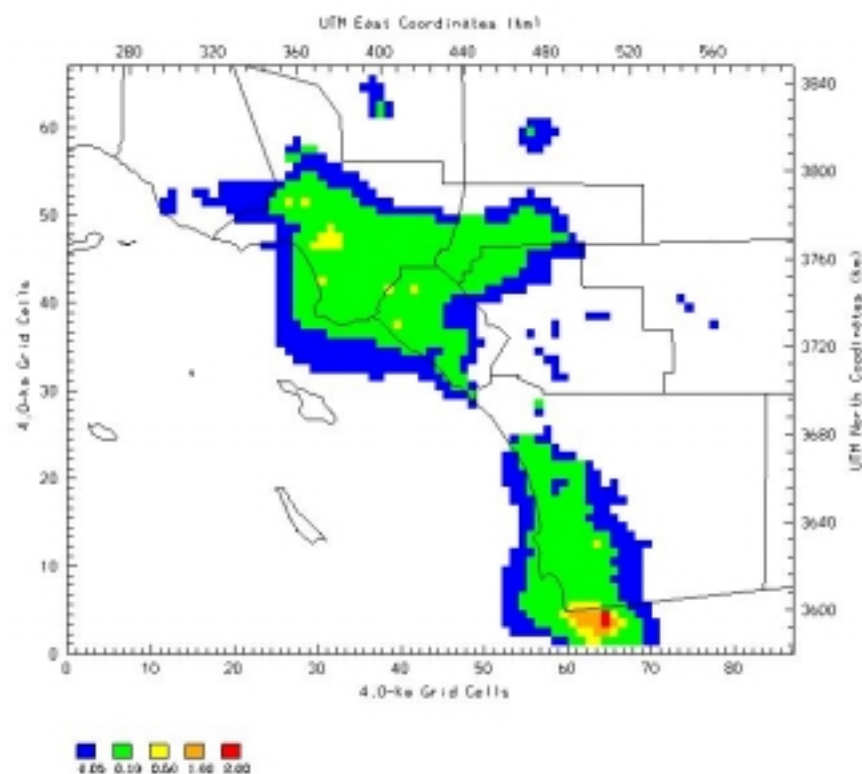
Figure 5.24 - Predicted annual average concentrations for 1,3-Butadiene using CALGRID (January 1-December 31, 1998)



1,3-Butadiene 1998 Annual Average (ppb).

Domain maximum of 1.51 ppb at (30,44)

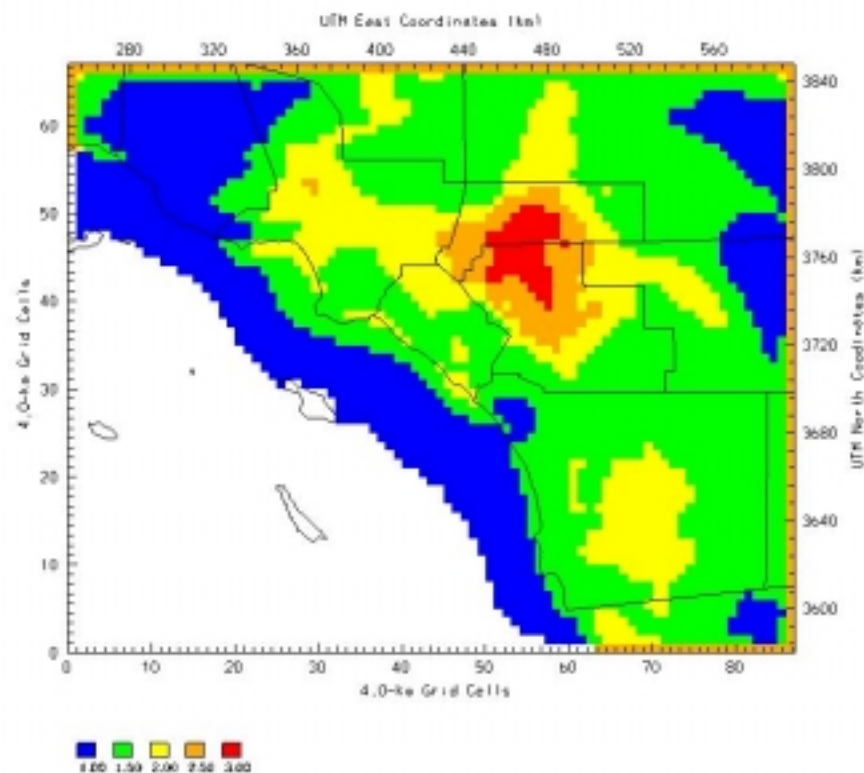
Figure 5.25 - Predicted annual average concentrations for Perchloroethylene using CALGRID (January 1-December 31, 1998)



Perchloroethylene 1998 Annual Average (ppb).

Domain maximum of 2.024 ppb at (65,5)

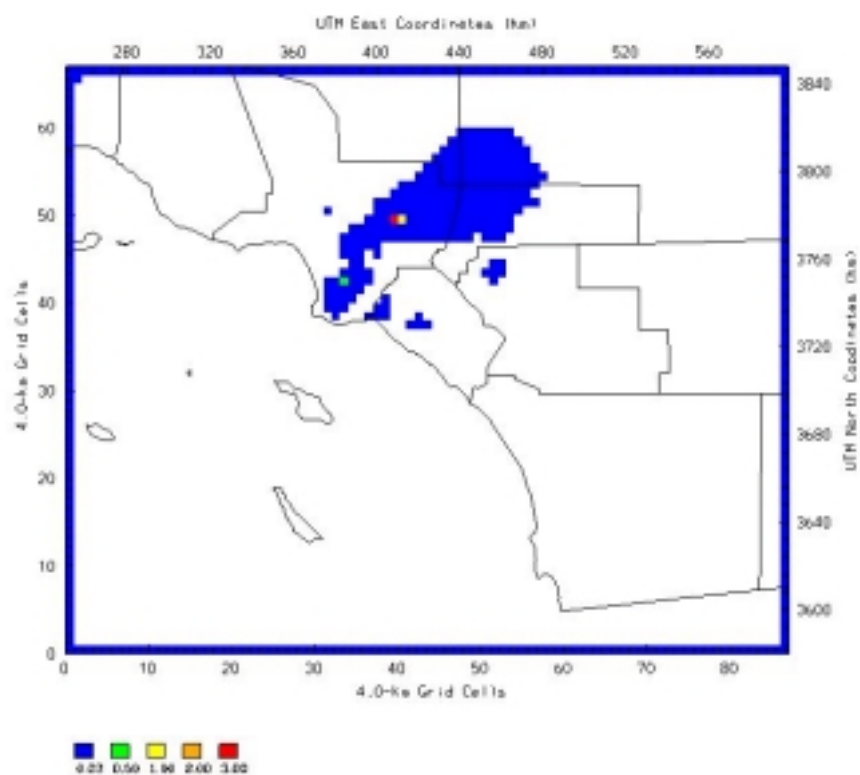
Figure 5.26 - Predicted annual average concentrations for Formaldehyde using CALGRID (January 1-December 31, 1998)



Formaldehyde 1998 Annual Average (ppb).

Domain maximum of 3.987 ppb at (57, 42)

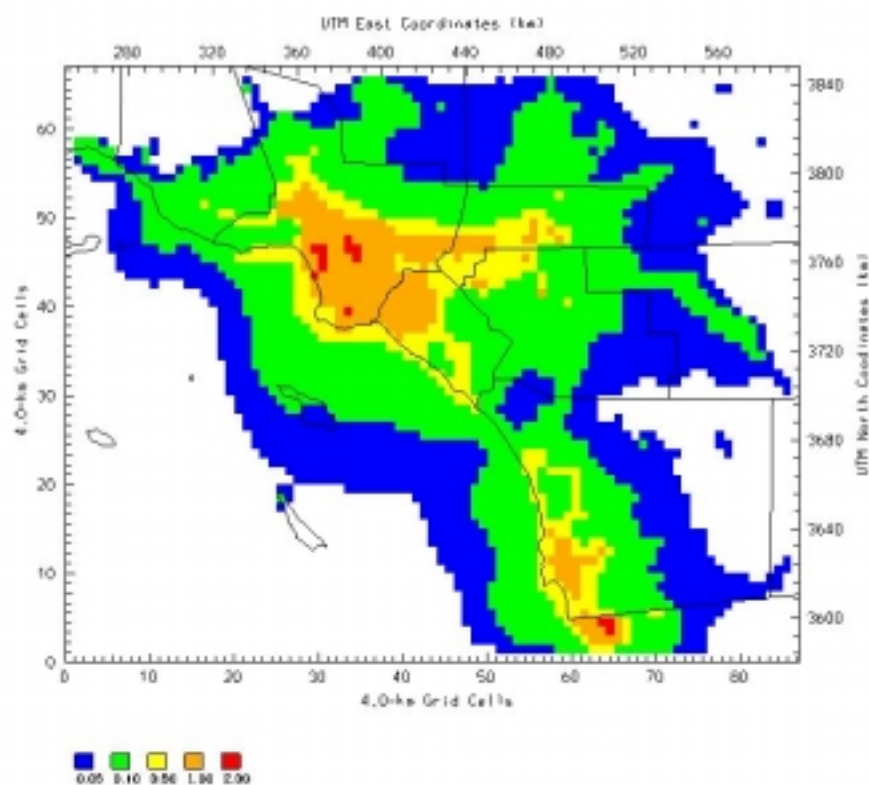
Figure 5.27 - Predicted annual average concentrations for Hexavalent Chromium using CALGRID (January 1-December 31, 1998)



Hexavalent Chromium 1998 Annual Average (ng/m³).

Domain maximum of 3.275 ng/m³ at (40, 50)

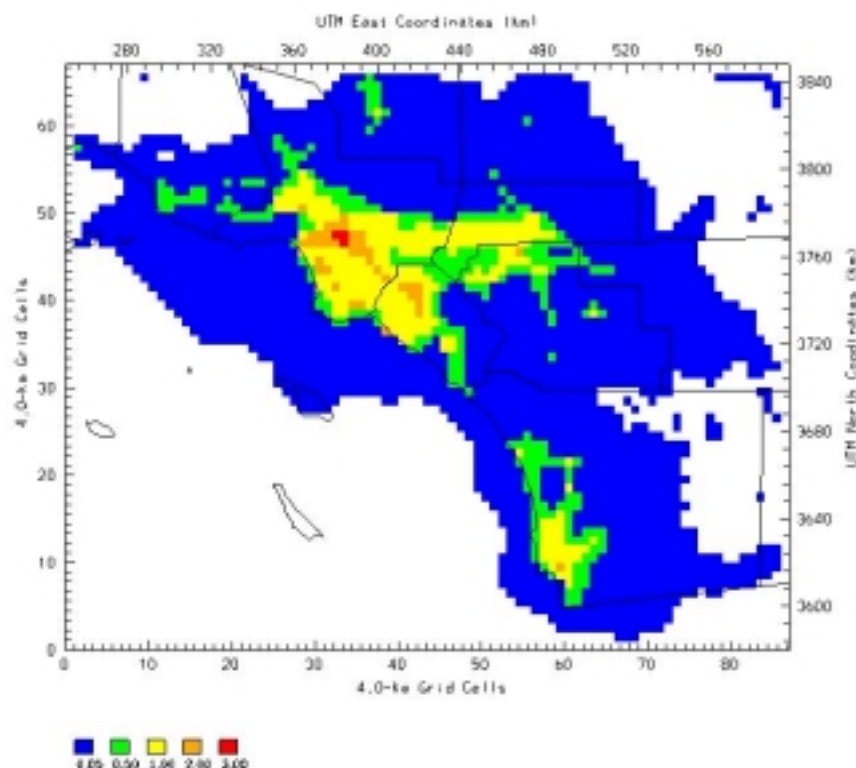
Figure 5.28 - Predicted annual average concentrations for Benzene using CALGRID (January 1-December 31, 1998)



Benzene 1998 Annual Average (ppb).

Domain maximum of 2.365 ppb at (65, 4)

Figure 5.29 - Predicted annual average concentrations for Diesel PM using CALGRID (January 1-December 31, 1998)



Diesel PM 1998 Annual Average ($\mu\text{g}/\text{m}^3$)

Domain maximum of $3.948 \mu\text{g}/\text{m}^3$ at (34, 48)

Background Concentrations in Barrio Logan

The term “background concentration” has widely different meanings depending on the effect being investigated (Collins, 1995). For this particular study, background concentration is defined as the concentration due to all sources outside the area of interest, specifically outside a given grid-cell in the domain. The concentrations due to sources outside the area of interest are a baseline upon which the effects of sources inside the area of interest are imposed.

The neighborhood of Barrio Logan is enclosed in a single 4-km x 4-km grid cell in the regional domain. Background toxic air pollutant concentrations in Barrio Logan are those concentrations due to emission sources outside the grid-cell where Barrio Logan is located. A simple way to estimate background levels is by eliminating emissions in the grid cell where Barrio Logan is located. However, because of the complex interaction of the atmospheric photochemistry, there is the concern that if we reduce the emissions of a reactive precursor in the Barrio Logan grid cell, it will impact the overall chemistry of the neighboring cells potentially affecting the predicted background

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concentrations for reactive species and secondary species. This is especially true for the reactive species like 1,3-butadiene, formaldehyde, and acetaldehyde. However, if the emissions inside the grid cell are very small compared to all sources outside that grid cell, a reduction or elimination of the emissions inside the grid cell would have little effect on the annual average concentrations at this location.

Table 5.25 shows the model species inventory at the county level and for the Barrio Logan cell for a typical summer weekday in 1998. Of note is that the emissions from the cell where Barrio Logan is located only represents a few percent of the total San Diego County emissions. As a result, it is expected that removal of the emissions from the cell where Barrio Logan is located will have a very small impact on predicted concentrations. However, other factors such as terrain topography and meteorology could affect this expectation.

To test the impacts of this assumption, two annual simulations were conducted using the CALGRID model. The first simulation includes all the emissions in the domain (baseline simulation) and the second annual simulation excludes all emissions from the grid cell where Barrio Logan is located. Table 5.26 shows that removing Barrio Logan emissions has very little impact on the predicted annual averages.

However, this will not be true at other locations. To illustrate this fact, we conducted an annual simulation omitting emissions in a grid-cell located in the Wilmington area. Table 5.27 shows that for this grid-cell, local sources significantly impact annual averages. One reason is that local topography and meteorology combine to produce a recirculation wind pattern in the Los Angeles area, which was not seen in the San Diego area.

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Table 5.25 - Emission Inventory in San Diego and Barrio Logan for a Typical Summer Weekday (1998)

Species	Model Species Emissions in San Diego County (kg/day)	Model Species Barrio Logan Cell Emissions (kg/day)	Percent of County
CO	1,416,728	26,873	1.9%
NOx	174,181	3,938	2.3%
1,3-butadiene	674	11	1.6%
Benzene	4,452	79	1.8%
p-dichlorobenzene	332	8	2.3%
Perchloroethylene	4,134	68	1.7%
Methylene dichloride	952	58	6.0%
Carbon Tetrachloride	0.03	0.00	
Styrene	211	3	1.3%
Toluene	22,532	690	3.1%
Trichloroethylene ^a	3,838	9	0.2%
Chloroform	0.2	0.003	1.2%
MTBE	11,795	203	1.7%
Xylenes	13,399	323	2.4%
Ethylene oxide	19	0.09	0.5%
Acrolein	212	2	1.1%
o-dichlorobenzene	0.1	0.00	2.1%
Ethylene chloride	3	0.03	1.1%
Vinyl chloride	29	0.3	1.1%
CRVI	0	0.00	
PM Arsenic	20	0.06	0.3%
PM Beryllium	21	0.3	1.5%
PM Cadmium	138	2.7	2.0%
PM Iron	7,198	141	2.0%
PM Lead	154	2.3	1.5%
PM Manganese	7	0.1	1.4%
PM Mercury	148	2.3	1.5%
PM Nickel	0	0.0	
PM Zinc	5	0.05	1.0%
Diesel PM	4,177	112	2.7%
VOC ^b	159,135	3,363	2.1%

a) Includes trichloroethane (TCA); b) Alk1+Alk2+Alk5+Aro1+Aro2+Ole1+Ole2

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Table 5.26 - Comparison of Predicted Barrio Logan Cell Annual Average Concentrations when Emissions in Barrio Logan Cell are Omitted from Baseline for Selected Toxic VOCs using CALGRID for 1998

Species	Annual Average Baseline Concentrations	Annual Average Concentrations w/o Barrio Logan Emissions ^a	Units	Percent change from Baseline Concentrations (%)
Acrolein	0.07	0.07	ppb	0.00%
1,3-Butadiene	0.273	0.272	ppb	-0.4%
Benzene	1.391	1.385	ppb	-0.4%
Toluene	6.757	6.742	ppb	-0.2%
Acetaldehyde	2.764	2.235	ppb	-1.05%
Carbon Tetrachloride	0.001	0.001	ppb	0.00%
Chloroform	0.002	0.002	ppb	0.00%
Dichloromethane	0.394	0.393	ppb	0.3%
Ethylene Oxide	0.007	0.007	ppb	0.00%
Formaldehyde	1.741	1.703	ppb	-2.2%
o-Dichlorobenzene	0.001	0.001	ppb	0.00%
Xylenes	3.247	3.239	ppb	-0.2%
p-Dichlorobenzene	0.130	0.124	ppb	-4.6%
Perchloroethylene	0.472	0.471	ppb	-0.2%
Styrene	0.041	0.041	ppb	0.00%
Ethylene dichloride	0.002	0.002	ppb	0.00%
Vinyl Chloride	0.009	0.009	ppb	0.00%
Diesel PM	2.219	2.210	µg/m3	-0.4%
Hexavalent Chromium	0.01432	0.01430	ng/m3	-0.1%
PM Arsenic	3.885	3.882	ng/m3	-0.1%
PM Beryllium	0.0143	0.0142	ng/m3	-0.1%
PM Cadmium	2.168	2.164	ng/m3	-0.2%
PM Lead	54.430	54.325	ng/m3	-0.2%
PM Manganese	48.998	48.890	ng/m3	-0.2%
PM Nickel	5.416	5.400	ng/m3	-0.3%
PM Zinc	52.693	52.581	ng/m3	-0.2%

a) Predicted by eliminating all emissions from cell (60,10) in gridded domain

Table 5.27 - Comparison of Predicted 1998 Wilmington Cell Annual Average Concentrations when Emissions in Wilmington Cell are Omitted with Baseline for Selected Toxic Air Pollutants Using CALGRID

Species	Annual Average Baseline Concentrations	Annual Average Concentrations w/o Wilmington Emissions ^a	Units	Percent change from Baseline Concentrations (%)
Acrolein	0.049	0.042	ppb	-14%
1,3-Butadiene	0.213	0.179	ppb	-16%
Benzene	2.198	1.164	Ppb	-47%
Toluene	4.584	3.373	ppb	-26%
Acetaldehyde	1.795	1.801	ppb	0.3%
Dichloromethane	0.537	0.422	ppb	-21%
Ethylene Oxide	0.004	0.003	ppb	-25%
Formaldehyde	1.83	1.823	ppb	-0.4%
o-Dichlorobenzene	0.003	0.001	ppb	-67%
Xylenes	2.41	2.022	ppb	-16%
p-Dichlorobenzene	0.141	0.128	ppb	-9%
Perchloroethylene	0.38	0.256	ppb	-33%
Styrene	0.077	0.071	ppb	-8
Vinyl Chloride	0.013	0.011	ppb	-15%
Diesel PM	1.89	1.13	µg/m3	-40.-23%
Hexavalent Chromium	0.06	0.05	ng/m3	-0.28%
PM Zinc	62.11	21.46	ng/m3	-65.45%

a) Predicted by eliminating all emissions from cell (34,40) in gridded domain

6) Inhalation Risk

Estimated lifetime inhalation cancer risk is estimated by multiplying annual average concentrations by an appropriate unit risk factor. Hence, the risk distribution for a given specie follows its concentration distribution (for example, see Figures 5.14 and 5.15). Risk plots can then be used to identify areas in the domain with potentially high risk to the people living there.

Table 5.28 shows the observed risk at Memorial Academy Charter School and the estimated risk from the model analysis of local emissions. Since there isn't a method to measure diesel PM, the observed risk from diesel PM is not calculated. As shown in the table, the observed risk from toxic air pollutants is 210 per million. The estimated risk for the same toxic air pollutants from the micro-scale air quality model analysis is 37 per million. The overall risk estimated from the regional modeling results, including diesel PM, is 990 per million (320 per million without diesel PM). ARB's 2004 Almanac of Emissions and Air Quality estimates the diesel PM risk for the San Diego air basin to be 420 in a million.

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Table 5.28 - Inhalation Risk Estimates (per Million) at Memorial Academy

Air Pollutant	Observed	Modeled Micro-scale (ISCST3/CAL3QHCR)					Modeled Regional (CALGRID)
		Stationary Sources	Motor Vehicles	Diesel Truck	Diesel Other	Total	
Diesel PM				27	107	134	670 ^g
1,3-butadiene	88	3	5			8	110
Benzene	74	1	4			5	130
Formaldehyde	16	1	1			2	13
Acetaldehyde	4	0	0			0 ^a	8
Perchloroethylene	3	0				0	19
Nickel	1	0				0	1
Methylene chloride	0	0				0	1
Trichloroethylene	0	0				0	- ^d
Hexavalent chromium	<LOD ^b	16				16	2
Other	23	5				5	35
Total w/o diesel PM	210	27	10			37	320
Total w/diesel PM						170	990 ^f

(a) 0 means less than 0.5 / million.
 (b) Cr (VI) was observed on occasion but is generally below Level Of Detect (30/million).
 A blank cell means no calculation for this cell.
 CALGRID results for trichloroethylene are not available because it was combined with trichloroethane. This has been corrected for future regional model runs such as for Wilmington.
 CMAQ simulations resulted in 640 per million risk for overall risk.

Regional Model Inhalation Risk Contour Plots

We found that 1,3-butadiene, benzene, and diesel PM are the main contributors to total risk exposure. This is shown in Table 5.29 for the domain and for Memorial Academy. Table 5.30 shows total estimated (cancer) risk from all toxic air pollutants at the locations with monitoring sites from CALGRID. Although the numerical values differ for each model, the order of magnitude is similar for most of the sites. Figures 5.30, 5.31, and 5.32 show risk plots for 1,3-butadiene, benzene, and diesel PM. Figure 5.33 shows risk plot from the contribution of all toxics.

