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 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 (OEHHA[2]) 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
1,2,3,4,6,7,89-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
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
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-FCM[3] and CMAQ, part of Models-3[4]. 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 SAPRC99[5] 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 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, NOx, 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 Guassian models as well as new and emerging models. The following models will be applied to estimate annual ambient concentrations for point and line sources:

- ISCST3[6] for point and area sources; this is the traditional U.S. EPA regulatory model;
- AERMOD[7] for point and area sources; this is an advanced U.S. EPA recommended model;
- CALPUFF[8] 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;
- CALINE[9] 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 model[10], 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 Riverside[11].

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.

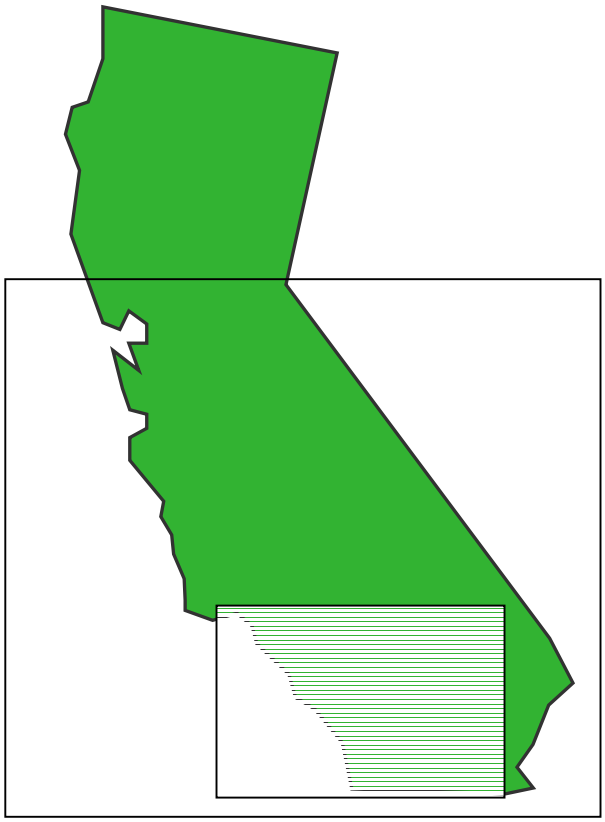
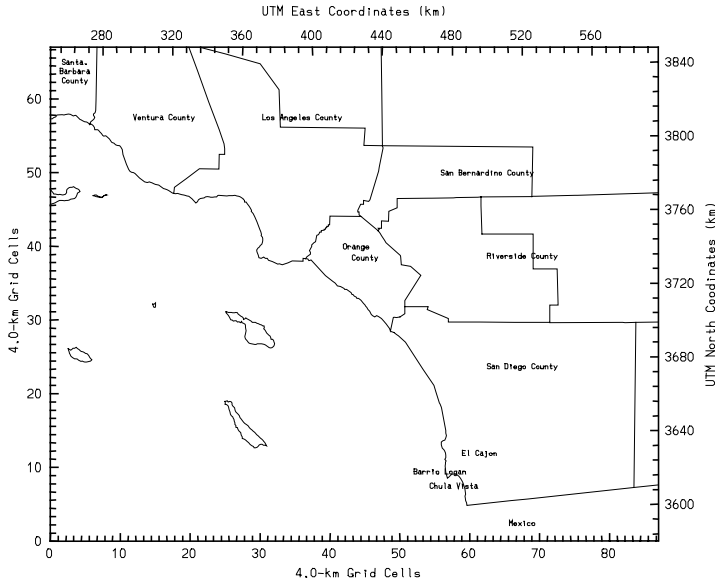


Figure 3.1.2 Regional scale inner nested modeling domain



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 my 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 EMFAC2000[12] will be used for the motor vehicle emissions inventory. 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 - CALMET[13] and MM5[14]. 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:

1) Use only surface and upper air observations obtained from the National Weather Service (NWS) network and other sources, including radar wind profilers;
2) 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 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^{o}N	34.76^{o}N	34.79^{o}N	32.35^{o}N
Longitude (deg)	-119.66^{o}W	-119.76^{o}W	-115.91^{o}W	-115.94^{o}W

