CHAPTER 4
REGIONAL MODELING AND EVALUATION

Chapter 4. Regional Modeling and Evaluation

4.1 Introduction

Regional air quality modeling is used to determine the concentration impact in time and space to the community due to emissions from a single or group of known toxic compounds and emissions sources. The model simulated concentration contours of toxic compounds are translated into a pattern of health risk based upon compound potency risk factor. The regional modeling provides a mechanism to disperse the emissions from a variety of source categories as well as individual sources to estimate a mass consistent impact throughout the modeling domain. This analysis complements the data analytical techniques used to assess concentration and risk from the data acquired at the fixed and mobile monitoring platforms.

For MATES III, the Comprehensive Air Quality Model with Extensions (CAMx) enhanced with a reactive tracer modeling capability (RTRAC) provided the dispersion modeling platform and chemistry used to simulate annual impacts of both gaseous and aerosol toxic compounds in the Basin. The version of the RTRAC "probing tool" in CAMx used in the modeling simulations includes an air toxics chemistry module that is used to treat the formation and destruction of reactive air toxic compounds.

Modeling was conducted on a domain that encompassed the Basin and the coastal shipping lanes located in the Southern California Bite portions of the Basin using a grid size of two squared kilometers. (Figure 4-1 depicts the MATES III modeling domain. The shaded portion of the grid area represents the extension of the domain beyond that used for MATES II). An updated version of the 2007 AQMP emissions inventory for model year 2005, which included detailed source profiles of air toxic sources, provided mobile and stationary source input for the MATES III CAMx/RTRAC simulations. Grid based, hourly meteorological fields generated from the MM5 mesoscale meteorological model using four dimensional data assimilation, and National Weather Service model initializations for 2005 provided the dispersion profile for the simulations.

4.2 Background

In the MATES II analysis, the Urban Airshed Model with TOX (UAMTOX) chemistry was used to simulate the advection and accumulation of toxic compound emissions throughout the Basin. UAMTOX was simulated for a slightly protracted two-squared kilometer grid domain that overlaid the Basin. The analysis relies on the 1997-98 emissions projection from the 1997 AQMP and meteorological data fields for 1997-98 generated from objective analysis using a diagnostic wind model. At this time, these tools were consistent with those used in both the 1997 and 2003 AQMP attainment demonstrations.

Peer review of the 2003 AQMP modeling strongly suggested that future AQMP attainment demonstrations utilize more state-of-the-sciences tools that utilize updated

chemistry modules, improved dispersion algorithms and mass consistent meteorological data. The recommendations were placed in action for the 2007 AQMP where the dispersion platform moved from UAM to CAMx and the diagnostic wind meteorological model was replaced by MM5 prognostic model. CAMx coupled with MM5 input using the "one atmosphere" gaseous and particulate chemistry was used to simulate both episodic ozone and annual concentrations of $PM_{2.5}$.