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Table 5.29 - Species Contribution to Potential Lifetime Cancer Risk at Memorial Academy and at the Domain Location with the Highest Risk in 1998

Species ^a	Domain Maximum		Memorial Academy	
	Percent Contribution	Risk ^b (in a million)	Percent Contribution	Risk ^a (in a million)
Diesel PM	74.11	1,137	67.59	670
Benzene	12.01	184	13.48	130
1,3-Butadiene	8.70	133	10.76	110
Perchloroethylene	1.11	17	1.98	20
Formaldehyde	1.06	16	1.35	13
p-Dichlorobenzene	0.98	15	0.90	9
Acetaldehyde	0.56	8.6	0.80	8
PM Cadmium	0.37	5.7	0.92	9
Hexavalent Chromium	0.33	5.1	0.21	2
Methylene Chloride	0.31	4.8	0.14	1.4
PM Arsenic	0.19	2.9	1.30	13
Vinyl Chloride	0.08	1.2	0.19	2
PM Nickel	0.07	1.1	0.14	1
Ethylene Oxide	0.06	1.0	0.11	2
PM Lead	0.03	0.5	0.07	1
Carbon Tetrachloride	0.02	0.3	0.03	0.3
Ethylene dichloride	0.01	0.1	0.01	1
PM Beryllium	0.002	0.04	0.00	0.05
Chloroform	0.002	0.03	0.00	0.03
Total	100.00	1,530	100.00	990

a) Only the results from the regional model are show

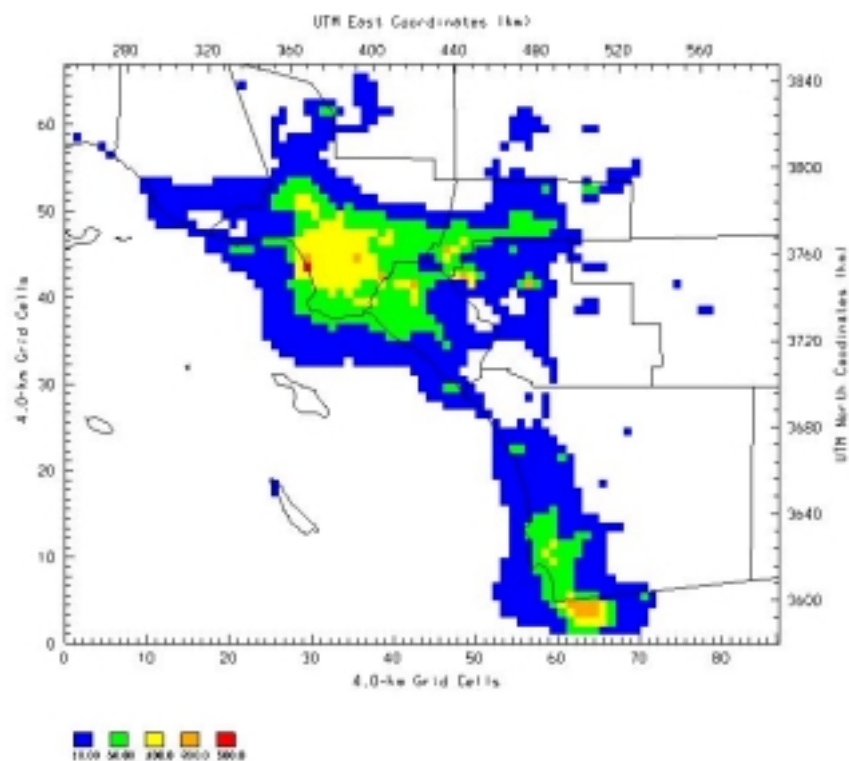
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Table 5.30 - Predicted lifetime risk from exposure to toxics at selected sites in the domain for 1998

Site	Risk ^a Estimated by CALGRID (per million)
Anaheim	950
Memorial Academy	990
Burbank	750
Los Angeles (Downtown)	1,160
Chula Vista	470
Fontana	470
Long Beach	810
Pico Rivera	730
Riverside-Rubidoux	480
Simi Valley	2870
Upland	260
Wilmington	930
Domain Maximum	1,530

a) Net risk doesn't include TCE.

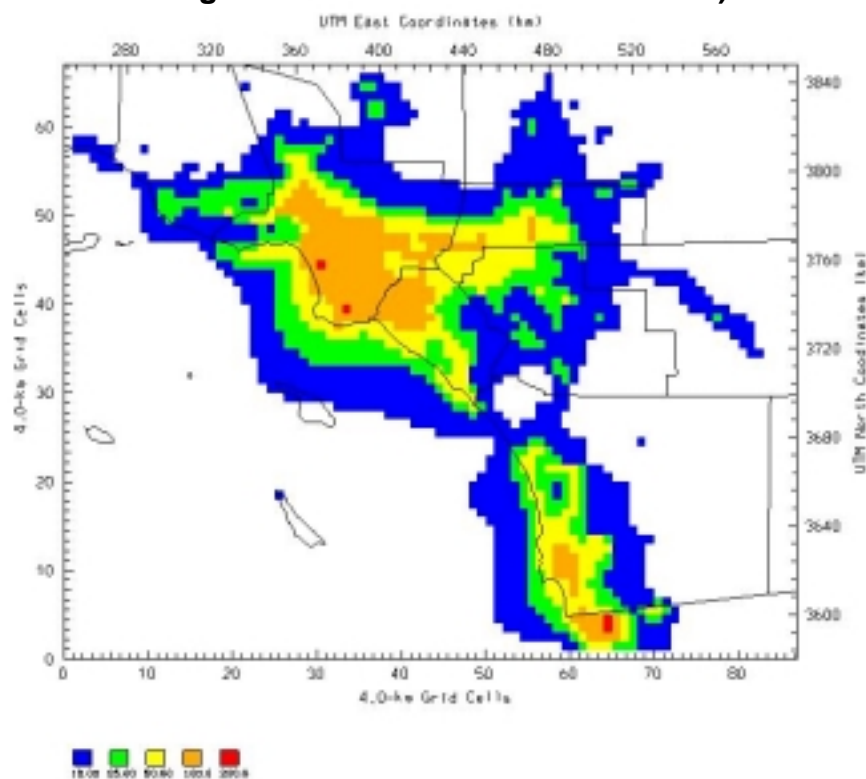
Figure 5.30 - Predicted lifetime risk from exposure to 1,3-Butadiene. (Only the results from the regional model CALGRID are shown).



1,3-Butadiene Estimated Lifetime Risk (in a million).

Domain maximum of 563 in a million at (30, 44)

Figure 5.31 - Predicted lifetime risk from exposure to Benzene. (Only the results from the regional model CALGRID are shown)

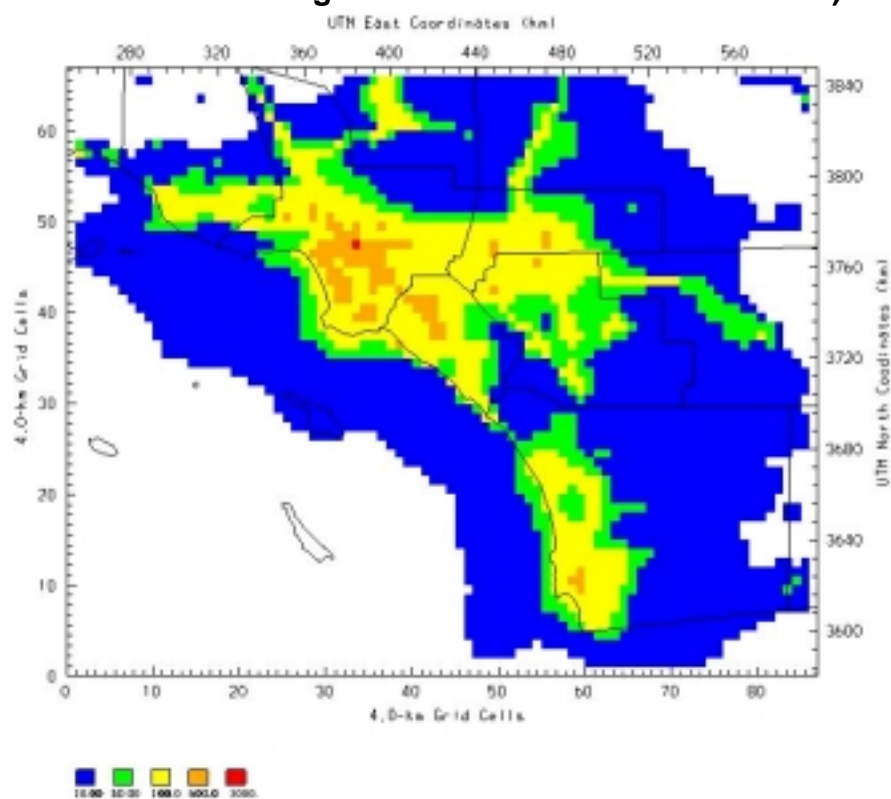


Benzene Estimated Lifetime Risk (in a million).

Domain maximum of 217 in a million at (65, 4)

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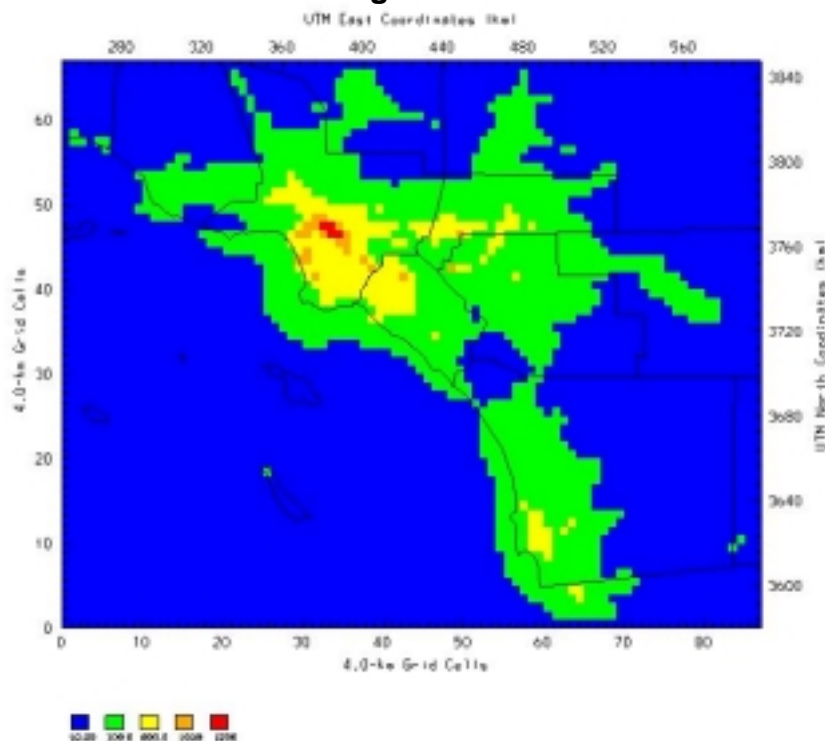
Figure 5.32 - Predicted lifetime risk from exposure to Diesel PM. (Only the results from the regional model CALGRID are shown).



Diesel PM Estimated Lifetime Risk (in a million).

Domain maximum of 1,137 in a million at (65, 4)

Figure 5.33 - Predicted total lifetime risk from all toxic species simulated. (Only the results from the regional model CALGRID are shown).



Estimated Lifetime Risk (in a million).

Domain maximum of 1,534 in a million at (34, 48)

C) Combining Micro-Scale and Regional Modeling Results

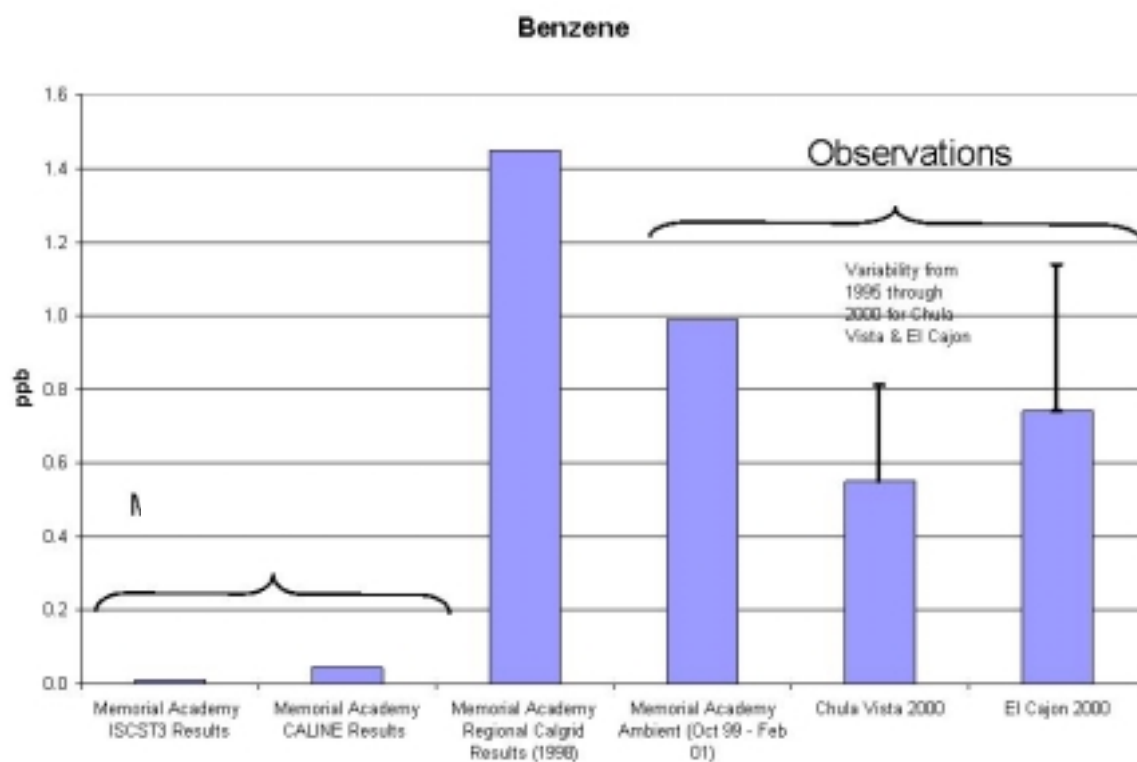
Micro-scale results are representative of near field impacts on the order of meters, while the regional modeling results are impacts from far sources and regional sources on the order of kilometers. Combining these results would ideally result in the total predicted concentrations and could be compared to observations. Below we discuss some of the issues associated with combining regional and micro-scale models. This work continues in our effort in Wilmington. Therefore we are not making a final recommendation on the best methodology to use at this time.

1) Benzene

Figure 5.34 shows the model predictions from regional and local scale modeling for benzene at Memorial Academy Charter School. The regional CALGRID model results overpredict the observations at Memorial Academy Charter School. In addition, the nearest toxic air pollutant monitoring sites, Chula Vista and El Cajon, also show lower observations than predicted at Memorial Academy Charter School. The local scale model results are small compared to the regional model results. The motor vehicle

component of benzene impacts for local scale modeling are greater than the point source component as shown by the CAL3QHCR results compared to the ISCST3 results.

Figure 5.34 - Model predictions from regional and local scale modeling for benzene at Memorial Academy



Year-to-Year Variability

As seen in Figure 5.34 and summarized in Table 5.31, regional model estimates are for 1998. The micro-scale estimates are mostly based on meteorological data for 2000 and on-road mobile source emissions are for 1999. The micro-scale emissions inventory for non-motor vehicle emissions (e.g., point sources) is basically reflective of 2000 because they were the best available at the time of the analysis. Observations at Memorial Academy Charter School are mostly for year 2000. For Chula Vista and El Cajon, observations are for 1995 – 2000.

Table 5.31 – Base Year Data for Modeling

Data	Regional Model	Micro-scale Model
Meteorological	1998	11/99 – 10/00
Emissions Inventory	1998	1999 motor vehicle, 2000 other

As seen in Figure 5.34, the year-to-year variability in the observations at Chula Vista and El Cajon can be 40% to 50% for benzene. This observational variability can be due to year-to-year meteorological conditions or to emission control measures. For the modeled data, the year-to-year variability is not presented even though it can be significant based on the observation data shown in Figure 5.34. To obtain the year-to-year variability in the model estimates would require five times the model runs for a five-year period in addition to the five databases required for the meteorological and emissions inventory data. Since the Barrio Logan analysis is a pilot study, we determined that it would be prohibitive to make multiple production runs with the models.

Double Counting

The regional modeling estimate is based on emissions from outside as well as within the grid cell. Double counting of emissions would result if we simply superimposed the model results from the local scale modeling with the model results from the regional scale modeling.

We performed sensitivity studies with the CALGRID model to determine if the air quality models are sensitive to the double counting of local scale emissions. It was determined that in Barrio Logan, the regional model results are insensitive to double counting. This was shown in Table 5.26 where the impact of eliminating emissions from all sources in Barrio Logan was less than 1% on the concentrations of most air pollutants. However, this is not the case in all areas. For example, local scale emissions in Wilmington are contributors to the regional scale model results in Wilmington (see Table 5.27). These results imply that the impact of local emissions on ambient concentrations varies significantly across the domain. This will be discussed further in the study on Wilmington air emissions.

For the sensitivity study, the CALGRID model was run twice. The first model run was a standard run with all emissions included. The second model run had zero emissions in the grid cell coincident with Barrio Logan. The results of the two model runs showed less than a 1% difference. Therefore, in the case of Barrio Logan, it may be possible to sum the local scale model results with the regional model results to obtain a combined result without observing the effect of double counting.

Emissions from the Barrio Logan grid cell of the regional modeling represents a very low percentage of county-wide emissions (see table 5.26). However, the impact of local emissions may be significant in other areas (see table 5.27).

Other sensitivity studies were also conducted for Barrio Logan regional modeling. Changing the boundary conditions had a very small impact on annual average toxic concentrations. Another sensitivity study looked into the feasibility of shortening model run time. The annual average was simulated using two methods – a) running a complete annual simulation, and b) running one month per season. The result of the

shorter simulation time, four months, is about 10% higher risk than the 12-month average.

D) Summary of Findings for the Regional Photochemical Modeling

Regional modeling for toxic air pollutants was conducted for the period January 1 through December 31, 1998 using the CALGRID air quality model. As a corroborative tool, the CMAQ air quality model was used to simulate the toxics concentrations in ambient air from January, April, August, and November, of the same year. Emission inputs were prepared for each season, distinguishing between weekday and weekend emissions. Both models used the same initial and boundary conditions, and used the same chemical mechanism (SAPRC-99). However, each model was driven by a different meteorology; CALGRID used meteorological fields from CALMET, and CMAQ from MM5. Each model was subjected to an extensive performance evaluation comparing model predictions with measurements for all toxic air pollutants and other pollutants, such as ozone. The predictions from the CALGRID/CALMET package were used to estimate background concentrations at Barrio Logan and to create risk plots for each species in the domain. Specific finding/lessons are summarized below.

1) General Findings

Both CALGRID and CMAQ were found to have similar model performance for ozone, for each toxic air pollutant simulated, and for other species. The ozone and toxic air pollutant model performance is similar to that obtained from other studies. This suggests that although different models will tend to predict different values for specific toxic air pollutants, they tend to have a general agreement on the magnitude of the predictions if care has been exercised in preparing model inputs. Toxic air pollutant performance is an added demand to the air quality models and model inputs. Rather than trying to decide which model is “correct” it should be recognized that the underlying science is similar in all models and that they will respond to the quality of inputs that are used. Models should then be used in a relative sense rather than in an absolute sense.

2) Model Performance for Ozone

For each day of the period simulated with each model, we calculated ozone model performance for CALGRID and CMAQ. We used a different ozone thresholds for March-October (60 ppb) and for January-February and November-December (30 ppb). This was done with the objective of conducting a complete ozone evaluation for all days in the year. For the entire year and domain, CALGRID shows an over-prediction of peak 1-hr ozone of 5%, with a normalized error of 21% and a normalized bias of minus 3%. CMAQ shows, on average, a 13% under-prediction of peak ozone, an 18% normalized gross error, and a minus 8% bias. These values are typical of episodic performance, and agree with the results of an ozone annual simulation done by Winer and Cass (1999).

The cumulative distribution of ozone concentrations from 72 sites in the domain was compared with those predicted by CALGRID and CMAQ. Both models show a similar cumulative distribution for March-October but differ during the colder months.

3) Model Performance for Toxic Air Pollutants

We compared the air quality model predictions from CALGRID and CMAQ against the measured toxic air pollutant concentrations obtained from 11 toxic air pollutant monitoring sites in ARB's toxic air pollutant monitoring network during the period January 1 through December 31, 1998. Summary annual statistics were prepared for each organic and particulate matter species (averaged over all 11 sites). We also added acetone, methyl t-butyl ether, methyl ethyl ketone, and PM iron for model evaluation. No thresholds were used in this toxic air pollutant performance evaluation.

Domain contour plots of annual average concentrations were created for each toxic air pollutant species. Risk plots was also estimated. We found that most of the risk to exposure to all toxics is due to diesel (~70%), benzene (10%), and 1,3-butadiene (~10%).

Gaseous Toxic Air Pollutants

Annual predictions by both models for most of the organic toxic air pollutant gases (such as benzene and 1,3-butadiene) were within a factor of 2-3 of observations, which is in agreement with previous studies. Maximum predicted concentrations over the domain are of the same order of magnitude as the measurements during 1998. Bias and error are significant for most gaseous species. Both models provided similar results.

Relative to the micro-scale results, the regional modeling results provided a much better estimate of concentrations at the Memorial Academy site. For example (see Figure 5.30), at Memorial Academy the regional model predicts a benzene annual average concentration of 1.45 ppb, while the microscale model predicts under 0.05 ppb. The observed annual average for benzene is 1.0 ppb that compares well with model predictions.

Particulate species and hexavalent chromium

For most PM species, the predicted annual average concentrations are significantly below observations, except for some species at some sites. For some species, such as hexavalent chromium, it is most likely the result of a large number of observations below the detection limit, which is much higher than the levels predicted through the air quality modeling. For other species, the emissions inventory may be deficient. For those species that are emitted by localized sources, like hexavalent chromium emissions from chrome plating activities, the regional model is not likely to be effective near the source (i.e., below the grid size resolution). In such cases, it is necessary to combine microscale and regional modeling to capture the small scale concentration gradients resulting from such emissions.

Since Diesel PM is not measured directly, we compared our model predictions for elemental carbon against observed elemental carbon measurements. The results did not compare favorably, as the observed annual average values were about 5 times higher than the predicted levels, again suggesting emissions inventory deficiencies.

4) Model Sensitivity Analyses

We investigated the impact of using cleaner boundary conditions on the average toxic concentrations at Barrio Logan. The months of February and August were simulated with cleaner boundaries and compared with the baseline. The impact of cleaner boundary conditions at Barrio Logan was found to be insignificant for the PM species (less than 1%). However, for the toxic VOCs, the impact depended on the month simulated. For example, formaldehyde and acetaldehyde both decrease by about 10% in February and decrease about 2% in August when using cleaner boundaries. Styrene showed the largest dependency (a decrease of 34% in February and 21% in August). Other species, such as perchloroethylene and 1,3-butadiene, decrease by 2% in August, but the effect was less than 1% in February. Although only two months were simulated, the results suggest that the effect of the choice of boundary conditions and annual averages can be important for some toxic species.

We used the results of the CALGRID air quality model, which was applied for each day in 1998 (baseline simulation), to see the impact of simulating a reduced number of periods in the year. Specifically, we investigated using one month each quarter, two weeks each quarter, every other month, and two weeks of each month. Other options, such as modeling the typical episodes and adjusting for the frequency of such episodes, were not investigated. The number of surface grid-cell in the domain that differ from baseline concentrations by 10%, 30%, and 50% were calculated for selected species. In general, the coarser the resolution, the larger the number of grid cells that differ from the baseline by over 30%. The less coarse scenarios, such as those using two weeks in each month or every other month, appear to introduce less error (compared to the other scenarios). Further investigation is clearly needed.

We compared the measured wind fields at five sites in the domain with those predicted by the two meteorological models used in this study. We found that although the wind field from CALMET and CMAQ differ on a day-to-day basis, both tended to agree on the general wind flow pattern over an extended period.

5) Model Limitations

We identified a few model limitations that warrant evaluation in future modeling efforts. One is that the SAPRC-99 mechanism only has “place holder” reactions for chlorinated VOCs. The result is that potentially the model can under or over-predict concentrations of the chlorinated species. Smog chamber experiments are necessary to elucidate the reaction mechanisms of chlorinated species. In addition, neither model had a module to

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recognize inert species separately. In both CALGRID and CMAQ, pseudo-reactions were used in the chemical mechanism to incorporate these species in the model. The potential impact is that significant under or over predictions can be introduced if the representation chosen is not adequate for the model.

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CHAPTER 6 - FINDINGS AND CONCLUSIONS

Detailed findings for the major topics in this report are presented in the respective chapters. This chapter summarizes those major findings and presents the final conclusions of the Barrio Logan effort. The Barrio Logan project provided us with a new understanding of how to evaluate air pollution at the neighborhood scale. We will build upon these findings as we continue our work in the Neighborhood Assessment Program in the Wilmington area of Los Angeles.