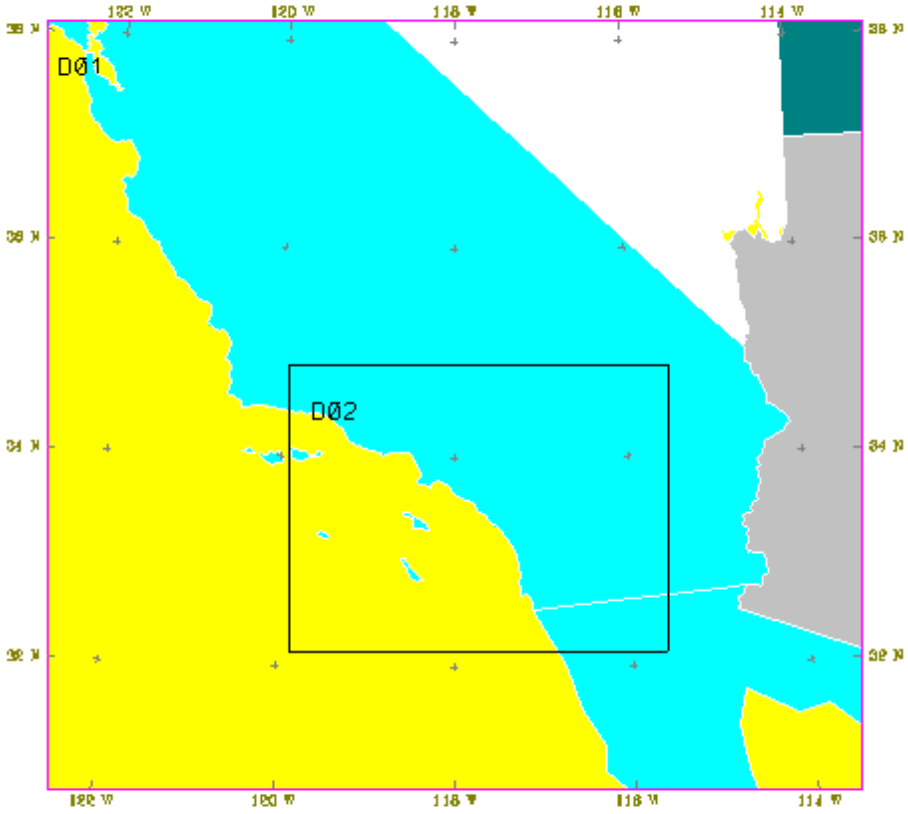
Although CALMET diagnostic meteorological model provides the necessary input parameters for the UAM air quality model, the model output can be more reliable if there is a rich network of observational data from a large number of surface and upper air stations obtained at frequent time intervals. For the initialization of the diagnostic CALMET model, all available surface stations (including10 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^{o}N	34.84^{o}N	34.84^{o}N	32.14^{o}N
Longitude (deg)	-119.84^{o}W	-119.92^{o}W	-115.55^{o}W	-115.64^{o}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 (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 SCOS97[15]. 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 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.