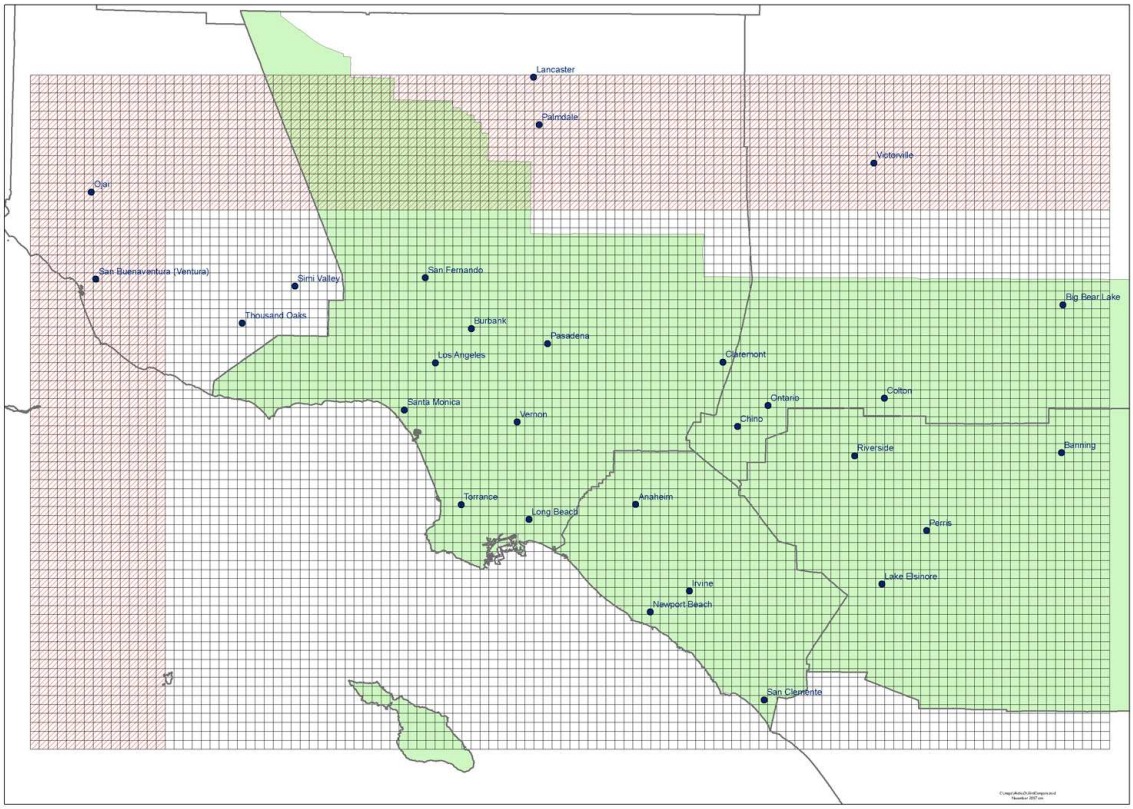

Figure 4-1
MATES III Modeling Domain.
(Shaded area highlights the grid extension to the MATES II modeling domain).

The MATES II modeling analysis was conducted using the UAMTOX model and diagnostic meteorological model. However, in order to take into account the advances in annual particulate modeling that was conducted as part of the 2007 $PM_{2.5}$ attainment demonstration and given the extensive effort in the 2007 AQMP to simulate particulates, using the peer recommended state-of-the-science art modeling tools, it was decided that a better comparison linking the AQMP $PM_{2.5}$ projections to the base year toxics analysis would be more complementary and up-to-date. As such, the MATES III simulations were conducted using the CAMx – MM5 couple with the RTRAC chemistry.

4.3 MATES III vs. MATES II: Key Modeling Assumptions

It is difficult to fully assess the impact caused by the major shift in modeling platforms and chemistry modules. Of the changes made to the modeling platform, moving to the MM5 model derived vertical diffusion characterization appears to have increased vertical dispersion throughout the modeling domain. The net impact from this modification is lower ground level concentrations. In addition, two other changes to emissions data preparation were implemented in the MATES III modeling. First, emissions from vessels in the shipping lanes were assumed emitted into the first two vertical modeling layers to better estimate plume rise from the hot stack emissions. Combined stack heights and plume rise for typical ocean-going (deep draft) vessels extend above 36 and below 73 meters (WRAP, 2007). MATES II held shipping emissions in the first vertical UAM layer. Due to the difference in vertical dispersion techniques used, the UAM model tends to produce higher concentrations than the CAMx model.

The second modification impacted the distribution of truck movement throughout the Basin. At the time of MATES II, no heavy-duty truck movement profile was available to characterize the truck distribution and travel on freeways, arterial and major streets. Truck travel was assigned the travel model characteristics designated for light-duty passenger vehicle travel. MATES III directly incorporated the output of the heavy-duty truck demand model to provide a more realistic characterization of weekday travel. Weekend travel was assigned the same routes but at substantially lowered demand. Table 4-1 summarizes the major differences in the toxic modeling between MATES III and MATES II.

4.4 Modeling Results

The results of the regional modeling analyses for the four toxic compounds that contributed the greatest risk throughout the domain (diesel particulate, benzene, 1,3 butadiene and formaldehyde) are depicted in Figures 4-2a through 4-2d. Such redistribution of truck activities would align diesel emissions along transportation corridors. Table 4-2 summarizes the projected concentrations at the eight MATES III monitoring sites that have complete monitoring records for 2005.