A) Ambient Air Monitoring Summary

1) Memorial Academy Charter School

Ambient air monitoring was conducted at Memorial Academy Charter School from October 1999 through February 2001. The monitoring was designed to evaluate the air pollution levels in Barrio Logan. Memorial Academy was chosen by the community for this project because it was believed that this school was representative of children's exposure to air pollution in Barrio Logan. The objectives of the study were to assess the differences in air pollution between Memorial Academy and other long-term monitoring sites in San Diego, and to use the results to evaluate the performance of modeling tools and inputs. Over 60 pollutants were measured during the 17-month study. The major findings are presented below.

- Based on the 17 months of ambient air measurements collected at Memorial Academy, we found that the air quality levels were similar to those measured at other air monitoring sites in the San Diego urban region. The toxic air pollutant levels were similar to those measured at El Cajon, and statewide urban averages, but slightly higher than Chula Vista. However, the potential cancer risks at Memorial Academy and Chula Vista are not statistically different. No monitoring method was available for diesel particulate matter, the largest contributor to known air pollution risk, so we were unable to measure diesel particulate as part of this study.
- The similarity of the air pollution concentrations at Memorial Academy and other regional monitoring stations indicates that exposure from the regional air monitoring network provides a good indication of the general exposure of the population to toxic air pollutants. This was confirmed by the regional modeling. However, the localized air monitoring also indicates that the regional sites may not be effective at identifying localized concentrations of toxic air pollutants.

2) Special Hexavalent Chromium Monitoring Study

To investigate the possibility of local-scale hot spots or pollution gradients, we conducted a short term monitoring project in Barrio Logan. Hexavalent chromium monitoring was conducted from December 3, 2001 to May 12, 2002 at various locations along Newton Avenue, a mixed use area of Barrio Logan which had both residences and two chrome platers in close proximity to each other. In January 2002, we found unexpectedly high levels of hexavalent chromium at a number of the monitoring sites. Working with community members and the San Diego County APCD, the monitoring continued in an effort to understand the source and magnitude of the emissions. Based on months of indoor and outdoor monitoring data, source testing, micro-scale modeling, and dust sample analysis, we determined that the decorative chrome plater was responsible for the hexavalent chromium emissions. The major findings are presented below.

- We found that one chrome plater in close proximity to residences had a high near source impact that was very localized, but the impact of the source dropped off quickly as the emissions dispersed.
- We found that chrome platers may emit chromium not only as part of the plating process but also as fugitive emissions resulting from housekeeping activities.
- The emission inventory estimates for the facility were significantly underestimated because they included only the plating tank emissions and not the fugitive dust associated with the housekeeping activities.
- It is possible that other “hot spots” may exist in close proximity to other air pollution sources in Barrio Logan that may impact nearby residences or other sensitive receptors.

3) General Findings

We were not able to actually monitor true toxic air pollutant gradients across the community of Barrio Logan because long-term monitoring was only conducted at one location. The air pollution levels monitored at Memorial Academy appeared to be more representative of regional air quality, and, aside from a few metals, there was little to differentiate the air quality at Memorial Academy from other parts of San Diego. The monitors in the hexavalent chromium study did show very localized areas of elevated hexavalent chromium levels but impacts dropped off very quickly with distance from the facility.

The difficulty of siting monitors to capture these types of gradients in communities makes the need for development of micro-scale modeling tools and accurate emission inventories essential. Future neighborhood monitoring studies should consider different siting criteria for the location of neighborhood monitors and multiple monitoring sites. The objectives of the ambient monitoring need to be clearer as to whether the focus is

on community air pollution levels (which may be more regional in nature), toxic air pollutant gradients, or localized hot spots.

B) Emission Inventory Summary

Both regional photochemical models and micro-scale dispersion models require inputs that properly characterize emissions and meteorology. To ensure this, the development of a complete and accurate emission inventory is essential. Chapter 4 discusses the development of the micro-scale inventory and how the regional emissions inventory was used under the Neighborhood Assessment Protocol. The major findings are presented below.

- Because of the relatively small zone of impact from localized emissions, it is critical that micro-scale inventories use accurate and complete information regarding site location and emission release points for proper spatial allocation of emissions.
- The development of micro-scale emission inventories requires supplementing the regional inventory with more detailed information than is typically collected to support regional air quality models. With few exceptions, the additional facilities did not greatly contribute to the overall emissions inventory; the regional inventory derived from the CEIDARS database was sufficient to capture most air pollutants from stationary sources located in the Barrio Logan community. Although in Barrio Logan the additional emissions did not make a large contribution to the overall inventory, this might not be true in other communities. We need to keep in mind that emissions from large point sources alone may not be adequate for neighborhood assessments.
- Whereas micro-scale inventories may be small contributors to the overall inventory of the region, micro-scale inventories are essential to understand and model localized near source impacts on a nearby receptor. This may be at a scale much smaller than the community or neighborhood.
- Emission inventories are based on various assumptions specific to each category, creating various levels of uncertainty. We base our work on the best information available and expect the methodology to change as we continue our work to develop neighborhood assessment tools.

The same questions arise here as in the ambient monitoring section; regional emission inventories seem to drive the overall risk modeled for the community. The addition of micro-scale inventories did not contribute greatly to the overall modeled risk. However, on a near-source basis, an accurate micro-scale emission inventory is needed to identify impacts on nearby residences, schools, or other sensitive receptors.

C) Micro-Scale Modeling Summary

Qualitatively, micro-scale modeling results show an expected, non-uniform spatial distribution of concentrations with strong spatial gradients. Simulated concentrations are much higher near the source and rapidly decrease with distance away from the source. However, quantitatively, the simulated concentrations from the micro-scale modeling are low as compared to ambient monitoring. Possible explanations for this are:

- The micro-scale emission inventory used in the model may not have captured all of the emissions from local sources.
- There are uncertainties in the micro-scale model formulations. For example, tracer studies indicate that micro-scale models generally tend to over-predict high concentrations in the near-field and under-predict lower concentrations observed at greater distances from a source.
- Air pollution from regional air pollution sources (i.e., sources outside of the micro-scale modeling domain) may overwhelm the air pollution contribution from local air pollution sources at the monitoring stations used for model performance purposes.
- The ambient observations collected in this study may be representative of a different scale. Memorial Academy, although selected as a community monitoring site, appears to reflect urban regional air quality and may not reflect conditions in other parts of the community.

Although the AERMOD model has undergone extensive evaluation, the CE-CERT tracer study is the first in which the meandering component of the model has been tested. This study demonstrates that AERMOD can provide reliable near-field concentration estimates from urban sources if turbulent velocity estimates close to a source are used to estimate plume direction. Future research should examine the relationship between urban morphology and meteorological parameters within the urban canopy.

D) Regional Photochemical Modeling Summary

To understand the contribution of regional air pollution to air quality in Barrio Logan, regional modeling of toxic air pollutants was conducted for the period January 1 through December 31, 1998 using the CALGRID air quality model and the CALMET meteorological model. To corroborate the CALGRID modeling results, the CMAQ air quality model was also run to simulate the toxic air pollutant concentrations in ambient air for January, April, August, and November 1998. The predictions from the CALGRID/CALMET package were used to estimate regional background toxic air pollutant concentrations at Barrio Logan and to create cancer risk plots for each specie in the domain.

Findings and Conclusions

Emission estimates were prepared for each season, distinguishing between weekday and weekend emissions (Chapter 4). Both models used the same initial and boundary conditions and used the same atmospheric reaction chemistry mechanism (SAPRC-99). However, each model was driven by different meteorological models; CALGRID utilized meteorological fields from CALMET, and CMAQ from MM5.

We compared the air quality model predictions from CALGRID and CMAQ against the measured toxic concentrations obtained from ARB's toxic air pollutant monitoring network and against the measurements taken at Memorial Academy Charter School. Each model was subjected to performance evaluation comparing model predictions with observations for all toxic species and other pollutants, such as ozone. Generally, both models exhibited similar performance. The major findings are presented below.

- The model performance for both annual ozone and toxic hydrocarbons was similar to that obtained in previous studies by other researchers.
- Observed annual organic toxic gases (such as benzene and 1,3-butadiene) were predicted within a factor of 2-3 of observations at several toxic sites and at Memorial Academy (which is in agreement with previous studies). Maximum predicted concentrations over the domain are of the same order of magnitude as the measurements made during 1998. Modeling results for toxic hydrocarbons compare well with observations and with results from previous studies.
- The PM species from models do not compare well with observations and suggest potential deficiencies in the model inputs. For some species, such as hexavalent chromium, the regional models predict annual average concentrations that are below the detection limit. Although, the regional model predictions are consistent with the observations, a direct comparison was not possible. For other species, the emissions inventory may be deficient.
- The regional model is appropriate to simulate emissions distributed in the domain (like benzene) or that are generated by secondary reactions (like formaldehyde). However, the regional models used were not appropriate to simulate pollutants that are emitted by a few localized sources. In those cases, microscale modeling was needed to represent the short-term air pollutant gradients.
- The impact of local emissions on local concentrations will vary significantly from one area to another.
- The averaging scheme selected will have a large impact on the predicted annual average concentrations. This is an important consideration when modeling less than 365 days is considered to represent one year of air quality. As computer technology improves, this may not be a necessary step.

E) Integration of Regional and Micro-Scale Modeling Summary

As discussed in Chapters 4 and 5, micro-scale modeling results are representative of near-field impacts on the order of meters, while the regional modeling results are representative of regional sources on the order of kilometers. Ideally, using the NAP Protocol, combining the results from these two models would produce total predicted concentrations that match the observed concentrations measured during the field measurement program.

When combining the results from the regional and micro-scale models that were used, we found that levels of simulated micro-scale concentrations are very low compared to both ambient monitoring and regional model simulations, which dominate the combined model predictions. Further investigations into the causes of the high regional modeling concentration predictions (and whether this makes sense) are being conducted under the Wilmington study.

As described in Chapter 4, because the sources that are included in local scale modeling are also included in the regional scale modeling, the contribution of these sources would be counted twice if we combine the results from both models. This problem is referred to as 'double counting'. We performed some sensitivity studies with the CALGRID model to determine if the air quality models are sensitive to the double counting of local scale emissions. It was determined that, in Barrio Logan, the regional model results are insensitive to double counting, because the overall contribution from local emissions that we were able to identify was small relative to the impacts of regional air pollution. This is expected to vary by region, however, depending on the type and distribution of sources.

It is also important to note that the periods of record for meteorological and emissions input data to both the regional and micro-scale models differed (Chapter 5). However, the impact of this year-to-year variability was not assessed, because it would require multiple model runs. Micro-scale models require five years of meteorological data to account for variability. Since the Barrio Logan analysis is a pilot study, we determined that it would be prohibitive to make multiple production runs for the models.

We will continue to work on a methodology for the integration of the regional and micro-scale model in our work in Wilmington.

F) Risk Summary

Cancer risk estimates represent the chances of developing cancer assuming a person is continuously exposed to the average concentration for a 70-year lifetime. These estimated lifetime inhalation cancer risks are estimated by multiplying annual average concentrations by an appropriate unit risk factor. These risks were estimated with our ambient monitoring concentrations and also with our modeled air pollutant concentrations. Our findings include:

Findings and Conclusions

- Diesel Particulate Matter contributes the most to overall cancer risk. With our Diesel Risk Reduction Plan, we are taking steps to reduce diesel PM throughout the State. The other major risk drivers for cancer risk are benzene and 1,3-butadiene.
- The observed cancer risk estimates calculated for Memorial Academy were similar to those calculated for other long-term San Diego monitoring locations.
- Modeled regional cancer risk estimates without diesel PM are slightly higher than the cancer risk estimates based on air pollution monitoring data, except for hexavalent chromium levels measured in the vicinity of the chrome platers on Newton street.
- Using a variety of information sources and methods, we estimate that most of the risk from exposure to toxic air pollutants in the Barrio Logan area is due to diesel particulate (~70%), followed by benzene (10%) and 1,3-butadiene (~10%).

G) Conclusions and Recommendations

The Neighborhood Assessment Program was designed to develop assessment tools for evaluating and understanding air quality in California communities. This section discusses our conclusions and recommendations from our work in Barrio Logan.

Initially, we went into Barrio Logan expecting to find localized air pollution impacts. We were not able to actually monitor true toxic gradients across the community of Barrio Logan with the monitoring that was performed there. The data from Memorial Academy appeared to be representative of regional air quality, and aside from a few metals, we were unable to detect any unusual impacts from local sources of air pollution.

The monitoring data from the hexavalent chromium study showed very localized hot spots but the impacts fell off quickly. The difficulty in siting monitors to capture air pollution gradients across communities makes the need for the development of micro-scale modeling tools and accurate emission inventories essential. Monitoring for modeling can result in different site placement than when population exposure is needed. Each objective must be weighed in developing a monitoring plan. Future neighborhood monitoring studies should consider different siting criteria for the location of neighborhood monitors and the use of multiple monitoring sites. The objectives need to be clear as to whether the focus is on community air pollution levels, toxic gradients, or localized hot spots

Regional emission inventories seem to drive the overall risk modeled for the community. The addition of micro-scale inventories did not contribute greatly to the overall modeled risk. However, on a near-source basis, an accurate micro-scale emission inventory is needed to identify impacts on nearby residences, schools or other sensitive receptors. For example, in Barrio Logan, we identified a decorative chrome plater that was having a significant impact on a nearby residence. We eventually found that the source of the emissions from this chrome plater was from the plating activities and fugitive dust that

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was collecting on the floor of the facility. This fugitive dust was not previously accounted for in the emissions estimates.

Air dispersion and photochemical models were tested to determine their capabilities for use in neighborhood assessments. The regional modeling results indicated that the models generally performed well overall, but did not perform well for most PM species. The micro-scale modeling results showed a non-uniform spatial distribution of concentrations with strong spatial gradients, where simulated concentrations are much higher near the source and rapidly decrease with distance away from the source. Levels of simulated concentrations are low as compared to observed concentrations. These differences may be attributed to:

- The uncertainties in the emission inventory and micro-scale models;
- Regional source influences may dominate the concentrations observed at the monitoring stations used for model performance; and
- Ambient observations may be representative of regional conditions and may not reflect worst case conditions in the community.

Below we discuss some of the issues associated with combining regional and micro-scale models. This work continues in our efforts in Wilmington. Therefore, we are not making a final recommendation on the best methodology at this time.

Micro-scale results are representative of near field impacts on the order of meters, while the regional modeling results are impacts from regional sources on the order of kilometers. Ideally using the NAP protocol, combining these results would show the total predicted concentrations matched the observed concentrations. Not surprisingly, we found that the problems found in each of the models individually carried into the integration of the modeling results. The regional modeling alone seemed to reflect the air quality measured at Memorial Academy and the model appeared to be insensitive to double counting when adding the micro-scale modeling results. This is expected to vary by region depending on the type and distribution of sources.

Based on the results of this study, our recommendations include;

- Ensure that ambient air monitors are sited for the studies purpose(s). This may necessitate several phases in monitoring given the different design characteristics of each objective.
- Ensuring that the most accurate and complete emission inventory is available; and
- Developing a new model formulation for micro-scale modeling.

The Barrio Logan Neighborhood Assessment was an intensive first step in developing tools for neighborhood assessments. The experience gained from this project will be used as we continue our neighborhood assessment tool development in Wilmington.

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APPENDIX A

***CONCEPTUAL MODELING PROTOCOL FOR THE
NEIGHBORHOOD ASSESSMENT PROGRAM***

CONCEPTUAL MODELING PROTOCOL FOR THE NEIGHBORHOOD ASSESSMENT PROGRAM

1. Introduction

This document describes the process that the Air Resources Board (ARB) will use to investigate the impacts of emissions for the "Neighborhood Assessment Program Work Plan" (Work Plan)¹. Although modeling is a dynamic and involved process, we believe that the approach described here provides the framework to improve the scientific basis for reliably estimating air pollutant concentrations.

The goals of the Neighborhood Assessment Program are:

- assess criteria and toxic air pollutant impacts in communities affected by multiple-emission sources; and,
- develop guidelines for evaluating strategies for reducing air pollution impacts at the neighborhood scale.

The technical objectives to achieve the goals are:

- develop and evaluate a methodology to estimate annual average ambient concentrations of various pollutants from multiple sources at the neighborhood scale; and,
- recommend a method to air districts to perform neighborhood assessments.

We organized a modeling working group, which includes more than 40 participants from government agencies, universities, industry, and environmental groups. We discussed the modeling approach and technical details at group meetings. The modeling protocol has undergone a peer review process. The peer review group includes the following members: Mr. John Irwin, Dr. Michael Kleeman, Dr. Christian Seigneur, and Dr. Akula Venkatram. We received valuable comments from the peer review group. A minority of the peer review group had a different opinion on the modeling approach. The concern was that superposition of two different types of models having different philosophies (plume models and photochemical models) is questionable. Therefore, it might be more efficient to use a photochemical grid model with a parameterization for selected grids. However, this would require major efforts on model development, which is currently beyond the scope of the project. We incorporated comments from the peer review group into the protocol.

2. Modeling Approach

To assess neighborhood impacts from local emission sources, ideally would require meteorological and air quality monitoring at many locations within the

References

neighborhood to determine where high concentrations may occur. Although desirable, it is not practicable considering the number of neighborhood assessment sites throughout the state, and the resources that are necessary to conduct such field monitoring. Thus, we need to rely on air quality models -- models that have been formulated based upon scientific principles -- models that have been tested and evaluated over a wide range of meteorological conditions and emissions.

We propose to apply air quality models to assess health impacts from direct inhalation only for both the micro and regional scales. Micro-scale modeling is for receptors located near emission sources, i.e., meters to few kilometers from the sources within the neighborhood area. Regional scale modeling is for distances of several kilometers, to hundreds of kilometers, to the size of air basins. The larger scale for regional modeling is necessary to simulate transport of pollutants from upwind areas that will contribute to concentrations in the micro-scale area. Regional modeling estimates ambient concentrations resulting from all emission sources in an area, whereas micro-scale modeling gives more detailed information in the vicinity of point and area sources on a local scale.

There are many toxic pollutants that are released into the atmosphere from emission sources. For the micro-scale (neighborhood) modeling we propose to model more than 100 pollutants. For the regional modeling we propose to model 30 toxic pollutants, which contribute to the majority of the health risk. This limited set of 30 pollutants is used for regional modeling due to limitations in emission inventory for regional modeling and also to reduce computational time. Table 2.1 below gives the toxic pollutants for which we have a chronic hazard index or a cancer unit risk factor (OEHHA²) to be modeled for the neighborhood scale applications. Table 2.2 shows a list of toxic pollutants to be modeled for the regional scale.

Table 2.1 - Toxic Air Contaminants, with one or more health values under development by the Office of Environmental Health Hazard Assessment.

1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	Dibenz[a j]acridine
1,1,2,2-Tetrachloroethane	Dibenzo[a e]pyrene
1,1,2-Trichloroethane	Dibenzo[a h]pyrene
1,2,3,4,6,7,8,9-Octachlorodibenzo-p-dioxin	Dibenzo[a i]pyrene
1,2,3,4,6,7,8-9-Octachlorodibenzofuran	Dibenzo[a l]pyrene
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	Diethanolamine
1,2,3,4,6,7,8-Heptachlorodibenzofuran	Dimethyl formamide
1,2,3,4,7,8,9-Heptachlorodibenzofuran	Epichlorohydrin
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	Ethyl benzene
1,2,3,4,7,8-Hexachlorodibenzofuran	Ethyl carbamate
1,2,3,6,7,8-Hexachlorodibenzofuran	Ethyl chloride
1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	Ethylene dibromide
1,2,3,7,8,9-Hexachlorodibenzofuran	Ethylene dichloride

References

1,2,3,7,8-Pentachlorodibenzo-p-dioxin	Ethylene glycol
1,2,3,7,8-Pentachlorodibenzofuran	Ethylene glycol monobutyl ether
1,2-Epoxybutane	Ethylene glycol monoethyl ether
1,3-Butadiene	Ethylene glycol monoethyl ether acetate
1,3-Propane sultone	Ethylene glycol monomethyl ether
1,4-Dichlorobenzene	Ethylene glycol monomethyl ether acetate
1,4-Dioxane	Ethylene oxide
1,6-Dinitropyrene	Ethylene thiourea
1,8-Dinitropyrene	Ethylidene dichloride
1-Nitropyrene	Formaldehyde
2,3,4,6,7,8-Hexachlorodibenzofuran	Glycol ethers
2,3,4,7,8-Pentachlorodibenzofuran	Hexachlorobenzene
2,3,7,8-Tetrachlorodibenzofuran	Hexachloroethane
2,4,6-Trichlorophenol	Hexamethylene-1,6-diisocyanate
2-Nitrofluorene	Hexane
2-Nitropropane	Hydrazine
3,3-Dichlorobenzidene	Hydrochloric acid
3-Methylcholanthrene	Hydrogen fluoride
4,4-Methylene bis(2-chloroaniline)	Hydrogen selenide
4,4-Methylenedianiline	Indeno[1,2,3-cd]pyrene
4-Nitropyrene	Inorganic Arsenic & arsenic compounds
5-Methylchrysene	Inorganic lead & Inorganic lead compounds
5-Nitroacenaphthene	Isophorone
6-Nitrochrysene	Lead compounds
7,12-Dimethylbenz[a]anthracene	Lindane
7H-Dibenzo[c g]carbazole	Maleic anhydride
Acetaldehyde	Manganese and compounds
Acetamide	Mercuric chloride
Acrolein	Mercury and compounds
Acrylamide	Methanol
Acrylic acid	Methyl bromide
Acrylonitrile	Methyl chloroform
Allyl chloride	Methyl ethyl ketone
Aniline	Methyl isocyanate
Antimony and compounds	Methyl methacrylate
Asbestos	Methyl tertiary butyl ether
Benz[a]anthracene	Methylene chloride
Benzene	Methylene diphenyl diisocyanate
Benzo[a]pyrene	N-Nitrosodimethylamine
Benzo[b]fluoranthene	N-Nitrosomorpholine
Benzo[j]fluoranthene	Naphthalene
Benzo[k]fluoranthene	Nickel and compounds
Benzyl chloride	Nitrobenzene
Beryllium and compounds	Particulate emissions from diesel-fueled engines
Bis(2-ethylhexyl)phthalate	Pentachlorophenol
Bis(chloromethyl)ether	Phenol
Cadmium and compounds	Phosgene
Carbon disulfide	Phosphine

References

Carbon tetrachloride	Phosphorus
Chlorinated dibenzo-p-dioxins	Phthalic anhydride
Chlorinated dibenzofurans	Polychlorinated biphenyls
Chlorine	Propylene oxide
Chlorobenzene	Selenium and compounds
Chloroform	Styrene
Chromium (VI)	Styrene oxide
Chromium and compounds	Toluene
Chrysene	Toluene-2,4-diisocyanate
Cobalt and compounds	Trichloroethylene
Cresols/Cresylic Acid	Triethylamine
Cyanide compounds	Vinyl acetate
Dibenz[a h]acridine	Vinyl chloride
Dibenz[a h]anthracen	Vinylidene chloride

Table 2.2 List of toxic species for the regional modeling

Reactive Species	Inert Species
Formaldehyde	Diesel PM
Acetaldehyde	Arsenic
1,3-Butadiene	Nickel
Benzene	Manganese
p-Dichlorobenzene	Iron
Perchloroethylene	Zinc
Methylene Chloride	Cadmium
Hexavalent Chromium	Lead
Carbon tetrachloride	Beryllium
Styrene	Mercury
Toluene	
Trichloroethylene	
Chloroform	
MTBE	
Xylenes	
Vinyl chloride	
Ethylene oxide	
Acrolein	
o-dichlorobenzene	
Ethylene dichloride	

Regional modeling provides ambient concentrations resulting from multiple emission sources: point, area, mobile, and biogenic. We propose to apply and test two grid-based models for regional modeling : UAM-FCM³ and CMAQ, part of Models-3⁴. The UAM (Urban Airshed Model) is the traditional regional model that has been applied for estimating ozone and precursor gas concentrations, while Models-3 represents the state-of-science model that has been developed by EPA scientists over the past six years. Both UAM and Models-3 will use the SAPRC99⁵ chemical mechanism modified to incorporate toxic chemistry.