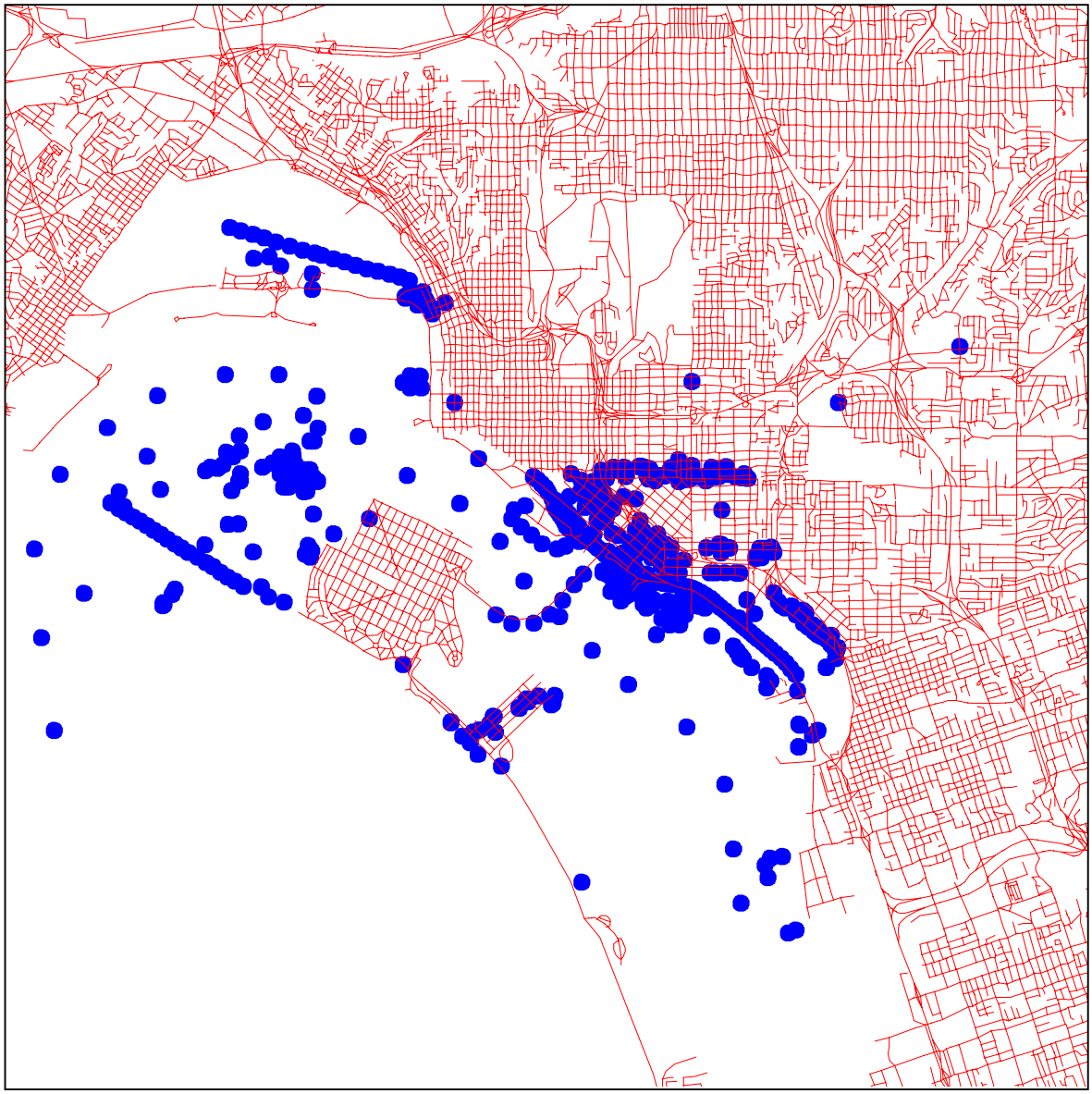
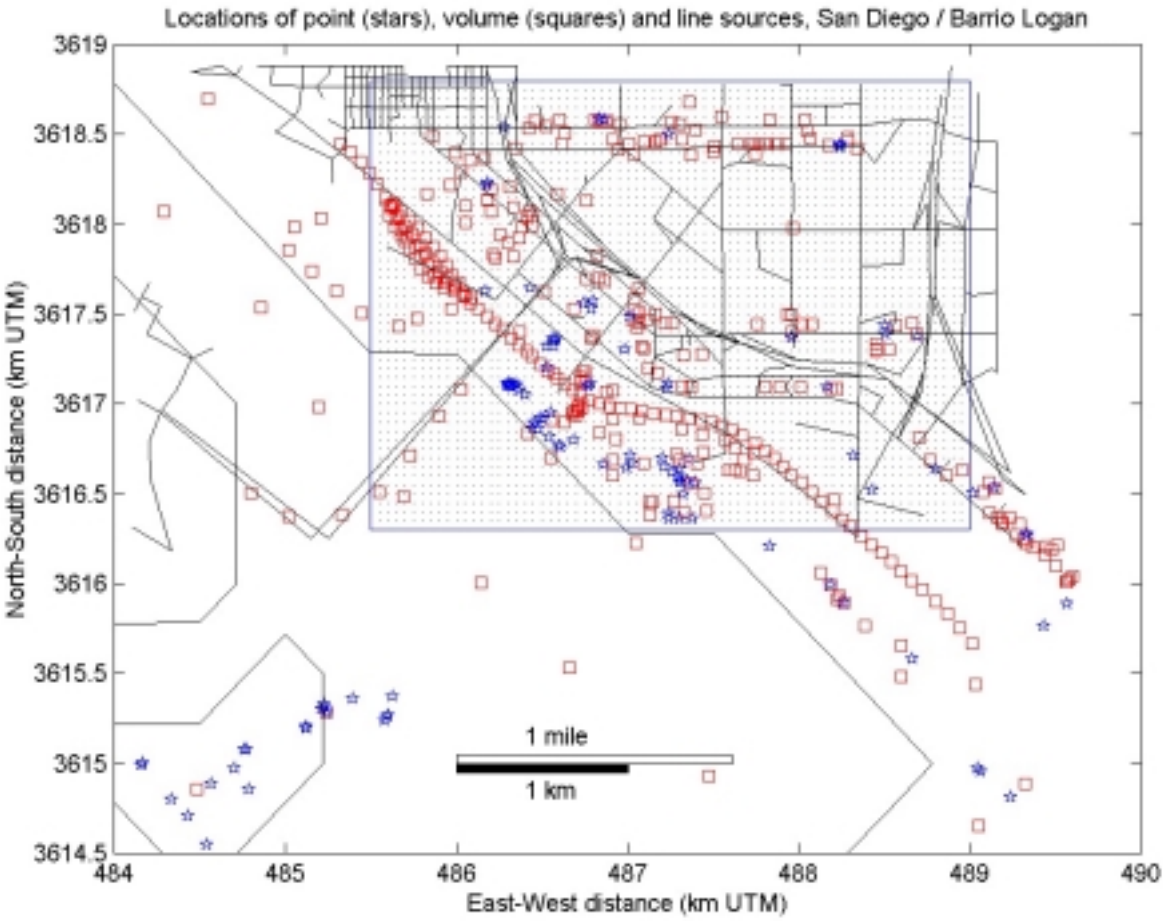