Table 4-1
Summary Comparison of Key Modeling Considerations Between
MATES III and MATES II

Parameter	MATES III	MATES II
Model Platform / Chemistry	CAMx / RTRAC	UAM/TOX
Meteorology Model /Layers	MM5 Prognostic / 7 layers	Diagnostic Wind Model / 5 layers
Vertical Diffusion	Blackadar PBL to determine grid-layer specific vertical diffusivity	Hourly grid specified mixing height
On-Road Truck Emissions	Caltrans/SCAG Truck Model	Used passenger vehicle pattern
Shipping Emissions Stack Height	Emissions spread through layers 1 and 2	Emissions released in layer 1 (variable size)
Emissions Inventory	2005 Projection from 2002 (2007 AQMP)	1998 Projection from 1997 (2003 AQMP)
Mobile Emissions	EMFAC2007	EMFAC7G

Figure 4-2a depicts the projected annual average concentration distribution of diesel particulates in the Basin. In general, the distribution of diesel particulates follows the major arterials. However, localized hot spots with annual average concentration ranging to 4.8 ug/m3 are observed in the central Los Angeles area and 8.5 ug/m3 at the Ports of Los Angeles and Long Beach. Figures 4-2b and 4-2c provide the distributions of benzene and 1,3 butadiene respectively whereby the toxic compounds are almost uniformly distributed throughout the Basin (reflecting patterns of light-duty fuel consumption). The formaldehyde profile (Figure 4-2d) depicts higher concentrations in the heavily traveled western and central Basin with additional hot spots in the downwind areas of the Basin that are impacted by higher levels of ozone formation (Santa Clarita and Crestline).

Table 4-2 provides a summary of the model performance to recreate measured 2005 annual average concentrations. For this comparison, the monitored data for eight stations are combined to provide an estimate of average Basin-wide conditions. Two stations, Huntington Park and Pico Rivera, did not have complete measurement records for the full 12 months and were excluded from the analysis. Simulated pollutant concentrations for the eight stations from the CAMx RTRAC analyses were calculated from the grid data using the distance weighted nine-cell average. No direct measurements of diesel $PM_{2.5}$ were available for comparison to simulate annual average concentrations. However, estimates of diesel based on ambient elemental carbon concentrations are discussed later in this section. Measured concentrations of naphthalene were available for Wilmington,

central Los Angeles, and Riverside. Each of the four counties is represented by at least one station, with the greatest concentration occurring in Los Angeles (five sites). Averaging the measured and simulated concentrations at the eight stations provides an estimate of the regional profile but with a bias towards impacts to the coastal communities in the heavily transited areas of the Basin. Moreover, the assessment provides a direct comparison for model performance evaluation.

Table 4-2

Toxic Compounds Simulated and Measured: 2005 Eight-Station Annual Average

Toxic Compound	Units	Measured Annual Average	Simulated Annual Average
$EC_{2.5}$	$\mu g/m^3$	1.83	1.73
Diesel (2.5)	$\mu g/m^3$	N/A	2.90
EC10	$\mu g/m^3$	2.08	2.18
Cr6 (TSP)	ng/m^3	0.23	0.08
As (2.5)	ng/m^3	0.51	1.06
As (TSP)	ng/m^3	0.75	2.48
Cd (2.5)	ng/m^3	1.60	0.60
Cd (TSP)	ng/m^3	1.55	0.88
Ni (2.5))	ng/m^3	4.08	4.62
Ni (TSP)	ng/m^3	5.31	7.19
Pb (2.5)	ng/m^3	5.43	2.49
Pb (TSP)	ng/m^3	10.68	8.40
Benzene	Ppb	0.57	0.52
Perchloroethylene	Ppb	0.06	0.09
p-Dichlorobenzene	Ppb	0.03	0.08
Methylene Chloride	Ppb	0.49	0.30
Trichloroethylene	Ppb	0.02	0.03
1,3Butadiene	Ppb	0.09	0.08
Fomaldehyde	Ppb	3.52	3.34
Acetaldehyde	Ppb	1.60	1.24
Naphthalene	Ppb	0.02*	0.02

* Three station average

In general, model simulated average annual toxic compound concentrations compare well with the measured annual average values. $EC_{2.5}$ and EC_{10} were well simulated as were the gaseous components. Arsenic and TSP nickel exhibit the greatest tendency for over prediction. Cadmium, hexavalent chromium, and lead concentrations tend to be under-predicted. In general, the concentrations of the gaseous compounds are closely recreated. Some uncertainty in prediction accuracy is introduced into the analysis due to the substitution of one-half level of detection for the metals data measured below the detection limit.