The mechanism designated as SAPRC-99 is a complete update of the SAPRC mechanism released in 1990. This mechanism was evaluated against the results

References

of approximately 1700 smog chamber experiments and represents the state-of-the science. Condensed versions of the SAPRC-99 mechanism have been developed for use in air quality model simulations, including fixed-parameter and variable-parameter versions. Appendix A lists all the reactions included in the condensed mechanism. The mechanism can be obtained at <http://helium.ucr.edu/~carter/SAPRC99.htm>. A condensed version of the SAPRC-99 chemical mechanism is selected for this project. The condensed versions include a few explicitly represented species such as ozone, NO_x, formaldehyde, acetaldehyde, acetone, and others. However, most of the organic species are lumped into classes (i.e., alkane, alkenes, aromatics, and terpenes) taking into account their reactivity. To address different toxics of concern, explicit mechanisms for 20 toxic VOCs were added to the condensed version of SAPRC-99. In addition, the simulation includes also 10 toxics that are treated as inert. A complete list of toxic species explicitly included in the mechanism is shown in Table 2.2 and a listing of the explicit mechanisms is given in Appendix B.

Since regional models estimate a uniform concentration field within a receptor grid of several square kilometers, we will use micro-scale models to obtain more detailed concentration field near emission sources. We propose to apply and test several types of micro-scale models. These models include traditional U.S. EPA Gaussian models as well as new and emerging models. The following models will be applied to estimate annual ambient concentrations for point and line sources:

- ISCST3⁶ for point and area sources; this is the traditional U.S. EPA regulatory model;
- AERMOD⁷ for point and area sources; this is an advanced U.S. EPA recommended model;
- CALPUFF⁸ for point and area sources; this model is also an advanced U.S. EPA recommended model for assessing impacts in complex terrain and for long-range transport;
- CALINE⁹ for mobile sources, e.g. emissions from motor vehicles on roadways; this is a traditional U.S. EPA approved model for line sources; in addition, this model has undergone performance evaluation for CO concentrations, and using inert tracers;
- Lagrangian particle dispersion model¹⁰, an advanced, state-of-the-science short-range model that will provide concentration estimates at scales of meters to tens of meters from a source. This model is being developed and evaluated by UC Riverside¹¹.

3. Regional Scale Modeling

3.1 Modeling Domains and Time Period

We propose a nested domain approach for regional modeling for meteorology and air quality. Figure 3.1.1 shows the coarse domain and one nested domain covering the central and southern parts of California. The air quality models will provide the results for the inner nested domain centered in San Diego and covering an area of approximately 300 by 300 km (Fig. 3.1.2). This domain covers the San Diego and portions of South Coast and Mojave air basins. The regional air quality models will be applied using an entire year of data for meteorology and monthly average emissions to estimate annual concentrations due to transport of pollutants from distant sources as well as background ambient air quality concentrations for the micro-scale areas.

Figure 3.1.1 Regional scale modeling domain.

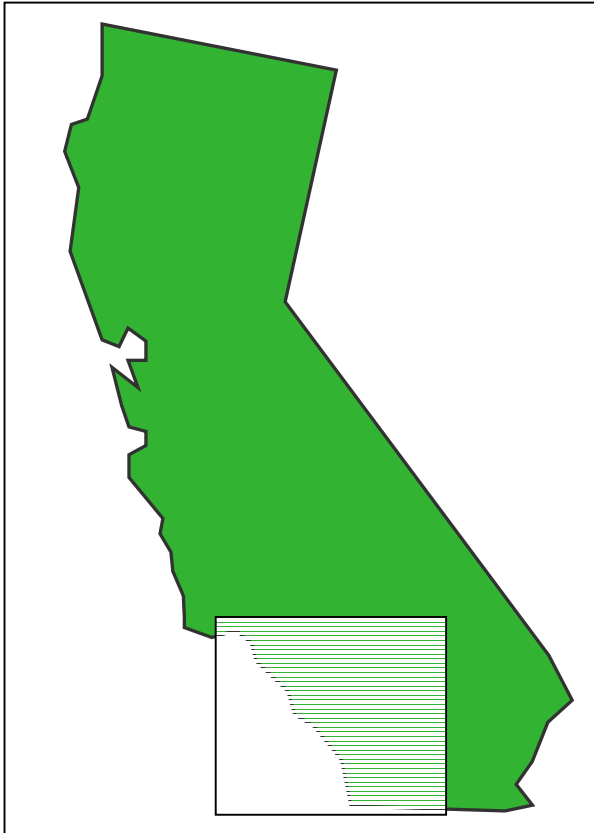
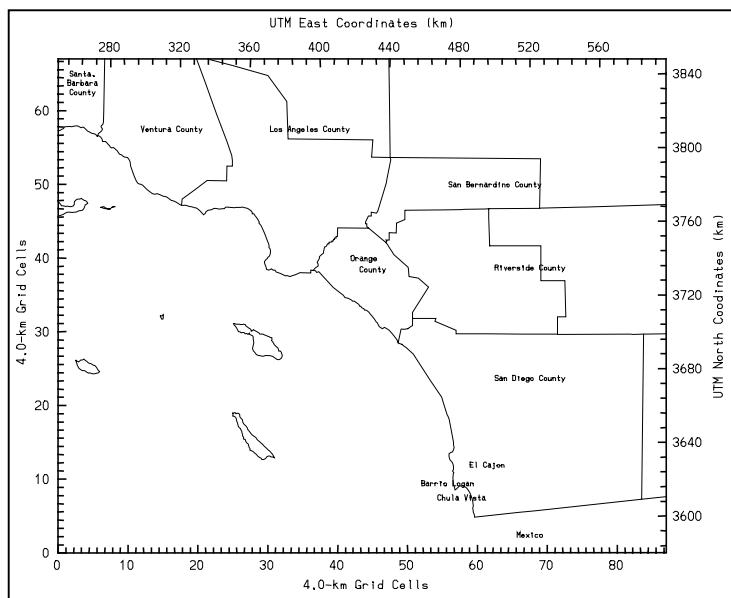


Figure 3.1.2 Regional scale inner nested modeling domain

The time period from December 31, 1997 12 GMT to January 1, 1999 12 GMT will be simulated to create high resolution gridded meteorological data to cover the entire year of 1998. This period was selected because enhanced upper air data (more than 10 wind profilers) are available and also the gridded emission inventory has already been developed to support the 1997 Southern California Ozone Study (SCOS97). The rich observational database of meteorological data is critical for the model evaluation. Future applications of regional models for NAP may have only routine meteorological data available. The 1998 database provides the opportunity to evaluate several meteorological models by comparing results with routine and special databases to determine which model performs best with routine data. For testing the methodologies at Barrio Logan, we assume that annual average concentrations estimated by regional models using evaluated 1998 meteorological inputs will be also representative for 1999/2000. We are planning to apply UAM using one full year of meteorology and CMAQ for selected episodes in summer and winter.

3.2 Inputs for Regional Model

Inputs for regional modeling require comprehensive databases for meteorology, emissions, and air quality. To generate a database from scratch, specifically for the emission inventory, would be a difficult task considering the time schedule and resources available. Thus, we propose to build upon the databases from previous photochemical modeling work conducted by ARB staff and air districts. We propose to update these databases to reflect seasonal variations of activity levels, temperature effects on emission rates, and update the toxic emissions as well. In addition, the latest version of EMFAC2000¹² will be used for the motor vehicle emissions inventory.

References

We will use CALMET to generate meteorological data for UAM and MM5 to generate data for Models-3. The UAM will be applied with five vertical layers and region top between 2 and 4 km. We will examine all available data from AIRS, ARB, and special studies to determine boundary conditions.

Meteorology

To generate the meteorological inputs for regional models, we propose to use two different meteorological models - CALMET¹³ and MM5¹⁴. CALMET is a diagnostic model and is the simpler of the two models. It requires inputs from observational data for surface and aloft winds as well as temperature data and generates three-dimensional meteorology fields to drive air quality models. CALMET includes a diagnostic wind field generator containing objective analysis and parameterized treatments of slope flows, kinematic terrain effects, terrain blocking effects, and a divergence minimization procedure, and a micro-meteorological model for over land and over water boundary layers. MM5 is an advanced state-of-science prognostic meteorological model that solves the conservation equations to simulate winds and temperatures. This is a limited area primitive equation model that uses sigma coordinate system in the vertical dimension with equally spaced rectangular grid in the horizontal on an Arakawa-Lamb B grid. The MM5 simulations will use the Blackadar high-resolution planetary boundary layer scheme, shallow convection, dry convective adjustment, the Grell cumulus scheme with explicit moisture that resolves mixed water-ice phase. Long and short wave radiation will be parameterized using Dudhia's scheme.

Two methods will be used to initialize the CALMET model:

Use only surface and upper air observations obtained from the National Weather Service (NWS) network and other sources, including radar wind profilers;
Use both surface and upper air observations and MM5 model output to improve the initial data for the CALMET model. The CALMET model results obtained using these two methods will be compared against each other and observed data to find out the performance of these two methods and which model best simulates flow features in the domain.

The CALMET model is set up with a single grid with 87x67 cells having 4 km grid spacing in x and y directions and 16 vertical layers with varying grid spacing for this study. The middle of the first vertical layer is set at 10 m above the surface to be compatible with the surface observations typically obtained by the NWS. The model top is located at 4 km above the surface. We will apply an interface program to extract data from CALMET outputs and generate inputs to UAM. Table 3.2.1 gives the UTM and latitude/longitude coordinate values of the numerical grid box used both in CALMET and UAM models. The CALMET model will be initialized using NWS hourly surface observations obtained by

References

automated surface stations, and twice-daily upper air observations obtained using rawinsonde stations.

Table 3.2.1. Coordinates of the numerical grid used in CALMET and UAM-IV models centered over San Diego County in Southern California.

	SW corner	NW corner	NE corner	SE corner
UTMX (km)	250.0	250.0	600.0	600.0
UTMY (km)	3580.0	3850.0	3850.0	3580.0
Latitude (deg)	32.33°N	34.76°N	34.79°N	32.35°N
Longitude (deg)	-119.66°W	-119.76°W	-115.91°W	-115.94°W

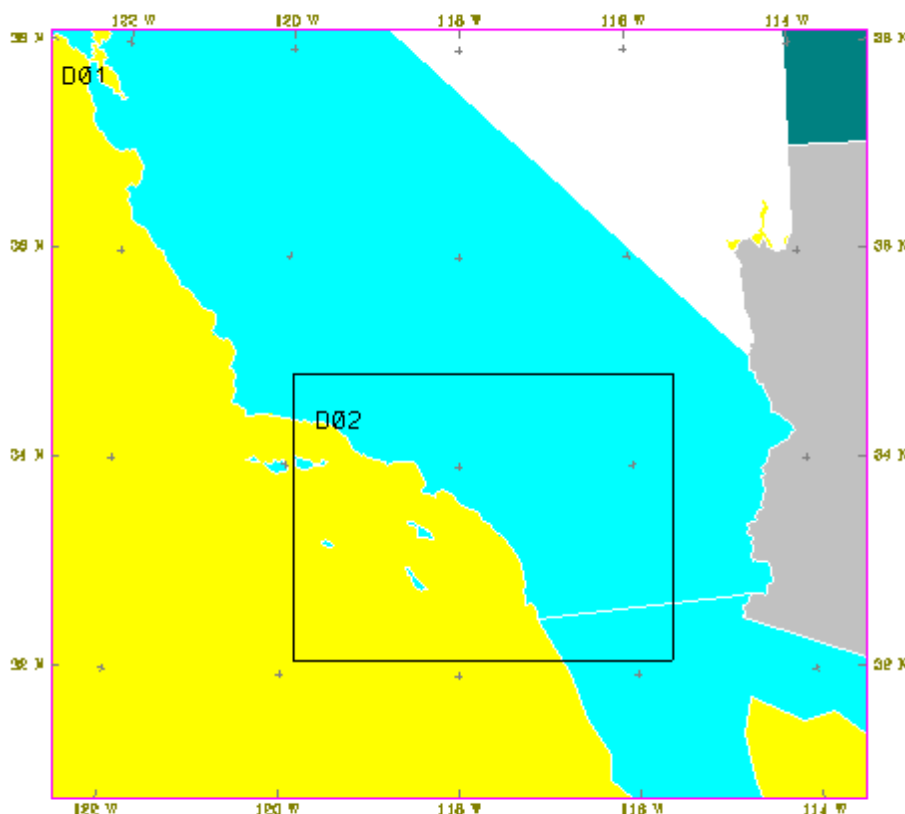
Although CALMET diagnostic meteorological model provides the necessary input parameters for the UAM air quality model, the model output can be more reliable if there is a rich network of observational data from a large number of surface and upper air stations obtained at frequent time intervals. For the initialization of the diagnostic CALMET model, all available surface stations (including 10 NWS stations, all Air Districts and ARB surface stations) and all available upper air rawinsonde stations (including 10 wind profilers) will be used. However, the surface stations are irregularly spaced and there can be missing data values because of operational problems. Furthermore, there is only one rawinsonde source available for the entire modeling domain. Therefore, domain wide coverage of the observational data are not available for numerical simulations. In order to improve the initialization of the diagnostic model, the Pennsylvania State/NCAR MM5 numerical model will be used to numerically simulate the evolution of the atmospheric circulation patterns within Southern California with an emphasis on San Diego County. This step is not required for the use of CALMET model, but is expected to improve the model performance by providing equally spaced data points both at the surface and upper levels within the modeling domain where observational data are not available.

The non-hydrostatic version of the MM5 model will be applied with one coarse and one nested domain. The grid has 27 levels in vertical sigma coordinates with resolution of approximately 10 m in the first layer and expanding towards the top of the modeling domain. The 1st, and 2nd grids will have 68x72 and 76x100 grid points with 12, and 4 km horizontal grid spacing, respectively. Table 3.2.2 provides the coordinates for the corners of the 12 km domain and offsets of 4 km domain from the lower left corner of the 12 km domain. Figure 3.2.1 shows the location of the grids used in the modeling study.

Table 3.2.2: Coordinates of the fine nested numerical grid used in MM5 centered over San Diego County in Southern California.

	SW corner	NW corner	NE corner	SE corner
UTMX (km)	231.05	233.85	633.04	628.05
UTMY (km)	3560.01	3859.79	3855.54	3556.34
Latitude (deg)	32.15°N	34.84°N	34.84°N	32.14°N
Longitude (deg)	-119.84°W	-119.92°W	-115.55°W	-115.64°W

Figure 3.2.1: Location of the coarse and fine grids used in MM5 model.



The MM5 numerical model will be initialized from the analysis files created by the National Climate and Environmental Prediction (NCEP) center using analysis nudging only. Atmospheric circulation patterns that were prevalent over the region during the case study period will be numerically simulated using 1st and 2nd grids with a two-way nested grid approach. In this approach, the effects of small-scale terrain on the evolution of the atmospheric circulation patterns will be captured by the fine scale 2nd grid. Preliminary results indicated that the model is capable of capturing the major flow features observed within the study domain.

Emissions

Gridded emission inventories for annual regional toxics modeling will be based on inventory development for the 1997 Southern California Ozone Study

References

(SCOS97). We propose to develop weekday and weekend inventories by month (a total of 24 different inventories) for this effort. The 1997 inventory will be adjusted to represent 1998 emissions.

All non-road emissions will be based on information provided from ARB's CEIDARS. Area sources will be spatially disaggregated using gridding surrogates developed by a contractor for SCOS97¹⁵. The surrogates are available at 2 km resolution, and can be grouped or re-mapped for other desired resolutions. Total Organic Gas (TOG) splits will be based on the ARB's latest organic gas profiles.

On-road emissions will be developed using two different methodologies:

- 1) For testing purposes, EMFAC2000 will be run for a two week period in January using hourly temperatures by county. Using a 1990 SCOS97 inventory as spatial surrogates, the various EMFAC2000 inventories will be allocated to grid cells.
- 2) As a best estimate of on-road emissions by month, the Caltrans Direct Travel Impact Model system DTIM4 will be run for each month using average grid cell temperatures and relative humidities. The DTIM4 runs will utilize the results from SCAG's heavy-duty truck model and weekday/weekend information developed in support of SCOS97 modeling.

Since micro-scale modeling will be performed for selected areas of the domain and combined with regional modeling results, there is a desire to minimize or avoid duplicating emissions for those areas. We propose to remove non-reactive emissions from those modeling cells in which micro-scale modeling will also be performed. However, photochemical mechanisms can be very sensitive to sudden changes in conditions, and we therefore propose to leave reactive emissions in for those cells. This will result in some double-counting of emissions, but should not drastically affect regional concentrations. We will test this assumption using a sensitivity test.

Biogenic emissions will be estimated using average seasonal temperatures and leaf mass by county. This will result in four biogenic inventories.

Diesel PM will be estimated using the EMFAC2000 diesel PM fraction of total on-road PM. Metals will be estimated by applying the ARB PM species fractions.

4. Neighborhood Scale Modeling

4.1 Modeling Domain and Time Period

The neighborhood scale modeling domain will cover an area of approximately 15 by 15km and includes a network of 961 receptors equally spaced 0.5 x 0.5-km apart. A schematic map of the modeling domain is shown in Figure 4.1.1. The

References

domain covers most of San Diego area and is centered at downtown San Diego. In this figure locations of point emission sources are shown as circles and the roadway and street network is shown as lines. We will also use a nested domain with a finer resolution of 50 m. A schematic map of the nested modeling domain is shown in Figure 4.1.2. In this figure 70 by 50 model receptors (central gridded area on the map) are shown as dots and all road links shown within the box area are used for micro-scale modeling.

Figure 4.1.1 Micro-scale modeling domain.

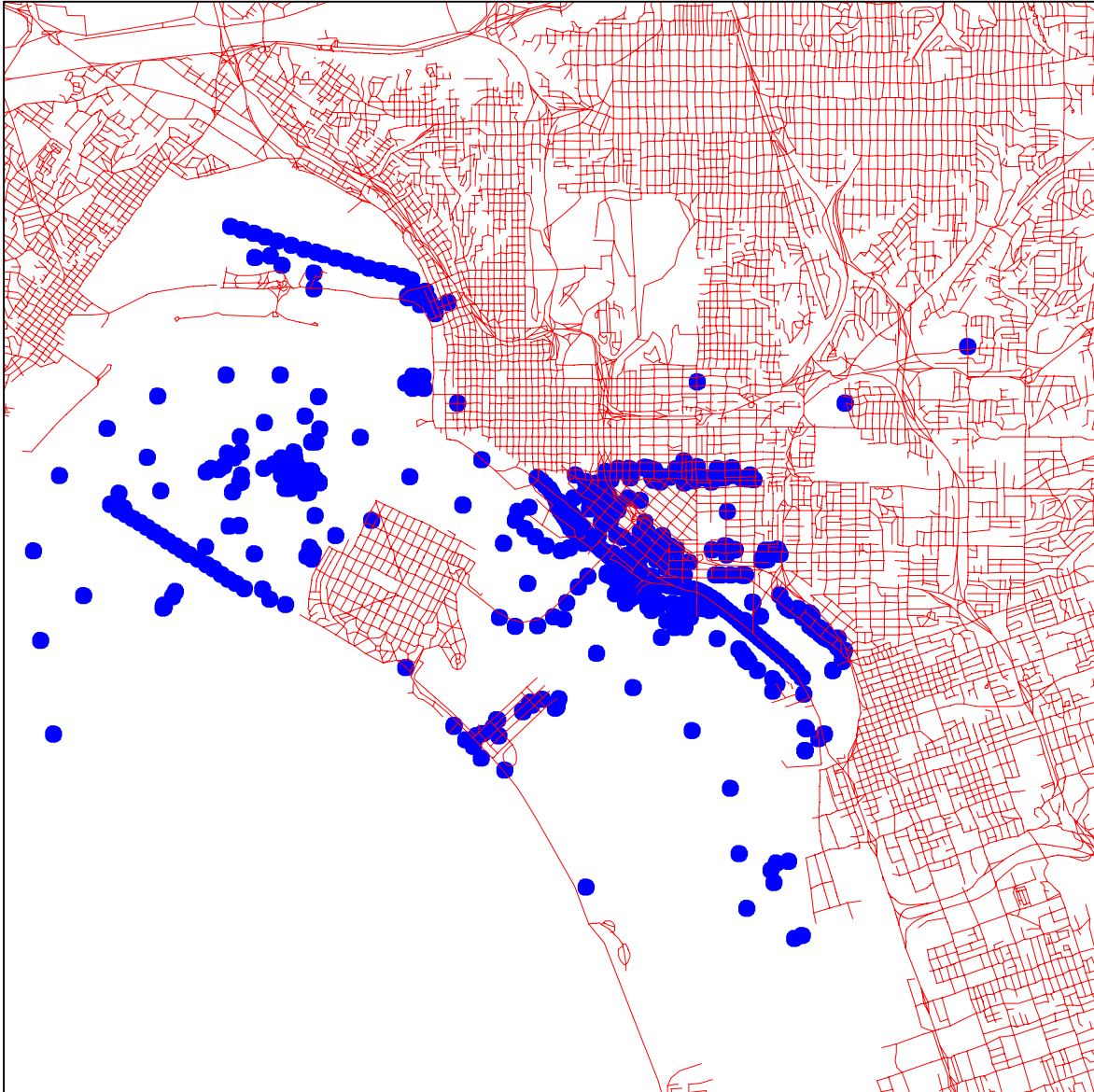
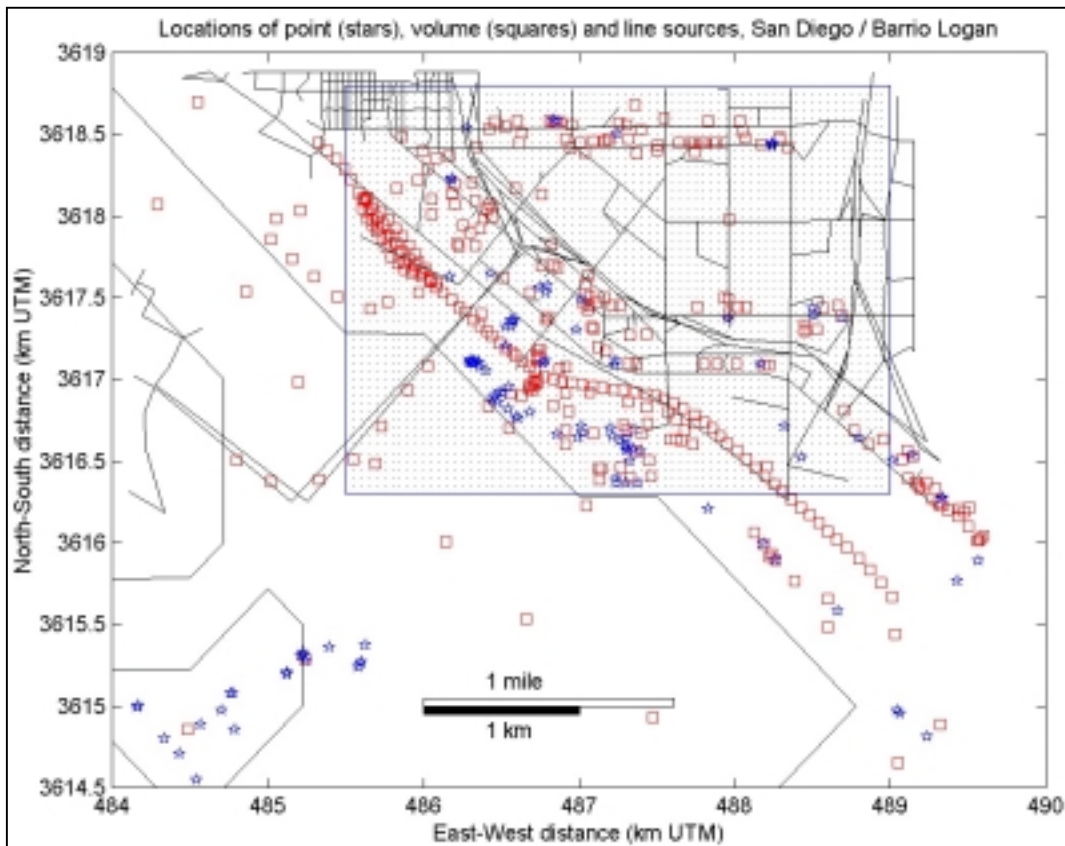


Figure 4.1.2 Micro-scale nested modeling domain.

