Chapter 5
Regional Model Evaluation

As part of the overall objectives of the MATES-II Program to estimate risk throughout the Basin, computer simulation models (state-of-science 3-dimensional computer models) were utilized. This chapter discusses the results of the regional modeling efforts. More detailed discussions of model input preparation are provided in Appendix V to this document.

5.1 3-Dimensional Simulation Models Evaluated

For the regional model simulations, the Urban Airshed Model (UAM) was used to simulate the dispersion of air toxic compounds based on their emission rates as discussed in Chapter 4. The UAM has been the U.S. Environmental Protection Agency's (U.S. EPA) recommended model for ozone attainment demonstrations. There are several models currently available for ozone simulation. These models are undergoing evaluations as potential models for the next Air Quality Management Plan (AQMP) revision. While the U.S. EPA's version of the UAM may be considered dated, the model has been proven for ozone air quality analysis. Specifically, the dispersion algorithms are still appropriate to analyze the dispersion of inert species (or compounds). As such, the UAM is used to simulate the dispersion of the toxic compounds discussed in Chapter 4.

In addition to the U.S. EPA's version of UAM, a special version of UAM (called UAM-TOX) is applied to simulate the atmospheric reactions of volatile organic compounds (VOCs) and oxides of nitrogen (NOx) to account for the formation and/or destruction of several toxic VOC compounds. Specifically, the UAM-TOX is used to model VOC compounds such as 1,3 butadiene, toluene and styrene (which react in the atmosphere) and carbonyls such as formaldehyde and acetaldehyde (which form in the atmosphere).

Figure 5-1 shows the modeling domain used in the modeling analysis. The horizontal modeling domain covers 210 km from west to east and 120 km from south to north. Each horizontal grid cell is 2 x 2 km in resolution. Five vertical layers are used in the simulation. The UAM and UAM-TOX are applied to a full year of hourly meteorological data. The simulations are for the MATES-II monitoring period from April 1, 1998 to March 31, 1999.

5.2 Toxic Compounds Modeled and Model Performance Goals

A total of 34 compounds are modeled, and 29 of the modeled compounds have measurements collected at the 10 MATES II sites. Table 5-1 provides the 10 MATES II site average of the modeled and measured annual average concentrations of the 29 toxic compounds. The field instrument's monitoring detection limit for the 29 compounds are also provided in Table 5-1. Several toxic compounds have measured average concentrations at or slightly above the detection limit. As such, model simulations of these compounds are typically lower than measured and are often not comparable to the detection limit levels.