4.5 Estimation of Risk

Figure 4-3 depicts the cumulative distribution of risk estimated from the predicted annual average concentrations of the key toxic compounds. Risk is calculated for each grid cell as follows:

$$\text{Risk}_{i,j} = \Sigma \text{ Concentration}_{i,j,k} \text{ X Risk Fisk Factor}_{i,j,k}$$

Where $_{i,j}$ is the grid cell (easting, nothing) and k is the toxic compound.

The Basin average risk summed for the toxic components valued 810 additional cases of cancer in a one-million person population. (The Basin average risk included all over-land cells that reside within the Basin portion of the modeling domain). The grid cell having the maximum simulated risk of 2,879 was located in the Port of Los Angeles/Long Beach. More specifically, the grids having the top 17 estimated risk values were located in adjacent cells around the port area. The cell having the highest risk outside of the port area occurred in South Los Angeles as part of a cluster of grids having high risk that extended from central Los Angeles to the southeast following Interstate-5. Other hot spot areas included the eastern Basin near the communities of Colton, Fontana and San Bernardino. As with the MATES II analysis, areas projected to have higher risk followed transportation corridors including freeways, and railways.

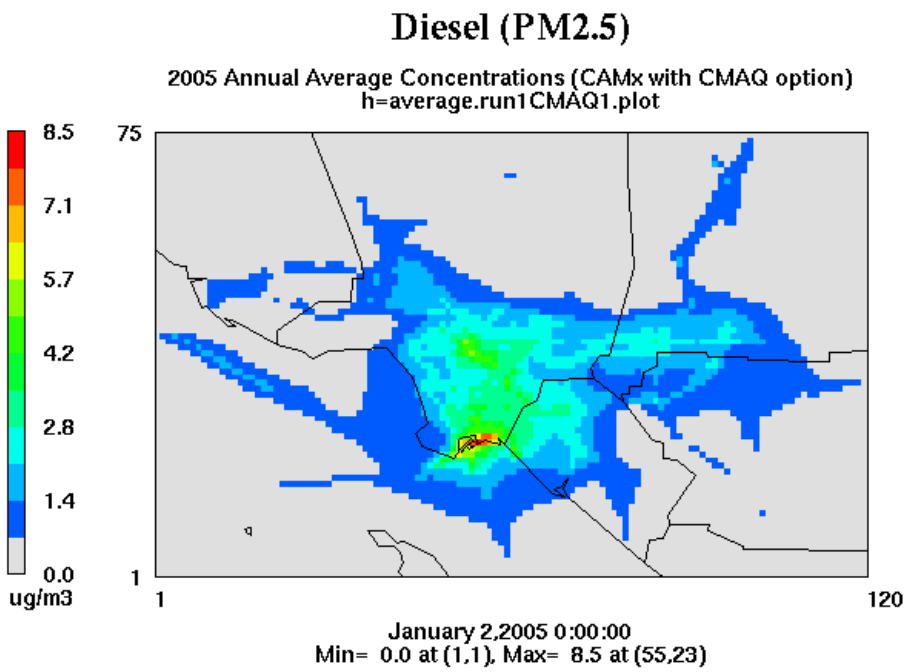

Figure 4-2a
Annual average concentration pattern for Diesel $PM_{2.5}$

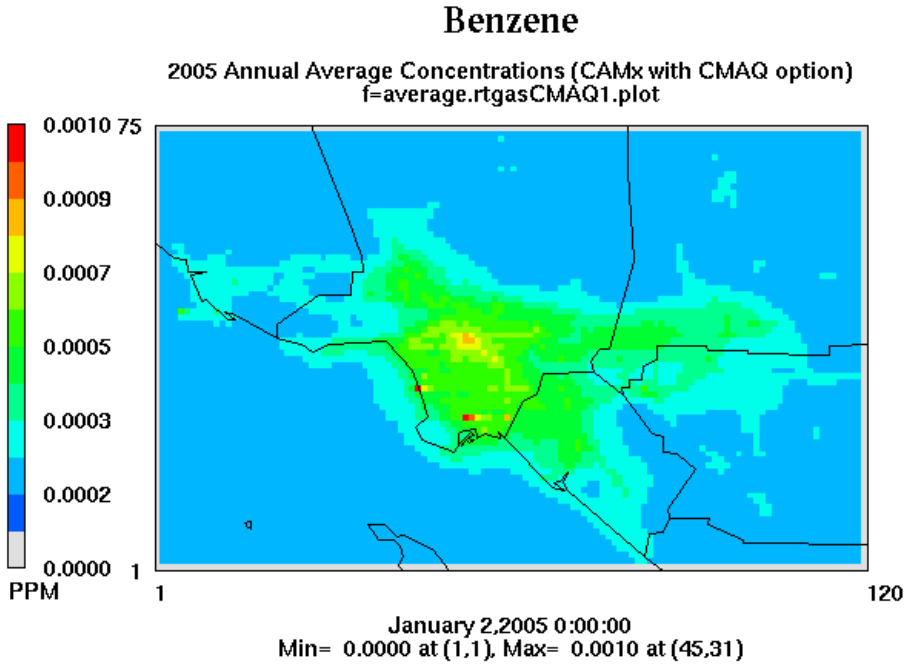

Figure 4-2b
Annual average concentration pattern for Benzene

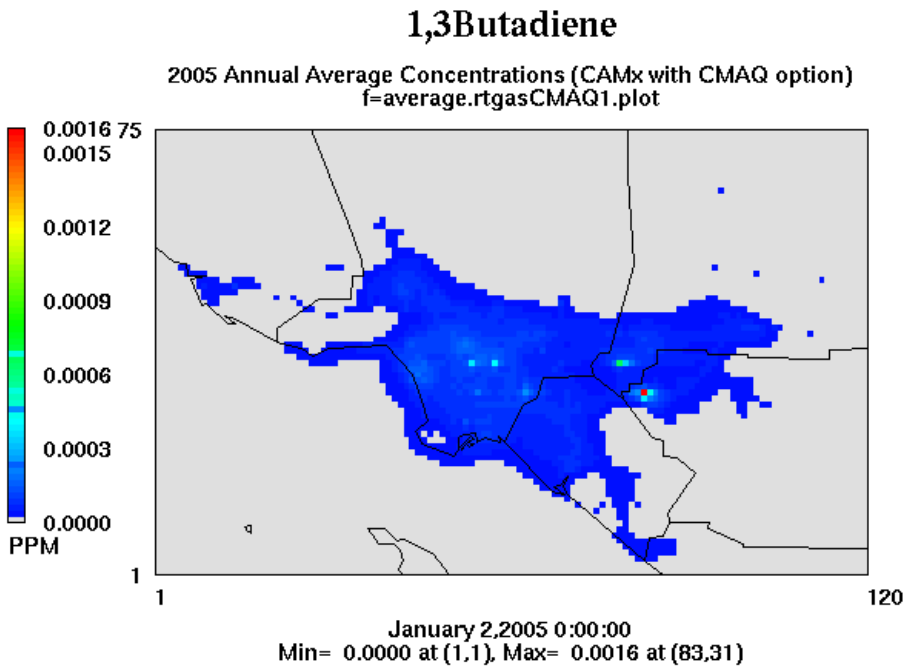

Figure 4-2c
Annual average concentration pattern for 1,3 Butadiene

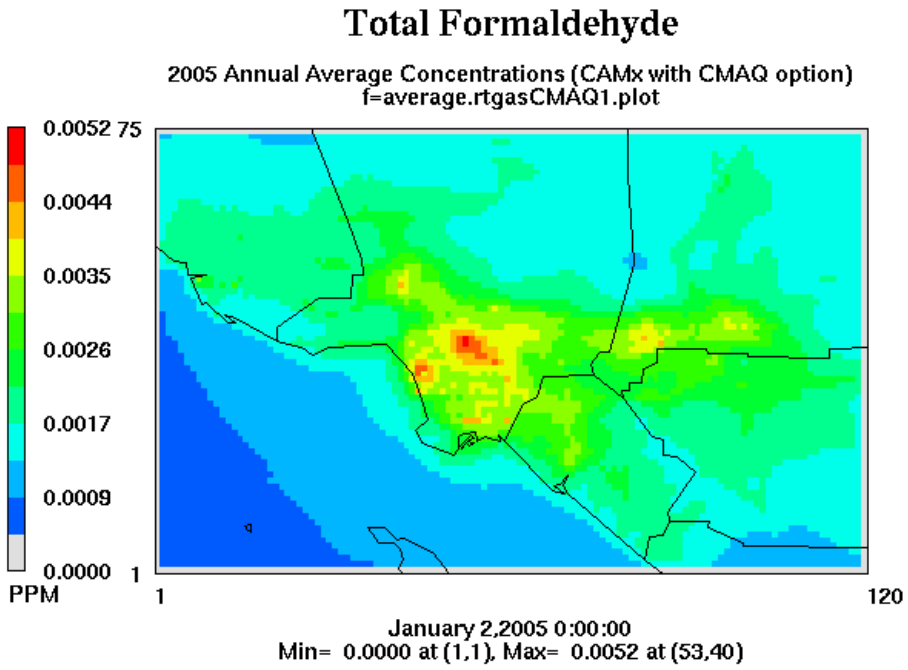

Figure 4-2d
Annual average concentration pattern for Total Formaldehyde

The MATES III Basin population weighted average risk (810 per million) is approximately 83% of the Basin average risk identified from the MATES II (981 per million) analysis. While it is desirable to try and compare the estimates of regional risk simulated for the Basin from MATES II to MATES III, a direct comparison should not be made. The 17% reduction in Basin risk can be attributed to many factors such as updated emissions estimates and spatial allocation, dispersion, and meteorological model selection. Also contributing to the uncertainty in a direct comparison is the variable weather profile between the two monitoring periods.