4.2 Inputs for Micro-scale Modeling

Inputs for the micro-scale modeling include the following types of data:

- meteorology (hourly surface observations and upper air data from local airports and on-site measurements);
- We propose to use wind speed, wind direction and temperature from on-site meteorological observations and other data required for modeling from the routine observations from the closest NWS stations. On-site data of wind speed, wind direction and ambient temperature are available at Logan Memorial Junior High School for a period of 10/30/99 – 02/01/01. We selected these data for micro-scale modeling since the data are representative of the Barrio Logan area.
- There are several meteorological stations in San Diego area that can be used to estimate atmospheric stability: Lindbergh Field, Miramar, Montgomery Field, and North Island. The closest meteorological station for the study area is Lindbergh Field. Unfortunately, hourly surface observations are not available for Lindbergh Field for the study period.

References

Hourly surface and upper air data are available only for Montgomery Field, the NWS station (32°49'N / 117°08'W, 127.1m (416.9') ASL). The data for a period of 1999-2000 are available from the Western Regional Climate Center for this station. Since the most recent on-site meteorological data are available we propose to use cloud data and surface observations for 1999-2000 for this station to calculate Pasquill-Gifford stability categories¹⁶.

- point source emissions (including some traditional “area wide” sources, e.g. dry cleaners)
- California maintains a comprehensive emissions inventory for point, area, and mobile sources. The point source inventory developed in California is one of the most comprehensive in the United States because the Hot Spots program requires some smaller facilities such as dry cleaners and autobody shops as well as all major sources to report their emissions to local air districts and the ARB. Also, California maintains a detailed area source inventory developed using top-down methods. In a top-down approach, commonly used for area sources, emissions are estimated for a large region and then allocated spatially using surrogates such as area or population. A detailed description of the emission inventory developed for Barrio Logan is given in Appendix C.
- More than 600 individual point sources, more than 100 individual pollutants, and diurnal variation of emissions by hour of day and by day of week are considered for the Barrio Logan area.
- mobile source emissions (hourly traffic volumes and emission factors)

The San Diego Association of Governments (SANDAG) provided the 1999 travel demand model results and traffic network for San Diego County. Total vehicle miles traveled in Barrio Logan is estimated as 898,292 [VMT/day] as compared to 70,036,699 [VMT/day] in San Diego County. San Diego County covers an area of 4260 square miles and contains 48,583 roadway links. Barrio Logan area covers approximately 2% of the San Diego County area (7sq.mi) and includes 985 road links.

The emission factors will be obtained from EMFAC2000 version 2.02r for an average summer day of calendar year 1999. The data include running emission factors in grams per hour for PM10 from diesel fueled vehicles by vehicle class, by relative humidity, by temperature and by speed. The composite emission factors are based on the default fleet for San Diego County. TOG values from catalyst-gasoline fueled and non-catalyst-gasoline fueled vehicles will be used to model concentrations from Volatile Organic Compounds (VOC). This output is generated using Caltrans' Impact Rate Summary (IRS) model. The speciation profile will be applied to identify pollutants shown in Table 4.1.

Table 4.1 Weight fractions of TOG for the specified organic chemicals

Weight Fraction of TOG	Non-cat. stabilized	Catalyst stabilized
Formaldehyde	0.0312	0.0173
Acetaldehyde	0.0075	0.0025
1,3-butadiene	0.0083	0.0056
Benzene	0.0344	0.0268
Styrene	0.0013	0.0013
Toluene	0.0679	0.0599
Xylenes	0.0600	0.0499
Acrolein	0.0018	0.0014
MTBE	0.0186	0.0198

5. Model Performance Evaluation

To ensure that the models are working properly and are estimating concentrations reliably, a performance evaluation for each model will be conducted. A model performance evaluation compares model estimates of concentrations with measured hourly concentrations for criteria pollutants, and 24-hour and annual concentrations for toxic pollutants where measurements are available. The procedures to evaluate model performance are identified in ARB's Technical Guidance Document¹⁷ on modeling. Standard statistical techniques such as bias and gross error will be calculated for annual model estimates of concentrations as well as for monthly and seasonal averaging times.

It is essential that meteorology, emissions, and air quality databases be available to test and evaluate a model's performance. To evaluate micro-scale models, a new database for short-range dispersion in urban areas will be collected through a field monitoring study for air quality and meteorological data. This field study will be conducted by researchers from UC Riverside¹¹. The field study will include the releases of known amounts of a tracer gas, SF₆, bag sampling and continuous monitoring of the tracer gas, and detailed meteorological measurements, which include six sonic anemometers and a mini-sodar.

To evaluate the regional air quality models, we propose to use the routine meteorological and air quality data collected from the monitoring networks operated by air districts and ARB. These include toxic data as well as criteria pollutants (both primary and secondary) and any other data gathered from special monitoring studies that may be useful. The evaluation process will be similar to that proposed for the micro-scale modeling in that similar statistical tests and diagnostic evaluations will be conducted to establish the reliability of model estimates. Although similar tests and evaluation procedures are proposed for regional as well as for micro-scale modeling, a greater level of resources is necessary to evaluate the regional model.

After evaluating the performance of each micro-scale and regional model, we will develop recommendations for guidelines, including technical protocols and methodologies. In addition, we will share our modeling results and

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recommendations with EPA's Emission Modeling and Analysis Division, OAQPS, which is currently developing guidelines for air dispersion modeling of toxic pollutants in urban areas.

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NAP Protocol - Appendix A

Listing of the SAPRC-99

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! SAPRC-99e Adjustable Parameter Mechanism
! Created from SAPRC99F.RXN, which was created
! from BASEMECH.XLS 10-Apr-2000 17:09
!-----
! Document:
! WPL Carter, 1999, "Documentation of the SAPRC-99 Chemical Mechanism
! for VOC Reactivity Assessment," Volume 1 of 2. Documentation Text.
! Final Report to CARB. Contract No. 92329, 95-308, May 8 2000.
! (available at www.cert.ucr.edu/pub/carter/pubs/s99txt.pdf)
!-----
! Adapted to UAM-FCM by Luis Woodhouse (9/2000)
!-----
! Small changes in nomenclature and species names were
! necessary for running in UAM-FCM:
! { to "
! } to "
! HO. to HO
! HO2. to HO2
! CCO3. to CCO3
! BZNO2O. to BZNO2O
! TBU-O. to TBUO
! BZ-O. to BZO
! HOCOO. to HOCOO
! R2O2. to R2O2
! METHACRO to METH
! MA-PAN to MPAN
! CCO-O2 to CCO3
! ISOPRENE to ISOP
! ISO-PROD to ISPD
! ETHENE to ETHE
! RCO-O2. to RCO3
! MA-RCO3. to MCO3
! CCO-OOH to CO3H
! CCO-OH to CO2H
! RCO-OOH to RC3H
! RCO-OH to RC2H
! HCOOH to HC2H
! C-O2. TO CXO2
! RO2-R. to RO2R
! RO2-N. to RO2N
! BZCO. to BZCO
! O*1D to O1D
! BZ(NO2)-O to BZNO2O
! Added an & at end of line in reactions that continue in following line
! Changed K0+K3M/1+K3M/K2 to K0+K3*M(1+K3*M/K2)
!
! Change the following four reaction labels
! O1OP to O1OA
! O2OP to O2OA
! T1OP to T1OA
! R1OP to R1OA
!-----
!
!
! RO2R = Represents effect of peroxyradicals that ultimately cause
! one NO=>NO2 and formation of HO2 when reacting with NO
! Has zero carbons
! RO2O2 = Effect of extra NO=>NO2 in multistep reactions
! RO2N = Reactions of peroxyradical with NO to form nitrates
!
! Explicitly represented and lumped molecule products
!
! HCHO, CCHO, RCHO (propionaldehyde and higher aldehydes), acetone,
! MEK, MEOH, COOH (methyl hydroperoxyde), ROOH (lumped higher peroxides),
! glyoxal, MGly (methyl glyoxal and higher alpha-dicarbonyl aldehydes),
! BACL (biacetyl and other alpha-dicarbonyl ketones), PHEN, CRES (cresols),
! NPHE (nitrophenols), BALD (benzaldehyde and other aromatic aldehydes),
! methacrolein, MVK (methyl vinyl ketone), ISOPRENE (4-product isoprene
! mechanism), ISOPROD (lumped isoprene products)
!
! Lumped parameter products:
!
! PROD2 = Lumped higher reactivity non-aldehyde oxygenates
! represents ketones and alcohols and other reactive non-aromatic
! and non-double-bond-containing oxygenated products with rate
! constants higher than 5x10**12 cm3 molec-1 s-1.
! See Table 3, page 22 in SAPRC-99 documentation for molecular
! weight (C6H12O2)
! RNO3 = Lumped organic nitrate products (other than PAN or PAN analogues)
! DCB1 = Uncharacterized ring-opening that do not undergo significant
! decomposition to form radicals (from benzene, naphthalene,
! unsaturated diketones (replaces AFG1)
! DCB2 DCB3= Represent highly photoreactive ring opening products formed

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References

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!      from alkylbenzenes. DCB2 is used to represent products with
!      an action spectra like alpha-dicarbonyl, and DCB3 uses action
!      spectra of acrolein.
!      Mechanism from CH3C(O)CH=CHCHO (MW=98.10237 g/mol) -see page
!      25 in documentation.
! ALK1  = Alkane and other non-aromatics that react only with OH and
!         kOH <5x10**+2 ppm-1min-1. Mainly ethane
! ALK2  = Alkane and other non-aromatics that react only with OH and
!         5x10**+2 ppm-1min-1 < kOH < 2.5x10+3 ppm-1min-1. Mainly propane
!         and acetylene.
! ALK3  = Alkane and other non-aromatics that react only with OH and
!         2.5x10**+3 ppm-1min-1 < kOH < 5x10+3 ppm-1min-1.
! ALK4  = Alkane and other non-aromatics that react only with OH and
!         5x10**+3 ppm-1min-1 < kOH < 1x10+4 ppm-1min-1.
! ALK5  = Alkane and other non-aromatics that react only with OH and
!         kOH > 1x10**+4 ppm-1min-1
! ARO1  = Aromatics with kOH < 2x10**+4 ppm-1min-1
! ARO2  = Aromatics with kOH > 2x10**+4 ppm-1min-1
! OLE1  = Alkenes (other than ethene) with kOH < 7x10**+4 ppm-1min-1
! OLE2  = Alkenes with kOH > 7x10**+4 ppm-1min-1
! ALD1  = higher aldehydes
! KET1  = higher ketones
! ACR1  = acroleins
!
! Unreactive product species
!
! CO2, NROG (non-reactive voc or non-reactive voc oxidation products),
! XC (lost carbon), XN (lost nitrogen), H2, SULF (formation of SO3 from SO2)
!
!
FORMAT=2
!
!-----
!      Conc(0) Mwt #C's #N's
!
!
.ACT
O3      0.0 48.00 0.0 0
NO      0.0 30.01 0.0 1
NO2     0.0 46.01 0.0 1
HO2     0.0 33.01 0.0 0
NO3     0.0 62.01 0.0 1
N2O5   0.0 108.02 0.0 2
HO      0.0 17.0 0.0 0
CXO2   0.0
RO2R   0.0
R2O2   0.0
RO2N   0.0
CCO3   0.0
RCO3   0.0
MCO3   0.0
BZCO   0.0
!
DCB1   0.0 84.07 5. 0
DCB3   0.0 98.10 5. 0
PROD2  0.0 116.16 6.0 0
!
.SLO
HNO3   0.0 63.02 0.0 1
HONO   0.0 47.02 0.0 1
HNO4   0.0 79.02 0.0 1
HCHO   0.0 30.03 1.0 0
CCHO   0.0 44.05 2.0 0
RCHO   0.0 58.08 3.0 0
ACET   0.0 58.08 3.0 0
MEK    0.0 72.11 4.0 0
RNO3   0.0 133.15 5.0 1
CO     0.0 28.01 1.0 0
CO2    0.0 44.01 1.0 0
HO2H   0.0 34.02 0.0 0
PAN    0.0 121.05 2.0 1
PAN2   0.0 135.08 3.0 1
GLY    0.0 58.04 2.0 0
MGLY   0.0 72.07 3.0 0
PHEN   0.0 94.11 6.0 0
CRES   0.0 108.14 7.0 0
BALD   0.0 106.13 7.0 0
NPHE   0.0 139.11 6.0 1
PBZN   0.0 183.13 7.0 1
ETHE   0.0 28.05 2.0 0
SO2    0.0 64.06 0.0 0
H2     0.0 2.02 0.0 0
XC     0.0 0.00 1.0 0
XN     0.0 0.00 0.0 1
CH4    1.79 16.04 1.0 0
MEOH   0.0 46.07 2.0 0
!TERP  0.0 131.09 10.0 0
ISOP   0.0 68.12 5. 0
METH   0.0 70.09 4. 0
MVK    0.0 70.09 4. 0
ISPD   0.0 0.0 5. 0
MPAN   0.0 0.0 4. 1
DCB2   0.0 98.10 5. 0

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References

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SULF 0.0 81.07 0. 0
CO3H 0.0
CO2H 0.0
RC3H 0.0
RC2H 0.0
HC2H 0.0
INERT 0.0 0.0 0. 0
ROOH 0.0 62.07 2. 0
COOH 0.0 48.04 1. 0
BACL 0.0 86.09 4. 0
!
!           Lumped groups (parameters emissions-dependent)
!
= ALK1 + ALK2 + ALK3 + ALK4 + ALK5 + ARO1 + ARO2 + OLE1 + OLE2 + TRP1
= KET1 + ALD1 + ACR1
!
.CON
O2 2.09E+5 32.00 0.0 0
M 1.00E+6 28.85 0.0 0
H2O 2.00E+4 18.02 0.0 0
HV 1.0 0.00 0.0 0
H2 0.00E+0
!
.STS
=O3P + O1D2 + TBUO + BZO + BZNO2O + HOCOO
!

.RXN
1) PF=NO2 ;NO2 + HV = NO + O3P
2) 5.68e-34 0.000 -2.80 ;O3P + O2 + M = O3 + M
3) 8.00e-12 4.094 0.00 ;O3P + O3 = #2 O2
4) 1.00e-31 0.000 -1.60 ;O3P + NO + M = NO2 + M
5) 6.50e-12 -0.238 0.00 ;O3P + NO2 = NO + O2
6) FALLOFF ;O3P + NO2 = NO3 + M
9.00e-32 0.000 -2.00
2.20e-11 0.000 0.00
0.80 1.0
8) 1.80e-12 2.722 0.00 ;O3 + NO = NO2 + O2
9) 1.40e-13 4.908 0.00 ;O3 + NO2 = O2 + NO3
10) 1.80e-11 -0.219 0.00 ;NO + NO3 = #2 NO2
11) 3.30e-39 -1.053 0.00 ;NO + NO + O2 = #2 NO2
12) FALLOFF ;NO2 + NO3 = N2O5
2.80e-30 0.000 -3.50
2.00e-12 0.000 0.20
0.45 1.0
13) FALLOFF ;N2O5 = NO2 + NO3
1.00e-03 21.859 -3.50
9.70e+14 22.018 0.10
0.45 1.0
14) 2.60e-22 ;N2O5 + H2O = #2 HNO3
17) 4.50e-14 2.504 0.00 ;NO2 + NO3 = NO + NO2 + O2
18) PF=NO3NO ;NO3 + HV = NO + O2
19) PF=NO3NO2 ;NO3 + HV = NO2 + O3P
20) PF=O3O3P ;O3 + HV = O3P + O2
21) PF=O3O1D ;O3 + HV = O1D2 + O2
22) 2.20e-10 ;O1D2 + H2O = #2 HO
23) 2.09e-11 -0.189 0.00 ;O1D2 + M = O3P + M
24) FALLOFF ;HO + NO = HONO
7.00e-31 0.000 -2.60
3.60e-11 0.000 -0.10
0.60 1.0
25) PF=HONO-NO ;HONO + HV = HO + NO
26) PF=HONO-NO2 ;HONO + HV = HO2 + NO2
27) 2.70e-12 -0.517 0.00 ;HO + HONO = H2O + NO2
28) FALLOFF ;HO + NO2 = HNO3
2.43e-30 0.000 -3.10
1.67e-11 0.000 -2.10
0.60 1.0
29) 2.00e-11 ;HO + NO3 = HO2 + NO2
30) K0+K3M/1+K3M/K2 ;HO + HNO3 = H2O + NO3
7.20e-15 -1.560 0.00
4.10e-16 -2.862 0.00
1.90e-33 -1.441 0.00
31) PF=HNO3 ;HNO3 + HV = HO + NO2
32) K1+K2[M] ;HO + CO = HO2 + CO2
1.30e-13
3.19e-33
33) 1.90e-12 1.987 0.00 ;HO + O3 = HO2 + O2
34) 3.40e-12 -0.537 0.00 ;HO2 + NO = HO + NO2
35) FALLOFF ;HO2 + NO2 = HNO4
1.80e-31 0.000 -3.20
4.70e-12 0.000 0.00
0.60 1.0
36) FALLOFF ;HNO4 = HO2 + NO2
4.10e-05 21.164 0.00
5.70e+15 22.197 0.00
0.50 1.0
37) PF=HO2NO2 ;HNO4 + HV = #.61 "HO2 + NO2" + #.39 "HO + NO3"
38) 1.50e-12 -0.715 0.00 ;HNO4 + HO = H2O + NO2 + O2
39) 1.40e-14 1.192 0.00 ;HO2 + O3 = HO + #2 O2
40A) K1+K2[M] ;HO2 + HO2 = HO2H + O2
2.20e-13 -1.192 0.00
1.85e-33 -1.947 0.00

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References

40B) K1+K2[M] ;HO2 + HO2 + H2O = HO2H + O2 + H2O
3.08e-34 -5.564 0.00
2.59e-54 -6.319 0.00
41) 4.00e-12 O2" ;NO3 + HO2 = #.8 "HO + NO2 + O2" + #.2 "HNO3 + &
42) 8.50e-13 4.869 0.00 ;NO3 + NO3 = #2 NO2 + O2
43) PF=H2O2 ;HO2H + HV = #2 HO
44) 2.90e-12 0.318 0.00 ;HO2H + HO = HO2 + H2O
45) 4.80e-11 -0.497 0.00 ;HO + HO2 = H2O + O2
S2OH) FALLOFF ;HO + SO2 = HO2 + SULF
4.00e-31 0.000 -3.30
2.00e-12 0.000 0.00
0.45 1.0
H2OH) 7.70e-12 4.173 0.00 ;HO + H2 = HO2 + H2O
MER1) 2.80e-12 -0.566 0.00 ;CXO2 + NO = NO2 + HCHO + HO2
MER6) 5.90e-13 1.011 0.00 ;CXO2 + CXO2 = #2 "HCHO + HO2"
RRNO) 2.70e-12 -0.715 0.00 ;RO2R + NO = NO2 + HO2
RRH2) 1.90e-13 -2.583 0.00 ;RO2R + HO2 = ROOH + O2 + #3 XC
RRN3) 2.30e-12 ;RO2R + NO3 = NO2 + O2 + HO2
RRME) 2.00e-13 ;RO2R + CXO2 = HO2 + #.75 HCHO + #.25 MEOH
RRR2) 3.50e-14 ;RO2R + RO2R = HO2
R2NO) SAMEK RRNO ;R2O2 + NO = NO2
R2H2) SAMEK RRH2 ;R2O2 + HO2 = HO2
R2N3) SAMEK RRN3 ;R2O2 + NO3 = NO2
R2ME) SAMEK RRME ;R2O2 + CXO2 = CXO2
R2RR) SAMEK RRR2 ;R2O2 + RO2R = RO2R
R2R3) SAMEK RRR2 ;R2O2 + R2O2 =
RNN0) SAMEK RRNO ;RO2N + NO = RNO3
RNH2) SAMEK RRH2 ;RO2N + HO2 = ROOH + #3 XC
RNME) SAMEK RRME ;RO2N + CXO2 = HO2 + #.25 MEOH + #.5 "MEK + &
PROD2" + #.75 HCHO + XC
RNN3) SAMEK RRN3 ;RO2N + NO3 = NO2 + O2 + HO2 + MEK + #2 XC
RNR2) SAMEK RRR2 ;RO2N + RO2R = HO2 + #.5 "MEK + PROD2" + O2 + &
XC
RNR2) SAMEK RRR2 ;RO2N + R2O2 = RO2N
RNRN) SAMEK RRR2 ;RO2N + RO2N = MEK + HO2 + PROD2 + O2 + #2 XC
APN2) FALLOFF ;CCO3 + NO2 = PAN
2.70e-28 0.000 -7.10
1.20e-11 0.000 -0.90
0.30 1.0
DPAN) FALLOFF ;PAN = CCO3 + NO2
4.90e-03 24.045 0.00
4.00e+16 27.026 0.00
0.30 1.0
APNO) 7.80e-12 -0.596 ;CCO3 + NO = CXO2 + CO2 + NO2
APH2) 4.30e-13 -2.067 0.00 ;CCO3 + HO2 = #.75 "CO3H + O2" + &
#.25 "CO2H + O3"
APN3) 4.00e-12 ;CCO3 + NO3 = CXO2 + CO2 + NO2 + O2
APME) 1.80e-12 -0.994 0.00 ;CCO3 + CXO2 = CO2H + HCHO + O2
APRR) 7.50e-12 ;CCO3 + RO2R = CO2H
APR2) SAMEK APRR ;CCO3 + R2O2 = CCO3
APRN) SAMEK APRR ;CCO3 + RO2N = CO2H + PROD2
APAP) 2.90e-12 -0.994 0.00 ;CCO3 + CCO3 = #2 "CXO2 + CO2" + O2
PPN2) 1.20e-11 0.000 -0.90 ;RCO3 + NO2 = PAN2
PAN2) 2.00e+15 25.436 0.00 ;PAN2 = RCO3 + NO2
PPNO) 1.25e-11 -0.477 ;RCO3 + NO = NO2 + CCHO + RO2R + CO2
PPH2) SAMEK APH2 ;RCO3 + HO2 = #.75 "RC3H + O2" + &
#.25 "RC2H + O3"
PPN3) SAMEK APN3 ;RCO3 + NO3 = NO2 + CCHO + RO2R + CO2 + O2
PPME) SAMEK APME ;RCO3 + CXO2 = RC2H + HCHO + O2
PPRR) SAMEK APRR ;RCO3 + RO2R = RC2H + O2
PPR2) SAMEK APRR ;RCO3 + R2O2 = RCO3
PPRN) SAMEK APRR ;RCO3 + RO2N = RC2H + PROD2 + O2
PPAP) SAMEK APAP ;RCO3 + CCO3 = #2 CO2 + CXO2 + CCHO + &
RO2R + O2
PPPP) SAMEK APAP ;RCO3 + RCO3 = #2 "CCHO + RO2R + CO2"
BPN2) 1.37e-11 ;BZCO + NO2 = PBZN
BPAN) 7.90e+16 27.821 0.00 ;PBZN = BZCO + NO2
BPNO) SAMEK PPNO ;BZCO + NO = NO2 + CO2 + BZO + R2O2
BPH2) SAMEK APH2 ;BZCO + HO2 = #.75 "RC3H + O2" + &
#.25 "RC2H + O3" + #4 XC
BPN3) SAMEK APN3 ;BZCO + NO3 = NO2 + CO2 + BZO + R2O2 + O2
BPME) SAMEK APME ;BZCO + CXO2 = RC2H + HCHO + O2 + #4 XC
BPRR) SAMEK APRR ;BZCO + RO2R = RC2H + O2 + #4 XC
BPR2) SAMEK APRR ;BZCO + R2O2 = BZCO
BPRN) SAMEK APRR ;BZCO + RO2N = RC2H + PROD2 + O2 + #4 XC
BPAP) SAMEK APAP ;BZCO + CCO3 = #2 CO2 + CXO2 + BZO + &
R2O2
BPPP) SAMEK APAP ;BZCO + RCO3 = #2 CO2 + CCHO + RO2R + &
BZO + R2O2
BPBP) SAMEK APAP ;BZCO + BZCO = #2 "BZO + R2O2 + CO2"
MPN2) SAMEK PPN2 ;MCO3 + NO2 = MPAN
MPPN) 1.60e+16 26.800 0.00 ;MPAN = MCO3 + NO2
MPNO) SAMEK PPNO ;MCO3 + NO = NO2 + CO2 + HCHO + CCO3
MPH2) SAMEK APH2 ;MCO3 + HO2 = #.75 "RC3H + O2" + &
#.25 "RC2H + O3" + XC
MPN3) SAMEK APN3 ;MCO3 + NO3 = NO2 + CO2 + HCHO + CCO3 + O2
MPME) SAMEK APME ;MCO3 + CXO2 = RC2H + HCHO + XC + O2
MPRR) SAMEK APRR ;MCO3 + RO2R = RC2H + XC
MPR2) SAMEK APRR ;MCO3 + R2O2 = MCO3
MPRN) SAMEK APRR ;MCO3 + RO2N = #2 RC2H + O2 + #4 XC
MPAP) SAMEK APAP ;MCO3 + CCO3 = #2 CO2 + CXO2 + HCHO + &
CCO3 + O2