Figure 4.1.2 Micro-scale nested modeling domain.



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. 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 categories[16].

- 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 Document[17] 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 Riverside[11]. The field study will include the releases of known amounts of a tracer gas, SF_6, 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 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.

6. References

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17. Air Resources Board, April 1992: Technical Guidance Document: Photochemical Modeling.

Appendix A

Listing of the SAPRC-99

```
! 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.
!     Finale 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 gloxal and higher alpha-dicarbonyl adehydes),
! 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, naphtalene,
!            unsaturated diketones (replaces AFG1)
! DCB2 DCB3= Represent highly photoreactive ring opening products formed
!            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
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
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              ;NO3 + HO2 = #.8 "HO + NO2 + O2" + #.2 "HNO3 + &
                             O2"
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 =
RNNO) 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
RNRR) 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
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 + &
                              #.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 + &
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                              #.376 RO2R + #.173 RO2N + #.596 R2O2 + &
                              #.01 HCHO + #.439 CCHO + #.213 RCHO + #.006 ACET + &
                              #.177 MEK + #.048 PROD2 + #.31 RNO3 + #.351 XN + &
                              #.56 XC
RNHV) 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 handlw 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 + #A1OHHN 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 + #A2OHHN 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 + #A3OHHN 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 + #A4OHHN 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 + &
       #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 + #A5OHCR CRES + #A5OHBL BALD + #A5OHD1 DCB1 + &
       #A5OHD2 DCB2 + #A5OHD3 DCB3 + #A5OHMA METH + &
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       #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 + #B1OHCR CRES + #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 + #B2OHCR CRES + #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 + #O1OHPH PHEN + #O1OHCR CRES + #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 CRES + #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 CRES + #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 CRES + #O1OPBL BALD + &
       #O1OPD1 DCB1 + #O1OPD2 DCB2 + #O1OPD3 DCB3 + &
       #O1OPMA METH + #O1OPMV MVK + #O1OPIP ISPD + #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 + #O2OHPH PHEN + #O2OHCR CRES + #O2OHBL BALD + &
       #O2OHD1 DCB1 + #O2OHD2 DCB2 + #O2OHD3 DCB3 + &
       #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
```