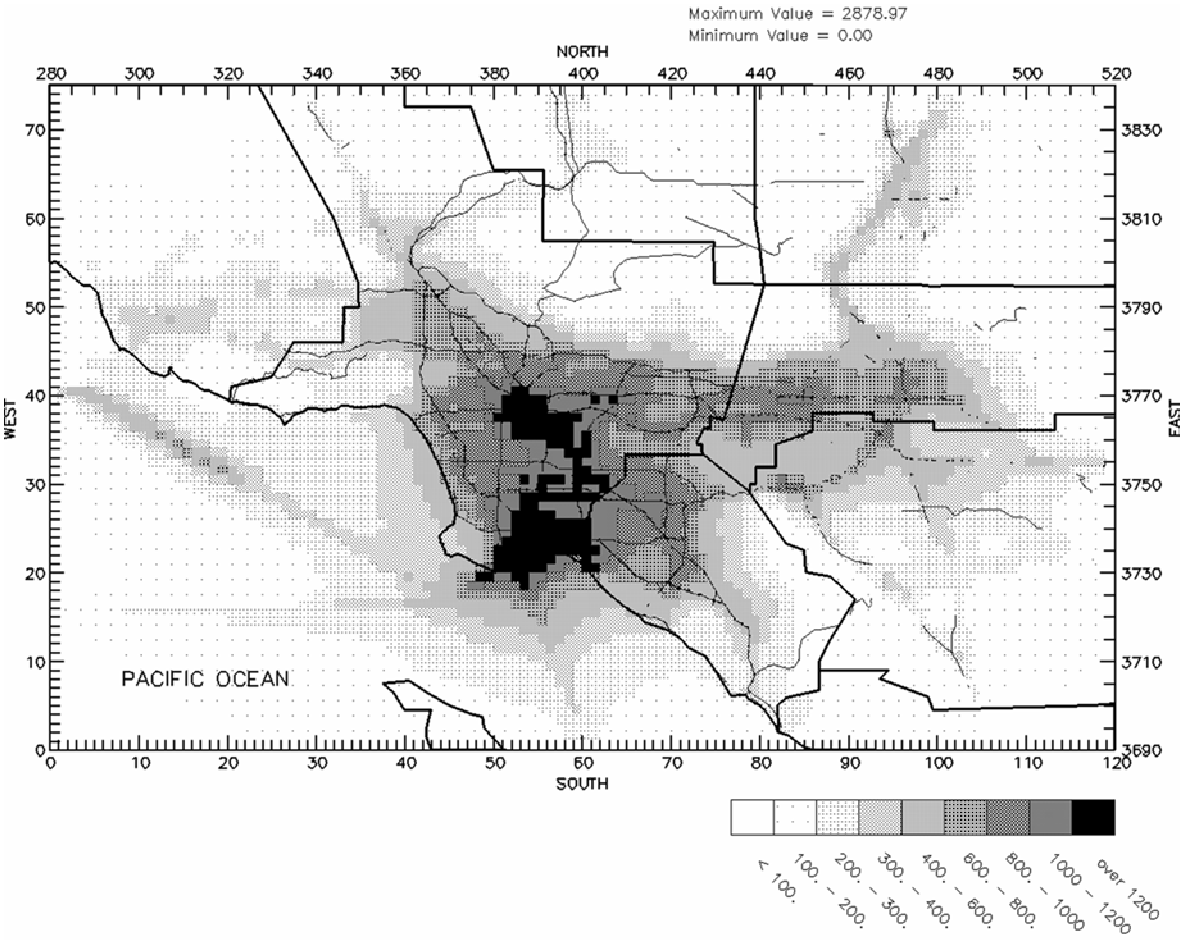

Figure 4-3
MATES III Simulated Cumulative Risk

Table 4-3 provides the county-wide breakdown of risk to the affected population. As presented in the spatial distribution, Los Angeles County bears the greatest average risk at 912 per one million person population. Orange County has the second highest number of projected risk at 724 per one million person population. Risk in the Eastern Basin is lower. The estimated risk for San Bernardino is 631 per million, and Riverside was estimated to have the lowest population weighted risk at 410. It should be noted that

these are county wide averages, and individual communities could have higher risks than the average if they are near emissions sources, such as railyards or intermodal facilities.

Table 4-3
County-Wide Population Weighted Risk

Region	Population	Average Risk (Per Million)
Los Angeles	9,305,726	912
Orange	2,579,794	724
Riverside	1,249,554	410
San Bernardino	1,269,919	631
SCAB	14,404,993	810

Table 4-4 provides the Basin average breakdown of risk associated with each of the key compounds simulated in the analysis. Diesel particulate ranked highest as the toxic compound contributing to the overall risk and development of excess cancers to the population. The next three highest contributors included benzene, 1,3 butadiene and secondary formaldehyde.

Table 4-5 provides the simulated risk at each of the eight stations (evaluated in Table 4-2) for the three main toxic compounds and the remaining aggregate based on the regional modeling. Risk is calculated using the predicted concentrations of each toxic component for the specific monitoring station location (based on a nine cell average concentration). The summary provides the comparison between simulated average risk for the eight station combine and the average risk calculated using the annual toxic compound measurements at those sites.