References

MPPP) SAMEK APAP ;MCO3 + RCO3 = HCHO + CCO3 + CCHO + &
 RO2R + #2 CO2
 MPBP) SAMEK APAP ;MCO3 + BZCO = HCHO + CCO3 + BZO + &
 R2O2 + #2 CO2
 MPMP) SAMEK APAP ;MCO3 + MCO3 = #2 "HCHO + CCO3 + CO2"
 TBON) 2.40e-11 ;TBUO + NO2 = RNO3 + #2 XC
 TBOD) 7.50e+14 16.200 0.00 ;TBUO = ACET + CXO2
 BRN2) 2.30e-11 -0.298 0.00 ;BZO + NO2 = NPHE
 BRH2) SAMEK RRH2 ;BZO + HO2 = PHEN
 BRXX) 1.00e-03 ;BZO = PHEN
 BNN2) SAMEK BRN2 ;BZNO2O + NO2 = #2 XN + #6 XC
 BNH2) SAMEK RRH2 ;BZNO2O + HO2 = NPHE
 BNXX) SAMEK BRXX ;BZNO2O = NPHE
 FAHV) PF=HCHO_R ;HCHO + HV = #2 HO2 + CO
 FAVS) PF=HCHO_M ;HCHO + HV = H2 + CO
 FAOH) 8.60e-12 -0.040 0.00 ;HCHO + HO = HO2 + CO + H2O
 FAH2) 9.70e-15 -1.242 0.00 ;HCHO + HO2 = HOCOO
 FAHR) 2.40e+12 13.910 0.00 ;HOCOO = HO2 + HCHO
 FAHN) SAMEK MER1 ;HOCOO + NO = HC2H + NO2 + HO2
 FAN3) 2.00e-12 4.830 0.00 ;HCHO + NO3 = HNO3 + HO2 + CO
 AAOH) 5.60e-12 -0.616 0.00 ;CCHO + HO = CCO3 + H2O
 AAHV) PF=CCHO_R ;CCHO + HV = CO + HO2 + CXO2
 AAN3) 1.40e-12 3.696 0.00 ;CCHO + NO3 = HNO3 + CCO3
 PAOH) 2.00e-11 ;RCHO + HO = #.034 RO2R + #.001 RO2N + &
 #.965 RCO3 + #.034 CO + #.034 CCHO + &
 #-0.003 XC
 PAHV) PF=C2CHO ;RCHO + HV = CCHO + RO2R + CO + HO2
 PAN3) 1.40e-12 3.520 ;RCHO + NO3 = HNO3 + RCO3
 K3OH) 1.10e-12 1.033 0.00 ;ACET + HO = HCHO + CCO3 + R2O2
 K3HV) PF=ACETONE ;ACET + HV = CCO3 + CXO2
 K4OH) 1.30e-12 0.050 2.00 ;MEK + HO = #.37 RO2R + #.042 RO2N + &
 #.616 R2O2 + #.492 CCO3 + #.096 RCO3 + &
 #.115 HCHO + #.482 CCHO + #.37 RCHO + #.287 XC
 K4HV) PF=KETONE QY=1.50e-1 ;MEK + HV = CCO3 + CCHO + RO2R
 MeOH) 3.10e-12 0.715 2.00 ;MEOH + HO = HCHO + HO2
 MER9) 2.90e-12 -0.378 0.00 ;COOH + HO = H2O + #.35 "HCHO + HO" + #.65 CXO2
 MERA) PF=COOH ;COOH + HV = HCHO + HO2 + HO
 LPR9) 1.10e-11 ;ROOH + HO = H2O + RCHO + #.34 RO2R + #.66 HO
 LPRA) PF=COOH ;ROOH + HV = RCHO + HO2 + HO
 GLHV) PF=GLY_R ;GLY + HV = #2 "CO + HO2"
 GLVM) PF=GLY_ABS QY=6.00e-3 ;GLY + HV = HCHO + CO
 GLOH) 1.10e-11 ;GLY + HO = #.63 HO2 + #1.26 CO + #.37 RCO3 + &
 #- .37 XC
 GLN3) 2.80e-12 4.722 ;GLY + NO3 = HNO3 + #.63 HO2 + #1.26 CO + &
 #.37 RCO3 + #- .37 XC
 MGHV) PF=MGLY_ADJ ;MGLY + HV = HO2 + CO + CCO3
 MGOH) 1.50e-11 ;MGLY + HO = CO + CCO3
 MGN3) 1.40e-12 3.765 ;MGLY + NO3 = HNO3 + CO + CCO3
 BAHV) PF=BACL_ADJ ;BACL + HV = #2 CCO3
 PHOH) 2.63e-11 ;PHEN + HO = #.24 BZO + #.76 RO2R + #.23 GLY + &
 #4.1 XC
 PHN3) 3.78e-12 ;PHEN + NO3 = HNO3 + BZO
 CROH) 4.20e-11 ;CRES + HO = #.24 BZO + #.76 RO2R + &
 #.23 MGLY + #4.87 XC
 CRN3) 1.37e-11 ;CRES + NO3 = HNO3 + BZO + XC
 NPN3) SAMEK PHN3 ;NPHE + NO3 = HNO3 + BZNO2O
 BZOH) 1.29e-11 ;BALD + HO = BZCO
 BZHV) PF=BZCHO QY=5.00e-2 ;BALD + HV = #7 XC
 BZNT) 1.40e-12 3.720 0.00 ;BALD + NO3 = HNO3 + BZCO
 MAOH) 1.86e-11 -0.350 0.00 ;METH + HO = #.5 RO2R + #.416 CO + &
 #.084 HCHO + #.416 MEK + #.084 MGLY + &
 #.5 MCO3 + #-0.416 XC
 MAO3) 1.36e-15 4.200 0.00 ;METH + O3 = #.008 HO2 + #.1 RO2R + &
 #.208 HO + #.1 RCO3 + #.45 CO + #.117 CO2 + &
 #.2 HCHO + #.9 MGLY + #.333 HC2H + #-0.1 XC
 MAN3) 1.50e-12 3.430 0.00 ;METH + NO3 = #.5 "HNO3 + RO2R + CO + &
 MCO3 " + #1.5 XC + #.5 XN
 MAOP) 6.34e-12 ;METH + O3P = RCHO + XC
 MAHV) PF=ACROLEIN ;METH + HV + #.9 = #.34 HO2 + #.33 RO2R + &
 #.33 HO + #.67 CCO3 + #.67 CO + #.67 HCHO + &
 #.33 MCO3 + #-0. XC
 MVOH) 4.14e-12 -0.900 0.00 ;MVK + HO = #.3 RO2R + #.025 RO2N + &
 #.675 R2O2 + #.675 CCO3 + #.3 HCHO + &
 #.675 RCHO + #.3 MGLY + #-0.725 XC
 MVO3) 7.51e-16 3.020 0.00 ;MVK + O3 = #.064 HO2 + #.05 RO2R + #.164 HO + &
 #.05 RCO3 + #.475 CO + #.124 CO2 + #.1 HCHO + &
 #.95 MGLY + #.351 HC2H + #-0.05 XC
 MVOP) 4.32e-12 ;MVK + O3P = #.45 RCHO + #.55 MEK + #.45 XC
 MVHV) PF=ACROLEIN QY=2.10e-3 ;MVK + HV = #.3 CXO2 + #.7 CO + #.7 PROD2 + &
 #.3 MCO3 + #-2.4 XC
 IPOH) 6.19e-11 ;ISPD + HO = #.67 RO2R + #.041 RO2N + &
 #.289 MCO3 + #.336 CO + #.055 HCHO + &
 #.129 CCHO + #.013 RCHO + #.15 MEK + #.332 PROD2 + &
 #.15 GLY + #.174 MGLY + #-0.504 XC
 IPO3) 4.18e-18 ;ISPD + O3 = #.4 HO2 + #.048 RO2R + &
 #.048 RCO3 + #.285 HO + #.498 CO + #.14 CO2 + &
 #.125 HCHO + #.047 CCHO + #.21 MEK + #.023 GLY + &
 #.742 MGLY + #.1 HC2H + #.372 RC2H + #- .33 XC
 IPN3) 1.00e-13 ;ISPD + NO3 = #.799 RO2R + #.051 RO2N + &
 #.15 MCO3 + #.572 CO + #.15 HNO3 + &
 #.227 HCHO + #.218 RCHO + #.008 MGLY + &
 #.572 RNO3 + #.28 XN + #- .815 XC
 IPHV) PF=ACROLEIN QY=4.10e-3 ;ISPD + HV = #1.233 HO2 + #.467 CCO3 + &

References

#.3 RCO3 + #1.233 CO + #.3 HCHO + #.467 CCHO + &
 #.233 MEK + #-233 XC
 K6OH) 1.50e-11 ;PROD2 + HO = #.379 HO2 + #.473 RO2R + &
 #.07 RO2N + #.029 CCO3 + #.049 RCO3 + &
 #.213 HCHO + #.084 CCHO + #.558 RCHO + #.115 MEK + &
 #.329 PROD2 + #.886 XC
 K6HV) PF=KETONE QY=2.00e-2 ;PROD2 + HV = #.96 RO2R + #.04 RO2N + &
 #.515 R2O2 + #.667 CCO3 + #.333 RCO3 + &
 #.506 HCHO + #.246 CCHO + #.71 RCHO + #.299 XC
 RNOH) 7.80e-12 ;RNO3 + HO = #.338 NO2 + #.113 HO2 + &
 #.376 RO2R + #.173 RO2N + #.596 R2O2 + &
 #.01 HCHO + #.439 CCHO + #.213 RCHO + #.006 ACET + &
 #.177 MEK + #.048 PROD2 + #.31 RNO3 + #.351 XN + &
 #.56 XC
 RNVH) PF=IC3ONO2 ;RNO3 + HV = NO2 + #.341 HO2 + #.564 RO2R + &
 #.095 RO2N + #.152 R2O2 + #.134 HCHO + &
 #.431 CCHO + #.147 RCHO + #.02 ACET + #.243 MEK + &
 #.435 PROD2 + #.35 XC
 D1OH) 5.00e-11 ;DCB1 + HO = RCHO + RO2R + CO
 D1O3) 2.00e-18 ;DCB1 + O3 = #1.5 HO2 + #.5 HO + #1.5 CO + &
 #.5 CO2 + GLY
 D2OH) 5.00e-11 ;DCB2 + HO = R2O2 + RCHO + CCO3
 D2HV) PF=MGLY_ABS QY=3.65e-1 ;DCB2 + HV = RO2R + #.5 "CCO3 + HO2" + CO + &
 R2O2 + #.5 "GLY + MGLY + XC"
 D3OH) 5.00e-11 ;DCB3 + HO = R2O2 + RCHO + CCO3
 ! FCM not suited to handle E+a only E-a:
 !D3HV) PF=ACROLEIN QY=7.28e+0 ;DCB3 + HV = RO2R + #.5 "CCO3 + HO2" + CO + &
 D3HV) PF=ACROLEIN QY=7.28 ;DCB3 + HV = RO2R + #.5 "CCO3 + HO2" + CO + &
 R2O2 + #.5 "GLY + MGLY + XC"
 c1OH) 2.15e-12 3.448 0.00 ;CH4 + HO = H2O + CXO2
 etOH) 1.96e-12 -0.870 0.00 ;ETHE + HO = RO2R + #1.61 HCHO + #.195 CCHO
 etO3) 9.14e-15 5.127 0.00 ;ETHE + O3 = #.12 HO + #.12 HO2 + #.5 CO + &
 #.13 CO2 + HCHO + #.37 HC2H
 etN3) 4.39e-13 4.535 2.00 ;ETHE + NO3 = RO2R + RCHO + #1 XC + XN
 etOA) 1.04e-11 1.574 0.00 ;ETHE + O3P = #.5 HO2 + #.2 RO2R + #.3 CXO2 + &
 #.491 CO + #.191 HCHO + #.25 CCHO + #.009 GLY + &
 #.5 XC
 isOH) 2.50e-11 -0.810 0.00 ;ISOP + HO = #.907 RO2R + #.093 RO2N + &
 #.079 R2O2 + #.624 HCHO + #.23 METH + &
 #.32 MVK + #.357 ISPD + #-0.167 XC
 isO3) 7.86e-15 3.800 0.00 ;ISOP + O3 = #.266 HO + #.066 RO2R + &
 #.008 RO2N + #.126 R2O2 + #.192 MCO3 + &
 #.275 CO + #.122 CO2 + #.592 HCHO + #.1 PROD2 + &
 #.39 METH + #.16 MVK + #.204 HC2H + &
 #.15 RC2H + #-0.259 XC
 isN3) 3.03e-12 0.890 0.00 ;ISOP + NO3 = #.187 NO2 + #.749 RO2R + &
 #.064 RO2N + #.187 R2O2 + #.936 ISPD + &
 #-0.064 XC + #.813 XN
 isOP) 3.60e-11 ;ISOP + O3P = #.01 RO2N + #.24 R2O2 + &
 #.25 CXO2 + #.24 MCO3 + #.24 HCHO + &
 #.75 PROD2 + #-1.01 XC
 !
 ! 5 Lumped groups for alkanes/others
 A1OH) ;ALK1 + HO = #A1OHN2 NO2 + #A1OHHO HO + #A1OHRH HO2 + #A1OHRR RO2R + &
 #A1OHNR RO2N + #A1OHR2 R2O2 + #A1OHME CXO2 + #A1OHQ1 CCO3 + &
 #A1OHQ2 RCO3 + #A1OHQM MCO3 + #A1OHTO TBUO + &
 #A1OHCO CO + #A1OHC2 CO2 + #A1OHNH HNO3 + #A1OHA1 HCHO + #A1OHA2 CCHO + &
 #A1OHA3 RCHO + #A1OHK3 ACET + #A1OHK4 MEK + #A1OHK6 PROD2 + &
 #A1OHGL GLY + #A1OHMG MGLY + #A1OHBA BACL + &
 #A1OHPH PHEN + #A1OHCR CRES + #A1OHBL BALD + #A1OHD1 DCB1 + &
 #A1OHD2 DCB2 + #A1OHD3 DCB3 + #A1OHMA METH + &
 #A1OHMV MVK + #A1OHIP ISPD + #A1OHN5 RNO3 + #A1OHZ1 HC2H + &
 #A1OHZ2 CO2H + #A1OHZ3 RC2H + #A1OHXX INERT + #A1OHXC XC + &
 #A1OHXN XN
 A2OH) ;ALK2 + HO = #A2OHN2 NO2 + #A2OHHO HO + #A2OHRH HO2 + #A2OHRR RO2R + &
 #A2OHNR RO2N + #A2OHR2 R2O2 + #A2OHME CXO2 + #A2OHQ1 CCO3 + &
 #A2OHQ2 RCO3 + #A2OHQM MCO3 + #A2OHTO TBUO + &
 #A2OHCO CO + #A2OHC2 CO2 + #A2OHNH HNO3 + #A2OHA1 HCHO + #A2OHA2 CCHO + &
 #A2OHA3 RCHO + #A2OHK3 ACET + #A2OHK4 MEK + #A2OHK6 PROD2 + &
 #A2OHGL GLY + #A2OHMG MGLY + #A2OHBA BACL + &
 #A2OHPH PHEN + #A2OHCR CRES + #A2OHBL BALD + #A2OHD1 DCB1 + &
 #A2OHD2 DCB2 + #A2OHD3 DCB3 + #A2OHMA METH + &
 #A2OHMV MVK + #A2OHIP ISPD + #A2OHN5 RNO3 + #A2OHZ1 HC2H + &
 #A2OHZ2 CO2H + #A2OHZ3 RC2H + #A2OHXX INERT + #A2OHXC XC + &
 #A2OHXN XN
 A3OH) ;ALK3 + HO = #A3OHN2 NO2 + #A3OHHO HO + #A3OHRH HO2 + #A3OHRR RO2R + &
 #A3OHNR RO2N + #A3OHR2 R2O2 + #A3OHME CXO2 + #A3OHQ1 CCO3 + &
 #A3OHQ2 RCO3 + #A3OHQM MCO3 + #A3OHTO TBUO + &
 #A3OHCO CO + #A3OHC2 CO2 + #A3OHNH HNO3 + #A3OHA1 HCHO + #A3OHA2 CCHO + &
 #A3OHA3 RCHO + #A3OHK3 ACET + #A3OHK4 MEK + #A3OHK6 PROD2 + &
 #A3OHGL GLY + #A3OHMG MGLY + #A3OHBA BACL + &
 #A3OHPH PHEN + #A3OHCR CRES + #A3OHBL BALD + #A3OHD1 DCB1 + &
 #A3OHD2 DCB2 + #A3OHD3 DCB3 + #A3OHMA METH + &
 #A3OHMV MVK + #A3OHIP ISPD + #A3OHN5 RNO3 + #A3OHZ1 HC2H + &
 #A3OHZ2 CO2H + #A3OHZ3 RC2H + #A3OHXX INERT + #A3OHXC XC + &
 #A3OHXN XN
 A4OH) ;ALK4 + HO = #A4OHN2 NO2 + #A4OHHO HO + #A4OHRH HO2 + #A4OHRR RO2R + &
 #A4OHNR RO2N + #A4OHR2 R2O2 + #A4OHME CXO2 + #A4OHQ1 CCO3 + &
 #A4OHQ2 RCO3 + #A4OHQM MCO3 + #A4OHTO TBUO + &
 #A4OHCO CO + #A4OHC2 CO2 + #A4OHNH HNO3 + #A4OHA1 HCHO + #A4OHA2 CCHO + &
 #A4OHA3 RCHO + #A4OHK3 ACET + #A4OHK4 MEK + #A4OHK6 PROD2 + &
 #A4OHGL GLY + #A4OHMG MGLY + #A4OHBA BACL + &
 #A4OHPH PHEN + #A4OHCR CRES + #A4OHBL BALD + #A4OHD1 DCB1 + &

References

#A4OHD2 DCB2 + #A4OHD3 DCB3 + #A4OHMA METH + &
#A4OHMV MVK + #A4OHIP ISPD + #A4OHN5 RNO3 + #A4OHZ1 HC2H + &
#A4OHZ2 CO2H + #A4OHZ3 RC2H + #A4OHXX INERT + #A4OHXC XC + &
#A4OHXN XN
A5OH) ;ALK5 + HO = #A5OHN2 NO2 + #A5OHHO HO + #A5OHRH HO2 + #A5OHRR RO2R + &
#A5OHNR RO2N + #A5OHR2 R2O2 + #A5OHME CXO2 + #A5OHQ1 CCO3 + &
#A5OHQ2 RCO3 + #A5OHQM MCO3 + #A5OHTO TBUO + &
#A5OHCO CO + #A5OHC2 CO2 + #A5OHHN HNO3 + #A5OHA1 HCHO + #A5OHA2 CCHO + &
#A5OHA3 RCHO + #A5OHK3 ACET + #A5OHK4 MEK + #A5OHK6 PROD2 + &
#A5OHGL GLY + #A5OHMG MGLY + #A5OHBA BACL + &
#A5OHPH PHEN + #A5OHC CRCS + #A5OHBL BALD + #A5OHD1 DCB1 + &
#A5OHD2 DCB2 + #A5OHD3 DCB3 + #A5OHMA METH + &
#A5OHMV MVK + #A5OHIP ISPD + #A5OHN5 RNO3 + #A5OHZ1 HC2H + &
#A5OHZ2 CO2H + #A5OHZ3 RC2H + #A5OHXX INERT + #A5OHXC XC + &
#A5OHXN XN

!