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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 + #T1OHNR RO2N + #T1OHR2 R2O2 + #T1OHME CXO2 + &
       #T1OHQ1 CCO3 + #T1OHQ2 RCO3 + #T1OHQM MCO3 + #T1OHTO TBUO + &
       #T1OHCO CO + #T1OHC2 CO2 + #T1OHHN HNO3 + #T1OHA1 HCHO + &
       #T1OHA2 CCHO + #T1OHA3 RCHO + #T1OHK3 ACET + #T1OHK4 MEK + &
       #T1OHK6 PROD2 + #T1OHGL GLY + #T1OHMG MGLY + &
       #T1OHBA BACL + #T1OHPH PHEN + #T1OHCR CRES + #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 + #L1OHNR RO2N + #L1OHR2 R2O2 + #L1OHME CXO2 + &
       #L1OHQ1 CCO3 + #L1OHQ2 RCO3 + #L1OHQM MCO3 + #L1OHTO TBUO + &
       #L1OHCO CO + #L1OHC2 CO2 + #L1OHHN HNO3 + #L1OHA1 HCHO + &
       #L1OHA2 CCHO + #L1OHA3 RCHO + #L1OHK3 ACET + #L1OHK4 MEK + &
       #L1OHK6 PROD2 + #L1OHGL GLY + #L1OHMG MGLY + &
       #L1OHBA BACL + #L1OHPH PHEN + #L1OHCR CRES + #L1OHBL BALD + &
       #L1OHD1 DCB1 + #L1OHD2 DCB2 + #L1OHD3 DCB3 + &
       #L1OHMA METH + #L1OHMV MVK + #L1OHIP ISPD + #L1OHN5 RNO3 + &
       #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 + #L1HVRR RO2R + #L1HVNR RO2N + #L1HVR2 R2O2 + &
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       #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 + &
       #L1HVBA BACL + #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 + &
       #K1OHRR RO2R + #K1OHNR RO2N + #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 + #K1OHPH 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 + #K1HVRR RO2R + #K1HVNR RO2N + #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 + &
       #K1HVBA BACL + #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 + &
       #R1OHRR RO2R + #R1OHNR RO2N + #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 + #R1OHPH 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 + &
       #R1N3Z1 HC2H + #R1N3Z2 CO2H + #R1N3Z3 RC2H + #R1N3XX INERT + &
       #R1N3XC XC + #R1N3XN XN
R1OA) ;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
R1HV) PF=ACROLEIN QY=R1HVQY ;ACR1 + HV = #R1HVN2 NO2 + #R1HVNO NO + #R1HVHO HO + &
       #R1HVRH HO2 + #R1HVRR RO2R + #R1HVNR RO2N + #R1HVR2 R2O2 + &
       #R1HVME CXO2 + #R1HVQ1 CCO3 + #R1HVQ2 RCO3 + #R1HVQM MCO3 + &
       #R1HVTO TBUO + #R1HVCO CO + #R1HVC2 CO2 + #R1HVHN HNO3 + &
       #R1HVA1 HCHO + #R1HVA2 CCHO + #R1HVA3 RCHO + #R1HVK3 ACET + #R1HVK4 MEK + &
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#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
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Appendix B

List of Toxics Mechanism

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! 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 + &
                            #.007 PROD2 + #.155 INERT + #.939 XC
!
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! 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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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.

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 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.

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.