The highest simulated risk was estimated for Wilmington followed by Los Angeles, Long Beach and Compton. The modeled risk at Anaheim essentially equaled the Basin population weighted risk while the remaining stations had risk lower than the Basin average. Taken as an eight-station average, the modeled risk (956 in a million) is higher than the Basin average population weighted risk (810). However, the simulated risk is lower than the risk calculated from the measured toxic compound concentrations and the estimates of diesel concentrations. The eight-station average risk based on measurement data exceeded the simulated risk eight-station average by approximately 11% (1,059 in a million) for the inventory-based diesel concentration and by 23% (1,175 in a million) based on the CMB method. The non-diesel- related portion (especially considering benzene and 1,3 butadiene) of risk for all three averages is essentially equivalent confirming that model performance was recreating ambient toxic compound concentrations with acceptable accuracy.

Table 4-4
Risk from Individual Toxic Compounds

Toxic Compound	Risk Factor	Annual Average Concentration	Units	Cumulative Risk (per million)	Percent Contribution
Diesel	3.00E-04	9.166	$\mu g/m^3$	681.62	84.1
Benzene	2.90E-05	1.029	ppb	43.46	5.4
1,3 Butadiene	1.70E-04	1.570	ppb	27.7	3.4
Primary Formaldehyde	6.00E-06	3.590	ppb	11.37	1.4
Secondary Formaldehyde	6.00E-06	1.765	ppb	11.16	1.4
Hexavalent Chromium 6	1.50E-01	0.002	ng/m^3	8.26	1.0
Arsenic	3.30E-03	0.022	ng/m^3	7.97	1.0
p-Dichlorobenzene	1.10E-05	0.209	ppb	5.02	0.6
Secondary Acetaldehyde	2.70E-06	0.967	ppb	4.02	0.5
Perchloroethylene	5.90E-06	0.368	ppb	3.67	0.5
Cadmium	4.20E-03	0.006	ng/m^3	2.40	0.3
Primary Acetaldehyde	2.70E-06	0.758	ppb	1.69	0.2
Methylene Chloride	1.00E-06	1.054	ppb	0.99	0.1
Nickel	2.60E-04	0.212	ng/m^3	0.90	0.1
Trichloroethylene	2.00E-06	0.339	ppb	0.33	< 0.1
Lead	1.20E-05	0.092	ng/m^3	0.09	< .01