! 2 Lumped Aromatic Groups

B1OH) ;ARO1 + HO = #B1OHN2 NO2 + #B1OHHO HO + #B1OHRH HO2 + #B1OHRR RO2R + &
#B1OHNR RO2N + #B1OHR2 R2O2 + #B1OHME CXO2 + #B1OHQ1 CCO3 + &
#B1OHQ2 RCO3 + #B1OHQM MCO3 + #B1OHTO TBUO + &
#B1OHCO CO + #B1OHC2 CO2 + #B1OHHN HNO3 + #B1OHA1 HCHO + #B1OHA2 CCHO + &
#B1OHA3 RCHO + #B1OHK3 ACET + #B1OHK4 MEK + #B1OHK6 PROD2 + &
#B1OHGL GLY + #B1OHMG MGLY + #B1OHBA BACL + &
#B1OHPH PHEN + #B1OHC CRCS + #B1OHBL BALD + #B1OHD1 DCB1 + &
#B1OHD2 DCB2 + #B1OHD3 DCB3 + #B1OHMA METH + &
#B1OHMV MVK + #B1OHIP ISPD + #B1OHN5 RNO3 + #B1OHZ1 HC2H + &
#B1OHZ2 CO2H + #B1OHZ3 RC2H + #B1OHXX INERT + #B1OHXC XC + &
#B1OHXN XN

B2OH) ;ARO2 + HO = #B2OHN2 NO2 + #B2OHHO HO + #B2OHRH HO2 + #B2OHRR RO2R + &
#B2OHNR RO2N + #B2OHR2 R2O2 + #B2OHME CXO2 + #B2OHQ1 CCO3 + &
#B2OHQ2 RCO3 + #B2OHQM MCO3 + #B2OHTO TBUO + &
#B2OHCO CO + #B2OHC2 CO2 + #B2OHHN HNO3 + #B2OHA1 HCHO + #B2OHA2 CCHO + &
#B2OHA3 RCHO + #B2OHK3 ACET + #B2OHK4 MEK + #B2OHK6 PROD2 + &
#B2OHGL GLY + #B2OHMG MGLY + #B2OHBA BACL + &
#B2OHPH PHEN + #B2OHC CRCS + #B2OHBL BALD + #B2OHD1 DCB1 + &
#B2OHD2 DCB2 + #B2OHD3 DCB3 + #B2OHMA METH + &
#B2OHMV MVK + #B2OHIP ISPD + #B2OHN5 RNO3 + #B2OHZ1 HC2H + &
#B2OHZ2 CO2H + #B2OHZ3 RC2H + #B2OHXX INERT + #B2OHXC XC + &
#B2OHXN XN

! 2 Lumped Alkene Groups

O1OH) ;OLE1 + HO = #O1OHN2 NO2 + #O1OHNO NO + #O1OHHO HO + #O1OHRH HO2 + &
#O1OHRR RO2R + #O1OHNR RO2N + #O1OHR2 R2O2 + #O1OHME CXO2 + &
#O1OHQ1 CCO3 + #O1OHQ2 RCO3 + #O1OHQM MCO3 + #O1OHTO TBUO + &
#O1OHCO CO + #O1OHC2 CO2 + #O1OHHN HNO3 + #O1OHA1 HCHO + &
#O1OHA2 CCHO + #O1OHA3 RCHO + #O1OHK3 ACET + #O1OHK4 MEK + &
#O1OHK6 PROD2 + #O1OHGL GLY + #O1OHMG MGLY + &
#O1OHBA BACL + #O1OHPP PHEN + #O1OHCR CRCS + #O1OHBL BALD + &
#O1OHD1 DCB1 + #O1OHD2 DCB2 + #O1OHD3 DCB3 + &
#O1OHMA METH + #O1OHMV MVK + #O1OHIP ISPD + #O1OHN5 RNO3 + &
#O1OHZ1 HC2H + #O1OHZ2 CO2H + #O1OHZ3 RC2H + #O1OHXX INERT + &
#O1OHXC XC + #O1OHXN XN

O1O3) ;OLE1 + O3 = #O1O3N2 NO2 + #O1O3NO NO + #O1O3HO HO + #O1O3RH HO2 + &
#O1O3RR RO2R + #O1O3NR RO2N + #O1O3R2 R2O2 + #O1O3ME CXO2 + &
#O1O3Q1 CCO3 + #O1O3Q2 RCO3 + #O1O3QM MCO3 + #O1O3TO TBUO + &
#O1O3CO CO + #O1O3C2 CO2 + #O1O3HN HNO3 + #O1O3A1 HCHO + &
#O1O3A2 CCHO + #O1O3A3 RCHO + #O1O3K3 ACET + #O1O3K4 MEK + &
#O1O3K6 PROD2 + #O1O3GL GLY + #O1O3MG MGLY + &
#O1O3BA BACL + #O1O3PH PHEN + #O1O3CR CRCS + #O1O3BL BALD + &
#O1O3D1 DCB1 + #O1O3D2 DCB2 + #O1O3D3 DCB3 + &
#O1O3MA METH + #O1O3MV MVK + #O1O3IP ISPD + #O1O3N5 RNO3 + &
#O1O3Z1 HC2H + #O1O3Z2 CO2H + #O1O3Z3 RC2H + #O1O3XX INERT + &
#O1O3XC XC + #O1O3XN XN

O1N3) ;OLE1 + NO3 = #O1N3N2 NO2 + #O1N3NO NO + #O1N3HO HO + #O1N3RH HO2 + &
#O1N3RR RO2R + #O1N3NR RO2N + #O1N3R2 R2O2 + #O1N3ME CXO2 + &
#O1N3Q1 CCO3 + #O1N3Q2 RCO3 + #O1N3QM MCO3 + #O1N3TO TBUO + &
#O1N3CO CO + #O1N3C2 CO2 + #O1N3HN HNO3 + #O1N3A1 HCHO + &
#O1N3A2 CCHO + #O1N3A3 RCHO + #O1N3K3 ACET + #O1N3K4 MEK + &
#O1N3K6 PROD2 + #O1N3GL GLY + #O1N3MG MGLY + &
#O1N3BA BACL + #O1N3PH PHEN + #O1N3CR CRCS + #O1N3BL BALD + &
#O1N3D1 DCB1 + #O1N3D2 DCB2 + #O1N3D3 DCB3 + &
#O1N3MA METH + #O1N3MV MVK + #O1N3IP ISPD + #O1N3N5 RNO3 + &
#O1N3Z1 HC2H + #O1N3Z2 CO2H + #O1N3Z3 RC2H + #O1N3XX INERT + &
#O1N3XC XC + #O1N3XN XN

O1OA) ;OLE1 + O3P = #O1OPN2 NO2 + #O1OPNO NO + #O1OPHO HO + #O1OPRH HO2 + &
#O1OPRR RO2R + #O1OPNR RO2N + #O1OPR2 R2O2 + #O1OPME CXO2 + &
#O1OPQ1 CCO3 + #O1OPQ2 RCO3 + #O1OPQM MCO3 + #O1OPTO TBUO + &
#O1OPCO CO + #O1OPC2 CO2 + #O1OPHN HNO3 + #O1OPA1 HCHO + &
#O1OPA2 CCHO + #O1OPA3 RCHO + #O1OPK3 ACET + #O1OPK4 MEK + &
#O1OPK6 PROD2 + #O1OPGL GLY + #O1OPMG MGLY + &
#O1OPBA BACL + #O1OPPH PHEN + #O1OPCR CRCS + #O1OPBL BALD + &
#O1OPD1 DCB1 + #O1OPD2 DCB2 + #O1OPD3 DCB3 + &
#O1OPMA METH + #O1OPMV MVK + #O1OPI IPSP + #O1OPN5 RNO3 + &
#O1OPZ1 HC2H + #O1OPZ2 CO2H + #O1OPZ3 RC2H + #O1OPXX INERT + &
#O1OPXC XC + #O1OPXN XN

O2OH) ;OLE2 + HO = #O2OHN2 NO2 + #O2OHNO NO + #O2OHHO HO + #O2OHRH HO2 + &
#O2OHRR RO2R + #O2OHNR RO2N + #O2OHR2 R2O2 + #O2OHME CXO2 + &
#O2OHQ1 CCO3 + #O2OHQ2 RCO3 + #O2OHQM MCO3 + #O2OHTO TBUO + &
#O2OHCO CO + #O2OHC2 CO2 + #O2OHHN HNO3 + #O2OHA1 HCHO + &
#O2OHA2 CCHO + #O2OHA3 RCHO + #O2OHK3 ACET + #O2OHK4 MEK + &
#O2OHK6 PROD2 + #O2OHGL GLY + #O2OHMG MGLY + &
#O2OHBA BACL + #O2OHPP PHEN + #O2OHCR CRCS + #O2OHBL BALD + &
#O2OHD1 DCB1 + #O2OHD2 DCB2 + #O2OHD3 DCB3 + &

References

#O2OHMA METH + #O2OHMV MVK + #O2OHIP ISPD + #O2OHN5 RNO3 + &
 #O2OHZ1 HC2H + #O2OHZ2 CO2H + #O2OHZ3 RC2H + #O2OHXX INERT + &
 #O2OHXC XC + #O2OHXN XN
 O2O3) ;OLE2 + O3 = #O2O3N2 NO2 + #O2O3NO NO + #O2O3HO HO + #O2O3RH HO2 + &
 #O2O3RR RO2R + #O2O3NR RO2N + #O2O3R2 R2O2 + #O2O3ME CXO2 + &
 #O2O3Q1 CCO3 + #O2O3Q2 RCO3 + #O2O3QM MCO3 + #O2O3TO TBUO + &
 #O2O3CO CO + #O2O3C2 CO2 + #O2O3HN HNO3 + #O2O3A1 HCHO + &
 #O2O3A2 CCHO + #O2O3A3 RCHO + #O2O3K3 ACET + #O2O3K4 MEK + &
 #O2O3K6 PROD2 + #O2O3GL GLY + #O2O3MG MGLY + &
 #O2O3BA BACL + #O2O3PH PHEN + #O2O3CR CRES + #O2O3BL BALD + &
 #O2O3D1 DCB1 + #O2O3D2 DCB2 + #O2O3D3 DCB3 + &
 #O2O3MA METH + #O2O3MV MVK + #O2O3IP ISPD + #O2O3N5 RNO3 + &
 #O2O3Z1 HC2H + #O2O3Z2 CO2H + #O2O3Z3 RC2H + #O2O3XX INERT + &
 #O2O3XC XC + #O2O3XN XN
 O2N3) ;OLE2 + NO3 = #O2N3N2 NO2 + #O2N3NO NO + #O2N3HO HO + #O2N3RH HO2 + &
 #O2N3RR RO2R + #O2N3NR RO2N + #O2N3R2 R2O2 + #O2N3ME CXO2 + &
 #O2N3Q1 CCO3 + #O2N3Q2 RCO3 + #O2N3QM MCO3 + #O2N3TO TBUO + &
 #O2N3CO CO + #O2N3C2 CO2 + #O2N3HN HNO3 + #O2N3A1 HCHO + &
 #O2N3A2 CCHO + #O2N3A3 RCHO + #O2N3K3 ACET + #O2N3K4 MEK + &
 #O2N3K6 PROD2 + #O2N3GL GLY + #O2N3MG MGLY + &
 #O2N3BA BACL + #O2N3PH PHEN + #O2N3CR CRES + #O2N3BL BALD + &
 #O2N3D1 DCB1 + #O2N3D2 DCB2 + #O2N3D3 DCB3 + &
 #O2N3MA METH + #O2N3MV MVK + #O2N3IP ISPD + #O2N3N5 RNO3 + &
 #O2N3Z1 HC2H + #O2N3Z2 CO2H + #O2N3Z3 RC2H + #O2N3XX INERT + &
 #O2N3XC XC + #O2N3XN XN
 O2OA) ;OLE2 + O3P = #O2OPN2 NO2 + #O2OPNO NO + #O2OPHO HO + #O2OPRH HO2 + &
 #O2OPRR RO2R + #O2OPNR RO2N + #O2OPR2 R2O2 + #O2OPME CXO2 + &
 #O2OPQ1 CCO3 + #O2OPQ2 RCO3 + #O2OPQM MCO3 + #O2OPTO TBUO + &
 #O2OPCO CO + #O2OPC2 CO2 + #O2OPHN HNO3 + #O2OPA1 HCHO + &
 #O2OPA2 CCHO + #O2OPA3 RCHO + #O2OPK3 ACET + #O2OPK4 MEK + &
 #O2OPK6 PROD2 + #O2OPGL GLY + #O2OPMG MGLY + &
 #O2OPBA BACL + #O2OPPH PHEN + #O2OPCR CRES + #O2OPBL BALD + &
 #O2OPD1 DCB1 + #O2OPD2 DCB2 + #O2OPD3 DCB3 + &
 #O2OPMA METH + #O2OPMV MVK + #O2OPIP ISPD + #O2OPN5 RNO3 + &
 #O2OPZ1 HC2H + #O2OPZ2 CO2H + #O2OPZ3 RC2H + #O2OPXX INERT + &
 #O2OPXC XC + #O2OPXN XN

!
 ! 1 Lumped terpene group
 T1OH) ;TRP1 + HO = #T1OHN2 NO2 + #T1OHNO NO + #T1OHHO HO + #T1OHRH HO2 + &
 #T1OHRR RO2R + #T1OHRN RO2N + #T1OHR2 R2O2 + #T1OHME CXO2 + &
 #T1OHQ1 CCO3 + #T1OHQ2 RCO3 + #T1OHQM MCO3 + #T1OHTO TBUO + &
 #T1OHCO CO + #T1OHC2 CO2 + #T1OHNN HNO3 + #T1OHA1 HCHO + &
 #T1OHA2 CCHO + #T1OHA3 RCHO + #T1OHK3 ACET + #T1OHK4 MEK + &
 #T1OHK6 PROD2 + #T1OHGL GLY + #T1OHMG MGLY + &
 #T1OHBA BACL + #T1OHPP PHEN + #T1OHR CRCS + #T1OHBL BALD + &
 #T1OHD1 DCB1 + #T1OHD2 DCB2 + #T1OHD3 DCB3 + &
 #T1OHMA METH + #T1OHMV MVK + #T1OHIP ISPD + #T1OHN5 RNO3 + &
 #T1OHZ1 HC2H + #T1OHZ2 CO2H + #T1OHZ3 RC2H + #T1OHXX INERT + &
 #T1OHXC XC + #T1OHXN XN
 T1O3) ;TRP1 + O3 = #T1O3N2 NO2 + #T1O3NO NO + #T1O3HO HO + #T1O3RH HO2 + &
 #T1O3RR RO2R + #T1O3NR RO2N + #T1O3R2 R2O2 + #T1O3ME CXO2 + &
 #T1O3Q1 CCO3 + #T1O3Q2 RCO3 + #T1O3QM MCO3 + #T1O3TO TBUO + &
 #T1O3CO CO + #T1O3C2 CO2 + #T1O3HN HNO3 + #T1O3A1 HCHO + &
 #T1O3A2 CCHO + #T1O3A3 RCHO + #T1O3K3 ACET + #T1O3K4 MEK + &
 #T1O3K6 PROD2 + #T1O3GL GLY + #T1O3MG MGLY + &
 #T1O3BA BACL + #T1O3PH PHEN + #T1O3CR CRES + #T1O3BL BALD + &
 #T1O3D1 DCB1 + #T1O3D2 DCB2 + #T1O3D3 DCB3 + &
 #T1O3MA METH + #T1O3MV MVK + #T1O3IP ISPD + #T1O3N5 RNO3 + &
 #T1O3Z1 HC2H + #T1O3Z2 CO2H + #T1O3Z3 RC2H + #T1O3XX INERT + &
 #T1O3XC XC + #T1O3XN XN
 T1N3) ;TRP1 + NO3 = #T1N3N2 NO2 + #T1N3NO NO + #T1N3HO HO + #T1N3RH HO2 + &
 #T1N3RR RO2R + #T1N3NR RO2N + #T1N3R2 R2O2 + #T1N3ME CXO2 + &
 #T1N3Q1 CCO3 + #T1N3Q2 RCO3 + #T1N3QM MCO3 + #T1N3TO TBUO + &
 #T1N3CO CO + #T1N3C2 CO2 + #T1N3HN HNO3 + #T1N3A1 HCHO + &
 #T1N3A2 CCHO + #T1N3A3 RCHO + #T1N3K3 ACET + #T1N3K4 MEK + &
 #T1N3K6 PROD2 + #T1N3GL GLY + #T1N3MG MGLY + &
 #T1N3BA BACL + #T1N3PH PHEN + #T1N3CR CRES + #T1N3BL BALD + &
 #T1N3D1 DCB1 + #T1N3D2 DCB2 + #T1N3D3 DCB3 + &
 #T1N3MA METH + #T1N3MV MVK + #T1N3IP ISPD + #T1N3N5 RNO3 + &
 #T1N3Z1 HC2H + #T1N3Z2 CO2H + #T1N3Z3 RC2H + #T1N3XX INERT + &
 #T1N3XC XC + #T1N3XN XN
 T1OA) ;TRP1 + O3P = #T1OPN2 NO2 + #T1OPNO NO + #T1OPHO HO + #T1OPRH HO2 + &
 #T1OPRR RO2R + #T1OPNR RO2N + #T1OPR2 R2O2 + #T1OPME CXO2 + &
 #T1OPQ1 CCO3 + #T1OPQ2 RCO3 + #T1OPQM MCO3 + #T1OPTO TBUO + &
 #T1OPCO CO + #T1OPC2 CO2 + #T1OPHN HNO3 + #T1OPA1 HCHO + &
 #T1OPA2 CCHO + #T1OPA3 RCHO + #T1OPK3 ACET + #T1OPK4 MEK + &
 #T1OPK6 PROD2 + #T1OPGL GLY + #T1OPMG MGLY + &
 #T1OPBA BACL + #T1OPPH PHEN + #T1OPCR CRES + #T1OPBL BALD + &
 #T1OPD1 DCB1 + #T1OPD2 DCB2 + #T1OPD3 DCB3 + &
 #T1OPMA METH + #T1OPMV MVK + #T1OPIP ISPD + #T1OPN5 RNO3 + &
 #T1OPZ1 HC2H + #T1OPZ2 CO2H + #T1OPZ3 RC2H + #T1OPXX INERT + &
 #T1OPXC XC + #T1OPXN XN

!
 ! 1 Lumped aldehyde group
 L1OH) ;ALD1 + HO = #L1OHN2 NO2 + #L1OHNO NO + #L1OHHO HO + #L1OHRH HO2 + &
 #L1OHRR RO2R + #L1OHRN RO2N + #L1OHR2 R2O2 + #L1OHME CXO2 + &
 #L1OHQ1 CCO3 + #L1OHQ2 RCO3 + #L1OHQM MCO3 + #L1OHTO TBUO + &
 #L1OHCO CO + #L1OHC2 CO2 + #L1OHNN HNO3 + #L1OHA1 HCHO + &
 #L1OHA2 CCHO + #L1OHA3 RCHO + #L1OHK3 ACET + #L1OHK4 MEK + &
 #L1OHK6 PROD2 + #L1OHGL GLY + #L1OHMG MGLY + &
 #L1OHBA BACL + #L1OHPP PHEN + #L1OHR CRCS + #L1OHBL BALD + &
 #L1OHD1 DCB1 + #L1OHD2 DCB2 + #L1OHD3 DCB3 + &
 #L1OHMA METH + #L1OHMV MVK + #L1OHIP ISPD + #L1OHN5 RNO3 + &

References

#L1OHZ1 HC2H + #L1OHZ2 CO2H + #L1OHZ3 RC2H + #L1OHXX INERT + &
 #L1OHXC XC + #L1OHXN XN
 L1N3) ;ALD1 + NO3 = #L1N3N2 NO2 + #L1N3NO NO + #L1N3HO HO + #L1N3RH HO2 + &
 #L1N3RR RO2R + #L1N3NR RO2N + #L1N3R2 R2O2 + #L1N3ME CXO2 + &
 #L1N3Q1 CCO3 + #L1N3Q2 RCO3 + #L1N3QM MCO3 + #L1N3TO TBUO + &
 #L1N3CO CO + #L1N3C2 CO2 + #L1N3HN HNO3 + #L1N3A1 HCHO + &
 #L1N3A2 CCHO + #L1N3A3 RCHO + #L1N3K3 ACET + #L1N3K4 MEK + &
 #L1N3K6 PROD2 + #L1N3GL GLY + #L1N3MG MGLY + &
 #L1N3BA BACL + #L1N3PH PHEN + #L1N3CR CRES + #L1N3BL BALD + &
 #L1N3D1 DCB1 + #L1N3D2 DCB2 + #L1N3D3 DCB3 + &
 #L1N3MA METH + #L1N3MV MVK + #L1N3IP ISPD + #L1N3N5 RNO3 + &
 #L1N3Z1 HC2H + #L1N3Z2 CO2H + #L1N3Z3 RC2H + #L1N3XX INERT + &
 #L1N3XC XC + #L1N3XN XN
 !L1HV) PF=C2CHO QY=L1HVQY ;ALD1 + HV = #L1HVN2 NO2 + #L1HVNO NO + #L1HVHO HO + &
 L1HV) PF=C2CHO ;ALD1 + HV = #L1HVN2 NO2 + #L1HVNO NO + #L1HVHO HO + &
 #L1HVRH HO2 + #L1HVRRO2R + #L1HVN2 NO2 + #L1HVR2 R2O2 + &
 #L1HVME CXO2 + #L1HVQ1 CCO3 + #L1HVQ2 RCO3 + #L1HVQM MCO3 + &
 #L1HVTO TBUO + #L1HVCO CO + #L1HVC2 CO2 + #L1HVHN HNO3 + &
 #L1HVA1 HCHO + #L1HVA2 CCHO + #L1HVA3 RCHO + #L1HVK3 ACET + #L1HVK4 MEK + &
 #L1HVK6 PROD2 + #L1HVGL GLY + #L1HVMG MGLY + &
 #L1HVB AACL + #L1HVPH PHEN + #L1HVCR CRES + #L1HVBL BALD + &
 #L1HVD1 DCB1 + #L1HVD2 DCB2 + #L1HVD3 DCB3 + &
 #L1HVMA METH + #L1HVMV MVK + #L1HVIP ISPD + #L1HVN5 RNO3 + &
 #L1HVZ1 HC2H + #L1HVZ2 CO2H + #L1HVZ3 RC2H + #L1HVXX INERT + &
 #L1HVXC XC + #L1HVXN XN

!

! 1 Lumped ketone group

K1OH) ;KET1 + HO = #K1OHN2 NO2 + #K1OHNO NO + #K1OHHO HO + #K1OHRH HO2 + &
 #K1OHRRO2R + #K1OHNRO2N + #K1OHR2 R2O2 + #K1OHME CXO2 + &
 #K1OHQ1 CCO3 + #K1OHQ2 RCO3 + #K1OHQM MCO3 + #K1OHTO TBUO + &
 #K1OHCO CO + #K1OHC2 CO2 + #K1OHHN HNO3 + #K1OHA1 HCHO + &
 #K1OHA2 CCHO + #K1OHA3 RCHO + #K1OHK3 ACET + #K1OHK4 MEK + &
 #K1OHK6 PROD2 + #K1OHGL GLY + #K1OHMG MGLY + &
 #K1OHBA BACL + #K1OHPPH PHEN + #K1OHCR CRES + #K1OHBL BALD + &
 #K1OHD1 DCB1 + #K1OHD2 DCB2 + #K1OHD3 DCB3 + &
 #K1OHMA METH + #K1OHMV MVK + #K1OHIP ISPD + #K1OHN5 RNO3 + &
 #K1OHZ1 HC2H + #K1OHZ2 CO2H + #K1OHZ3 RC2H + #K1OHXX INERT + &
 #K1OHXC XC + #K1OHXN XN
 K1N3) ;KET1 + NO3 = #K1N3N2 NO2 + #K1N3NO NO + #K1N3HO HO + #K1N3RH HO2 + &
 #K1N3RR RO2R + #K1N3NR RO2N + #K1N3R2 R2O2 + #K1N3ME CXO2 + &
 #K1N3Q1 CCO3 + #K1N3Q2 RCO3 + #K1N3QM MCO3 + #K1N3TO TBUO + &
 #K1N3CO CO + #K1N3C2 CO2 + #K1N3HN HNO3 + #K1N3A1 HCHO + &
 #K1N3A2 CCHO + #K1N3A3 RCHO + #K1N3K3 ACET + #K1N3K4 MEK + &
 #K1N3K6 PROD2 + #K1N3GL GLY + #K1N3MG MGLY + &
 #K1N3BA BACL + #K1N3PH PHEN + #K1N3CR CRES + #K1N3BL BALD + &
 #K1N3D1 DCB1 + #K1N3D2 DCB2 + #K1N3D3 DCB3 + &
 #K1N3MA METH + #K1N3MV MVK + #K1N3IP ISPD + #K1N3N5 RNO3 + &
 #K1N3Z1 HC2H + #K1N3Z2 CO2H + #K1N3Z3 RC2H + #K1N3XX INERT + &
 #K1N3XC XC + #K1N3XN XN
 K1HV) PF=KETONE QY=K1HVQY ;KET1 + HV = #K1HVN2 NO2 + #K1HVNO NO + #K1HVHO HO + &
 #K1HVRH HO2 + #K1HVRRO2R + #K1HVN2 NO2 + #K1HVR2 R2O2 + &
 #K1HVME CXO2 + #K1HVQ1 CCO3 + #K1HVQ2 RCO3 + #K1HVQM MCO3 + &
 #K1HVTO TBUO + #K1HVCO CO + #K1HVC2 CO2 + #K1HVHN HNO3 + &
 #K1HVA1 HCHO + #K1HVA2 CCHO + #K1HVA3 RCHO + #K1HVK3 ACET + #K1HVK4 MEK + &
 #K1HVK6 PROD2 + #K1HVGL GLY + #K1HVMG MGLY + &
 #K1HVB AACL + #K1HVPH PHEN + #K1HVCR CRES + #K1HVBL BALD + &
 #K1HVD1 DCB1 + #K1HVD2 DCB2 + #K1HVD3 DCB3 + &
 #K1HVMA METH + #K1HVMV MVK + #K1HVIP ISPD + #K1HVN5 RNO3 + &
 #K1HVZ1 HC2H + #K1HVZ2 CO2H + #K1HVZ3 RC2H + #K1HVXX INERT + &
 #K1HVXC XC + #K1HVXN XN

!