Table 4-5
Comparison of the 2005 Network Averaged Modeled Risk to Measured Risk at the Eight –MATES III Sites

Location	Benzene	Butadiene	Other	Diesel	Total
Anaheim	14	13	42	813	882
Burbank	14	11	38	582	645
Compton	16	24	60	873	973
Fontana	12	8	76	585	681
Long Beach	17	16	51	1158	1242
Los Angeles	20	21	60	1167	1268
Rubidoux	11	8	37	489	545
Wilmington	18	12	71	1314	1415
Average Modeled	15	14	54	873	956
Average Measured (EC2.5 * 1.72 for Diesel)	17	16	80	946	1059
Average Measured (CMB)	17	16	80	1004 - 1120	1117 - 1233

4.6 Evaluation

The population weighted average Basin risk (810 per million) simulated from the MATES III data for 2005 was estimated to be 17% lower than the similar average population weighted risk (981) estimated for the 1998-99 MATES II analysis. The areas of the Basin having maximum risk continued to be the Ports of Los Angeles and Long Beach with a secondary maximum occurring in an area starting in central Los Angeles and extending towards southeastern Los Angeles. The overall improvement in average risk and the impact observed in the metropolitan area reflect the combination of pollutant controls and changes made to the analysis from MATES II to MATES III.

The average simulated Basin risk based on the 2005 MATES III data is lower than the comparable average risk estimated for the 1998 MATES II analysis. This improvement stands despite a 2005 emissions increase compared with the MATES II 1998 diesel emissions. Diesel emissions estimated from the 2005 MATES III inventory were approximately 9.6% higher than for the 1998 MATES II inventory. However, back-casts of the 1998 diesel inventory from the current 2002 inventory results in an overall 4.7% decrease in diesel emissions from MATES II to MATES III after adjusting for inventory methodology changes. The percentage difference in emissions between 1998 and 2005 using the 2007 AQMP inventory methodology is less than the 17% change in population weighted risk.

Upgraded modeling and chemistry platforms provided similar results to those presented in the 2007 AQMP $PM_{2.5}$ attainment demonstration for elemental carbon values (only Wilmington displayed a higher predicated bias). Past evaluations conducted for the 2003 AQMP indicated that the UAM platform tended to predict higher peak pollutant

concentrations than CAMx for the same meteorology. Applying this observation to the current analysis can explain a portion of the difference in population weighted risk between MATES II and MATES III.

A sensitivity simulation conducted with emissions restricted to the first layer revealed that distributing the emissions from shipping through the first two fixed layers in the modeling domain resulted only in a nominal reduction in ground level Basin average diesel particulate concentrations.

General assessments of the meteorological profile suggest that the two monitoring periods were comparable in dispersion potential. Meteorological field development, however, was significantly different with MATES III exhibiting a set of more mass consistent data fields and better characterization of vertical diffusion. The MATES II vertical diffusion was based on objective analysis and extrapolation of daily vertical temperature profiles and may have understated the extent of diurnal mixing in the modeling domain.

The spatial distribution of diesel emissions between MATES II and MATES III is significant. The MATES II inventory placed a large percentage of the diesel emissions at the port area and offshore along the shipping lanes. The emissions from trucks were also spread more uniformly throughout the Basin following the travel pattern identified for gasoline vehicles. Diesel emissions remained high in the port areas for 2005 MATES III modeling inventory. However, refinements in truck travel routes and better characterization of rail emissions resulted in a pattern shift that is more clustered near the freeways in the coastal plain and metropolitan areas.

Taken collectively, each element of the analysis contributes to the improvement in estimating average Basin risk for 2005. Regardless, the MATES III modeling analysis represented the state-of-science application of regional modeling tools and chemistry applied to an updated set of meteorological and emissions input data. The model output compared well with the 2007 AQMP $PM_{2.5}$ attainment demonstration and should equally be considered state-of-the–science.

4.7 Reference

WRAP, (2007), Western Regional Air Partnership, Technical Support System, Emissions Method, Offshore Emissions, http://vista.cira.colostate.edu/TSS/Results/Emissions.as