! 1 Lumped group for acroleins

R1OH) ;ACR1 + HO = #R1OHN2 NO2 + #R1OHNO NO + #R1OHHO HO + #R1OHRH HO2 + &
 #R1OHRRO2R + #R1OHNRO2N + #R1OHR2 R2O2 + #R1OHME CXO2 + &
 #R1OHQ1 CCO3 + #R1OHQ2 RCO3 + #R1OHQM MCO3 + #R1OHTO TBUO + &
 #R1OHCO CO + #R1OHC2 CO2 + #R1OHHN HNO3 + #R1OHA1 HCHO + &
 #R1OHA2 CCHO + #R1OHA3 RCHO + #R1OHK3 ACET + #R1OHK4 MEK + &
 #R1OHK6 PROD2 + #R1OHGL GLY + #R1OHMG MGLY + &
 #R1OHBA BACL + #R1OHPPH PHEN + #R1OHCR CRES + #R1OHBL BALD + &
 #R1OHD1 DCB1 + #R1OHD2 DCB2 + #R1OHD3 DCB3 + &
 #R1OHMA METH + #R1OHMV MVK + #R1OHIP ISPD + #R1OHN5 RNO3 + &
 #R1OHZ1 HC2H + #R1OHZ2 CO2H + #R1OHZ3 RC2H + #R1OHXX INERT + &
 #R1OHXC XC + #R1OHXN XN
 R1O3) ;ACR1 + O3 = #R1O3N2 NO2 + #R1O3NO NO + #R1O3HO HO + #R1O3RH HO2 + &
 #R1O3RR RO2R + #R1O3NR RO2N + #R1O3R2 R2O2 + #R1O3ME CXO2 + &
 #R1O3Q1 CCO3 + #R1O3Q2 RCO3 + #R1O3QM MCO3 + #R1O3TO TBUO + &
 #R1O3CO CO + #R1O3C2 CO2 + #R1O3HN HNO3 + #R1O3A1 HCHO + &
 #R1O3A2 CCHO + #R1O3A3 RCHO + #R1O3K3 ACET + #R1O3K4 MEK + &
 #R1O3K6 PROD2 + #R1O3GL GLY + #R1O3MG MGLY + &
 #R1O3BA BACL + #R1O3PH PHEN + #R1O3CR CRES + #R1O3BL BALD + &
 #R1O3D1 DCB1 + #R1O3D2 DCB2 + #R1O3D3 DCB3 + &
 #R1O3MA METH + #R1O3MV MVK + #R1O3IP ISPD + #R1O3N5 RNO3 + &
 #R1O3Z1 HC2H + #R1O3Z2 CO2H + #R1O3Z3 RC2H + #R1O3XX INERT + &
 #R1O3XC XC + #R1O3XN XN
 R1N3) ;ACR1 + NO3 = #R1N3N2 NO2 + #R1N3NO NO + #R1N3HO HO + #R1N3RH HO2 + &
 #R1N3RR RO2R + #R1N3NR RO2N + #R1N3R2 R2O2 + #R1N3ME CXO2 + &
 #R1N3Q1 CCO3 + #R1N3Q2 RCO3 + #R1N3QM MCO3 + #R1N3TO TBUO + &
 #R1N3CO CO + #R1N3C2 CO2 + #R1N3HN HNO3 + #R1N3A1 HCHO + &
 #R1N3A2 CCHO + #R1N3A3 RCHO + #R1N3K3 ACET + #R1N3K4 MEK + &
 #R1N3K6 PROD2 + #R1N3GL GLY + #R1N3MG MGLY + &
 #R1N3BA BACL + #R1N3PH PHEN + #R1N3CR CRES + #R1N3BL BALD + &
 #R1N3D1 DCB1 + #R1N3D2 DCB2 + #R1N3D3 DCB3 + &
 #R1N3MA METH + #R1N3MV MVK + #R1N3IP ISPD + #R1N3N5 RNO3 + &

References

#R1N3Z1 HC2H + #R1N3Z2 CO2H + #R1N3Z3 RC2H + #R1N3XX INERT + &
#R1N3XC XC + #R1N3XN XN
R1OAJ :ACR1 + O3P = #R1OPN2 NO2 + #R1OPNO NO + #R1OPHO HO + #R1OPRH HO2 + &
#R1OPRR RO2R + #R1OPNR RO2N + #R1OPR2 R2O2 + #R1OPME CXO2 + &
#R1OPQ1 CCO3 + #R1OPQ2 RCO3 + #R1OPQM MCO3 + #R1OPTO TBUO + &
#R1OPCO CO + #R1OPC2 CO2 + #R1OPHN HNO3 + #R1OPA1 HCHO + &
#R1OPA2 CCHO + #R1OPA3 RCHO + #R1OPK3 ACET + #R1OPK4 MEK + &
#R1OPK6 PROD2 + #R1OPGL GLY + #R1OPMG MGLY + &
#R1OPBA BACL + #R1OPPH PHEN + #R1OPCR CRES + #R1OPBL BALD + &
#R1OPD1 DCB1 + #R1OPD2 DCB2 + #R1OPD3 DCB3 + &
#R1OPMA METH + #R1OPMV MVK + #R1OPIP ISPD + #R1OPN5 RNO3 + &
#R1OPZ1 HC2H + #R1OPZ2 CO2H + #R1OPZ3 RC2H + #R1OPXX INERT + &
#R1OPXC XC + #R1OPXN XN
R1HVJ PF=ACROLEIN QY=R1HVQY :ACR1 + HV = #R1HVN2 NO2 + #R1HVNO NO + #R1HVHO HO + &
#R1HVRH HO2 + #R1HVRR RO2R + #R1HVN2 RO2N + #R1HVR2 R2O2 + &
#R1HVME CXO2 + #R1HVQ1 CCO3 + #R1HVQ2 RCO3 + #R1HVQM MCO3 + &
#R1HVTO TBUO + #R1HVC CO + #R1HVC2 CO2 + #R1HVHN HNO3 + &
#R1HVA1 HCHO + #R1HVA2 CCHO + #R1HVA3 RCHO + #R1HVK3 ACET + #R1HVK4 MEK + &
#R1HVK6 PROD2 + #R1HVGL GLY + #R1HVMG MGLY + &
#R1HVBA BACL + #R1HVPH PHEN + #R1HVCR CRES + #R1HVBL BALD + &
#R1HVD1 DCB1 + #R1HVD2 DCB2 + #R1HVD3 DCB3 + &
#R1HVMA METH + #R1HVMV MVK + #R1HVIP ISPD + #R1HVN5 RNO3 + &
#R1HVZ1 HC2H + #R1HVZ2 CO2H + #R1HVZ3 RC2H + #R1HVXX INERT + &
#R1HVXC XC + #R1HVXN XN

NAP Protocol - Appendix B

List of Toxics Mechanism

! From s99appa.pdf.
 ! William P.L. Carter. "Documentation of the SAPRC-99 Chemical mechanism
 ! for VOC reactivity assessment." Final report to CARB. May 8, 2000.
 ! Appendix A. Mechanisms Listings and Tabulations.

```

!
!      Conc(0) Mwt  #C's  #N's
!
.SLO
FORM  0.0  30.03  1.0  0  !Emitted formaldehyde
ALD  0.0  44.05  2.0  0  !Emitted acetaldehyde
BUTD  0.0  54.09  4.0  0  !1,3-butadiene
C6H6  0.0  78.11  6.0  0  !benzene
CHLO  0.0  119.38  1.0  0  !chloroform
TEDC  0.0  98.96  2.0  0  !1,2-dichloroethane
ETOX  0.0  44.05  2.0  0  !ethylene oxide
MCHL  0.0  50.49  1.0  0  !methyl chloride
MTBE  0.0  88.15  5.0  0  !methyl t-butyl ether
PDCB  0.0  147.00  6.0  0  !p-dichlorobenzene
ODCB  0.0  147.00  6.0  0  !o-dichlorobenzene
STYR  0.0  104.15  8.0  0  !styrene
C7H8  0.0  92.14  7.0  0  !toluene
VCHL  0.0  62.50  2.0  0  !vinyl chloride
OXYL  0.0  106.17  8.0  0  !o-xylene (represents all xylenes)
PERC  0.0  165.85  2.0  0  !perchloroethylene
TCE  0.0  131.39  2.0  0  !trichloroethylene
ACRO  0.0  56.06  3.0  0  !acrolein
CTET  0.0  153.82  1.0  0  !carbon tetrachloride
DIES  0.0  1.00  0.0  0  !diesel pm10
CRVI  0.0  52.00  0.0  0  !hexavalent chromium
ARSE  0.0  74.92  0.0  0  !Arsenic
NICK  0.0  58.71  0.0  0  !nickel
MANG  0.0  54.94  0.0  0  !manganese
IRON  0.0  55.85  0.0  0  !iron
ZINC  0.0  65.37  0.0  0  !zinc
CADM  0.0  112.40  0.0  0  !cadmium
LEAD  0.0  201.19  0.0  0  !lead
BERY  0.0  9.01  0.0  0  !beryllium
MERC  0.0  200.59  0.0  0  !mercury

.RXN
!
!1,3-butadiene
BUTD) 1.48E-11 -0.89 0 ; BUTD + HO = #.961 RO2R + #.039 RO2N + &
      #.48 METH + #.48 ISPD + #.1.039 XC
!
! Emitted formaldehyde
FOR1) PF=HCHO_R ;FORM + HV = #2 HO2 + CO
FOR2) PF=HCHO_M ;FORM + HV = H2 + CO
FOR3) 8.60e-12 -0.040 0.00 ;FORM + HO = HO2 + CO + H2O
FOR4) 9.70e-15 -1.242 0.00 ;FORM + HO2 = HOCOO
FOR5) 2.00e-12 4.830 0.00 ;FORM + NO3 = HNO3 + HO2 + CO
!
! Emitted acetaldehyde
ALD1) 5.60e-12 -0.616 0.00 ;ALD + HO = CCO3 + H2O
ALD1) PF=CCHO_R ;ALD + HV = CO + HO2 + CXO2
ALD1) 1.40e-12 3.696 0.00 ;ALD + NO3 = HNO3 + CCO3
!
! benzene
BEN1) 2.47e-12 0.41 0.0 ; C6H6 + HO = #.236 HO2 + #.764 RO2R + &
      #.207 GLY + #.236 PHEN + #.764 DCB1 + &
      #1.114 XC
!
! chloroform
CHLO) 5.67e-13 1.0 2.0 ;CHLO + HO = RO2R + #.5 HCHO + #.5 RCHO
!
! 1,1-dichloroethane
!11DI) 2.60e-13 0.0 0.0 ; 11CL2 + HO = RO2R + #.5 HCHO + #.5 RCHO
!
! trans 1,2-dichloroethene
TEDC) 1.01e-12 -0.50 0.0 ; TEDC + HO = RO2R + #.5 HCHO + #.5 RCHO
!
! ethylene oxide
ETOX) 7.64e-14 ;ETOX + HO = RO2R + R2O2 + #.411 CO + #.071 CO2 + &
      #.071 HCHO + #.411 HC2H + #.518 INERT + #.518 XC
!
! methyl chloride
MCHL) 3.15e-13 1.16 2.0 ;MCHL + HO = RO2R + #.5 HCHO + #.5 RCHO
!
! MTBE
MTBE) 5.89e-13 -0.96 2.0 ;MTBE + HO = #.743 RO2R + #.078 RO2N + &
      #.381 R2O2 + #.162 CXO2 + #.016 TBUO + &
      #.234 HCHO + #.024 ACET + #.719 MEK + &

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References

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#007 PROD2 + #.155 INERT + #.939 XC
!
! p-dichlorobenzene
PDCB) 5.55e-13 ; PDCB + HO = #.236 HO2 + #.764 RO2R + #.207 GLY + &
      #.236 PHEN + #.764 DCB1 + #1.114 XC
!
! o-dichlorobenzene (rate constant from esc.syrres.com)
ODCB) 4.2e-13 ; ODCB + HO = #.236 HO2 + #.764 RO2R + #.207 GLY + &
      #.236 PHEN + #.764 DCB1 + #1.114 XC
!
! Styrene
STY1) 5.80e-11 ; STYR + HO = #.87 RO2R + #.13 RO2N + &
      #.87 HCHO + #.87 BALD + #.26 XC

STY2) 1.71e-17 ; STYR + O3 = #.4 HCHO + #.6 BALD + #.6 HC2H + &
      #.4 RC2H + #1.6 XC

STY3) 1.51e-13 ; STYR + NO3 = #.22 NO2 + #.65 RO2R + #.13 RO2N + &
      #.22 R2O2 + #.22 HCHO + #.22 BALD + #.65 RNO3 + &
      #1.56 XC + #.13 XN
!
STY4) 1.76e-11 ; STYR + O3P = PROD2 + #2 XC
!
! toluene
TOLU) 1.81e-12 -0.71 0.0 ; C7H8 + HO = #.234 HO2 + #.758 RO2R + &
      #.008 RO2N + #.116 GLY + #.135 MGLY + &
      #.234 CRES + #.085 BALD + #.46 DCB1 + &
      #.156 DCB2 + #.057 DCB3 + #1.178 XC
!
! vinyl chloride
VCHL) 1.69e-12 -0.84 0.0 ; VCHL + HO = RO2R + #5 HCHO + #.5 RCHO
!
! o-xylene (used to lump o-,m-,p-xylene)
OXYL) 1.37e-11 ; OXYL + HO = #.161 HO2 + #.831 RO2R + #.008 RO2N + &
      #.084 GLY + #.238 MGLY + #.139 BACL + #.161 CRES + &
      #.054 BALD + #.572 DCB1 + #.06 DCB2 + #.145 DCB3 + &
      #1.697 XC
!
! Perchloroethylene (adapted from SAPRC97 version in mtbephout)
OH152) 9.640E-12 2.403 0.000 ; PERC + HO = RO2R + #.5 HCHO + #.5 RCHO
!
! Trichloroethylene
TCE1) 5.63e-13 -0.85 0.0 ; TCE + HO = RO2R + #.5 HCHO + #.5 RCHO
!
! carbon tetrachloride (rate constant from esc.syrres.com)
TCE1) 1.2e-16 ; CTET + HO = RO2R + #.5 HCHO + #.5 RCHO
!
! Acrolein (LP)
ACRO1) 1.99e-11 ; ACRO + HO = #.25 RO2R + #.75 MCO3 + #.167 CO + &
      #.083 HCHO + #.167 CCHO + #.083 GLY + #.75 XC
!
ACRO2) 1.36e-15 5.01 0.0 ; ACRO + O3 = #.31 HO + #.81 HO2 + &
      CO + #.315 CO2 + #.5 HCHO + #.5 GLY + #.185 HC2H
!
ACRO3) 2.94e-15 ; ACRO + NO3 = #.031 RO2R + #.002 RO2N + #.967 MCO3 + &
      #.031 CO + #.031 RCHO + #1.003 XC + XN
!
ACRO4) 2.37e-12 ; ACRO + O3P = RCHO

ACRO5) PF=ACROLEIN QY=2.0e-3 ; ACRO + HV = #.172 HO + #1.01 HO2 + &
      #.172 CXO2 + #.33 MCO3 + #1.182 CO + #.046 CO2 + &
      #.34 HCHO + #.112 CO2H + #.046 INERT + #.284 XC

! Particulate species (treated as inert)
DIES) 0.0 ; DIES =
CRVI) 0.0 ; CRVI =
ARSE) 0.0 ; ARSE =
NICK) 0.0 ; NICK =
MANG) 0.0 ; MANG =
IRON) 0.0 ; IRON =
ZINC) 0.0 ; ZINC =
CADM) 0.0 ; CADM =
LEAD) 0.0 ; LEAD =
BERY) 0.0 ; BERY =
MERC) 0.0 ; MERC =
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NAP Protocol - Appendix C

Emission inventory for Barrio Logan

Early in the Barrio Logan project, ARB staff recognized a need to develop accurate emissions inventories in a greater detail than normally achieved, in order to characterize exposure to ambient air toxics in the community. Staff believed existing regionally developed emissions inventories would be inadequate to characterize risk because of the presence of many smaller facilities with the potential to emit air toxics, including automobile body and repair shops, metal platers, and metal fabrication facilities. Even though emissions from these facilities were expected to be low, many of these facilities were located in close proximity to residential receptors including houses and schools. As a result, ARB initiated efforts to develop much more detailed emissions inventory assessments for the Barrio Logan community.

The boundaries of the Barrio Logan / Logan Heights community were identified using maps from the San Diego Association of Governments and through discussions with local community organizations. Once the community was identified, ARB staff used information available from the San Diego Air Pollution Control District and business lists from the City of San Diego Business Tax Division to create a master list of facilities. ARB staff then visited approximately 200 facilities over three days to identify facility contacts, verify their location, business type, applicable SIC codes, and any emission points at each facility.

Once identified, emissions inventory information was collected for each facility. Facilities which emit greater than 10 tons per year of criteria pollutants are regulated through the Hot Spots program; thirty-eight facilities in Barrio Logan were found to comply. Facilities subject to this program are legally required to quantify all stationary point source emissions of air toxics at their facility using source tests, emission factors, and mass balance methods. However, the accuracy of these emissions estimates is not typically verified, and there may be substantial variability in the quality of reported emissions between facilities. The San Diego Air Pollution Control District (SDAPCD) evaluated all Hot Spots data, and provided the most current emissions inventory information for each facility. Under normal circumstances, data quality can be assessed by comparing emissions factors used in emissions inventory development for each facility. However, the SDAPCD was unable to provide process rate information for each facility, as a result, emissions factors could not be assessed. In addition, SDAPCD could not provide stack data for emissions from any of these facilities. As a result, emissions from these facilities were either considered area sources, treated as emitted from a generic point source, or previously submitted health risk assessments were used to identify emission release parameters.

References

Most industrial facilities in California do not generate emissions in quantities sufficient to trigger Hot Spots regulation. While some of these facilities have equipment permitted by local air districts, most do not. In most inventory assessments, emissions from these facilities are either treated as area sources by process category and allocated spatially using surrogates, or are excluded. ARB staff evaluated these facilities by using existing information on each facility, collecting information during initial facility visits, grouping facilities by industry type, and conducting detailed inspections of a sample of facilities identified by industry type. Emissions were allocated using information collected during initial facility visits and by making assumptions on stack parameters or treating emission locations as area sources.

In Barrio Logan, 30 facilities were permitted by local districts but exempt from Hot Spots regulation. SDAPCD permit files were examined by ARB staff, and contained information on each piece of equipment under permit, as well as annual compliance inspection records. Information from these files were used to identify processes generating emissions and process rates. Material safety data sheets and emission factors were then used to estimate emissions. Our method assumed the only emissions from these facilities originated from permitted equipment, unless emissions were identified during initial facility visits or detailed facility inspections. Overall, 19 facilities were assessed by permit data alone, while 11 facilities were assessed using permit information in conjunction with other information sources.

137 facilities in Barrio Logan were exempt from Hot Spots regulation and did not own equipment permitted by the SDAPCD. These facilities are assumed to operate equipment which either do not generate air emissions, generate air emissions in quantities below thresholds which would require the facility to obtain a permit, or generate emissions from unregulated equipment. Of these 137 unpermitted facilities, three types were predominant, including auto repair shops, welding and metal fabrication shops, and warehouse / distribution facilities. ARB staff inspected 28 of 84 unpermitted auto repair shops and developed emission inventory estimates for these facilities using data collected during inspections. Emissions estimates for the 28 inspected auto repair facilities were then averaged, and this average facility profile was applied to the other 56 facilities. ARB staff inspected 17 of 24 unpermitted welding / metal fabrication shops in Barrio Logan, and calculated emissions inventories for each facility. Inventories were averaged among the 17 facilities, and this average facility profile was assigned to the remaining 7 facilities. During development of the master facility list and initial facility visits, ARB staff excluded warehouse and distribution facilities; as a result a count to identify all warehouses and distribution facilities was not completed for Barrio Logan. ARB staff decided to inspect some warehouse facilities to determine the significance of diesel emissions. 12 warehouses were inspected and emissions were quantified for these facilities. ARB staff calculated diesel particulate emissions from stationary engines and equipment, idling trucks, operation of forklifts, and operation of transportation

References

refrigeration units. Results indicated some of these facilities produce significant contributions to diesel inventories.

22 facilities were assessed using information collected during initial facility visits. These facilities were grouped into several categories based on similarity of processes occurring at each facility including wood refinishing, small varnish coating and curing operations, print shops, and operation of Safety-Kleen degreasers. For each facility type, ARB staff made assumptions based on process rate including permit threshold process rate limits pursuant to SDAPCD regulation, or an average facility profile developed from ARB databases, and used emission factors or speciation profiles to generate emissions estimates.

Results indicated emissions from Hot Spots facilities constituted the vast majority of the overall community emissions inventory, even though these facilities represented only 18% of all facilities assessed. However, permitted equipment and processes from facilities exempt from Hot Spots regulation accounted for 40% of the toluene, 31% of the perchloroethylene (from dry cleaners not reporting to the Hot Spots program), and 14% of the methyl ethyl ketone from point sources. Emissions from unpermitted automobile related facilities were low, consisting of between 10-15% of the community point source inventory for methanol, toluene, and naphthalene. Emissions from non-permitted welding / metal fabrication activities were also low, but could be considered significant given one of these facilities contributed 3% of the total hexavalent chromium inventory from all point sources.

Development of diesel particulate emissions inventories was particularly problematic and inventory estimates in Barrio Logan are probably underestimated. Emissions were collected or calculated using the same methods for other facilities, but each data source posed additional difficulties for diesel inventory analysis. Diesel emissions sources were collected from Hot Spots facilities, but some diesel sources at these facilities are not required to be included in Hot Spots inventories, and historically these facilities have placed little emphasis on diesel inventory reporting. Emissions were also calculated from information in SDAPCD permit files. Many facilities had permits for portable diesel engines, which could not be allocated spatially within the community and were excluded as a result. In most cases, ARB staff expect these engines to be used at major facilities in Barrio Logan including National Steel and Shipbuilding, Continental Maritime, and Southwest Marine. While technically emissions from subcontractors should be included in Hot Spots inventories, there is no evidence to support this had been completed. Inspection methods proved to be an effective tool in estimating diesel emissions, but only a subset of facilities with diesel emissions could be assessed. For these reasons, the diesel particulate inventory likely underestimates actual diesel emissions in Barrio Logan. In future NAP communities, all diesel sources in a community will be assessed by inspection.

References

In conclusion, inventory collection methods were developed for this project in order to collect detailed community-specific emissions inventory data. Over 200 facilities were included in the inventory of which only 18% were regulated through the Hot Spots Program. Hot Spots facilities accounted for the vast majority of most pollutants; however, smaller facilities did contribute substantially to inventories of toluene, methyl ethyl ketone, perchloroethylene, and diesel exhaust. Emissions from several of these facilities appeared sufficiently significant to influence community health risk. Diesel exhaust emissions inventories were probably incomplete, and methods have been revised to improve diesel inventories in future NAP communities.