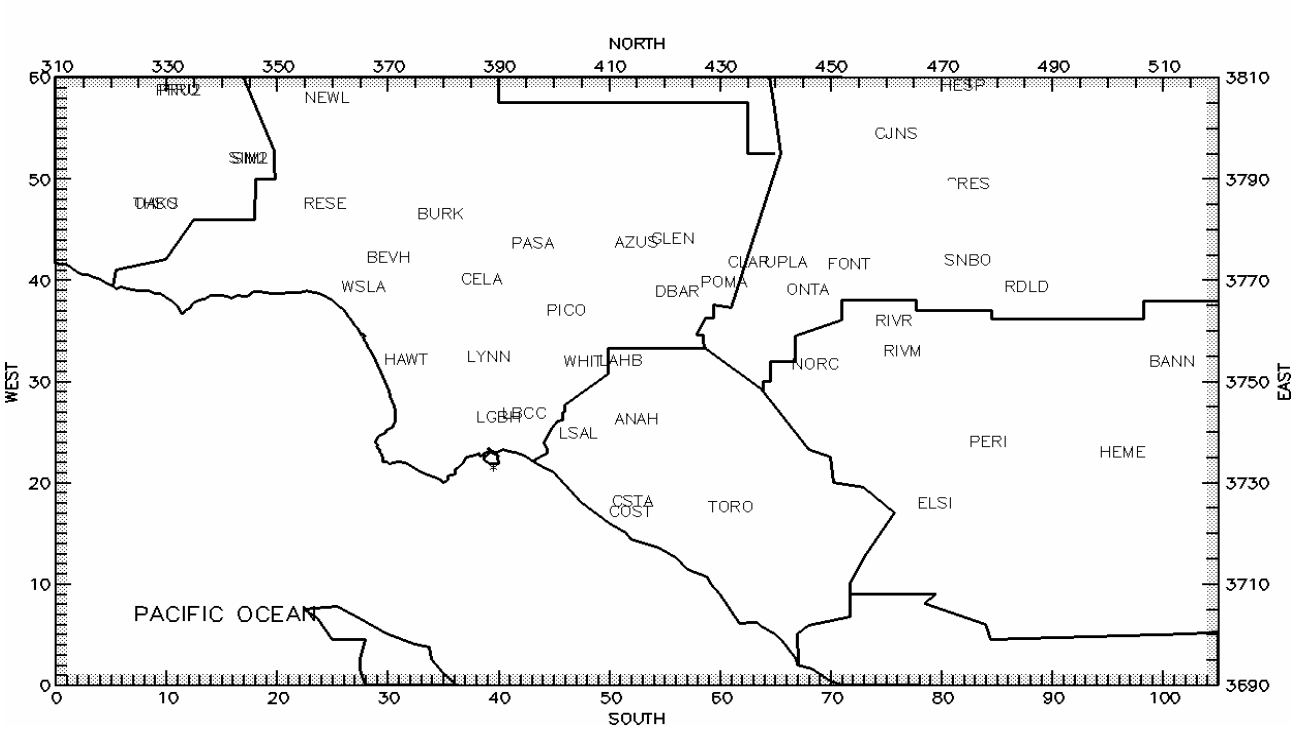

Figure 5-1 MATES-II Modeling Domain

The output of the UAM and UAM-TOX models is given as 24-hour average concentrations for the one-year period modeled. For the current analysis, the 24-hour average concentrations are compared to the corresponding measurements (that are also 24-hour average values). Traditionally, risk calculations are based on annual averaged concentrations. While variations may exist between model simulations and measurements on a daily basis, the longer-term averages tend to be more similar.

Model performance goals have not been established for simulating toxic compounds. However, based on prior ozone model evaluation experience, VOC model performance can vary by as much as an order of magnitude while ozone model performance can vary by as much as 50 percent. In addition, based on prior AQMP ozone modeling applications and recent information regarding mobile source emissions, it is anticipated that higher measured ozone levels will be underestimated in the current analysis. No attempt is made at this time to test the sensitivity of the model simulation. As such, it is expected that mobile source risk contributions will be underestimated by the simulation models.

Table 5-1
Toxic Compounds Modeled and Measured at the 10 MATES-II Sites

Toxic Compound	Modeled Annual Average ($\mu g/m^3$)	Measured Annual Average ($\mu g/m^3$)	Measurable Detection Limit ($\mu g/m^3$) [Percent Non-Detects]	
			ARB	AQMD
Benzene	3.13	3.53	0.639 [4]	0.319 [1]
1,3Butadiene	0.34	0.79	0.088 [4]	0.221 [14]
p-Dichlorobenzene	0.24	0.92	1.202 [-]	0.601 [47]
Methylene Chloride	1.08	2.65	3.476 [72]	0.348 [4]
Chloroform	0.08	0.24	0.098 [14]	0.488 [94]
Perchloroethylene	2.46	1.96	0.068 [3]	0.678 [17]
Trichloroethylene	0.26	0.43	0.107 [31]	0.537 [78]
Carbon Tetrachloride	0.78	0.65	0.126 [0]	1.258 [90]
Ethylene Dibromide	0.01	0.38	--	0.768 [100]
Ethylene Dichloride	0.10	0.26	--	0.405 [98]
Vinyl Chloride	0.01	0.26	--	0.511 [100]
Formaldehyde	5.49	4.82	0.123 [2]	0.123 [2]
Acetaldehyde	5.21	3.17	0.180 [3]	0.180 [3]
Acetone	2.78	5.00	--	0.238 [0]
Methyl Ethyl Ketone	1.72	1.06	0.295 [21]	0.295 [21]
Styrene	0.53	1.23	0.426 [-]	0.426 [25]
Toluene	12.17	12.98	0.754 [2]	0.377 [2]
1,1Dichloroethane	0.03	0.20	--	0.405 [100]
Chloromethane	1.24	1.31	--	0.206 [0]
Arsenic	1.69	1.56	0.003 [95]	0.004 [100]
Elemental Carbon	3.40	3.36	--	--
Organic Carbon	5.92	6.43	--	--
Chromium	0.01441	0.00487	0.002 [6]	0.002 [84]
Hexavalent Chromium	0.00024	0.00018	0.002 [84]	0.00006 [4]
Cadmium	0.00193	0.00605	--	0.001 [99]
Lead (point sources)	0.00292	0.0197	0.003 [0]	0.001 [-]
Lead (area sources)	0.04808	0.0197	0.003 [0]	0.001 [-]
Nickel	0.00775	0.00872	0.002 [9]	0.001 [2]
Selenium	0.00160	0.00197	0.002 [83]	0.001 [47]

However, when ARB finalizes the latest version of the on-road mobile source emissions factor model (EMFAC) and new off-road mobile source emissions, the model performance will be re-evaluated. Detailed discussions of the model performance are provided in Appendix V.

5.3 Model-Estimated Spatial Concentration Fields

Figure 5-2 shows spatial concentration fields simulated by the UAM for six of the 34 compounds (benzene, 1,3 butadiene, perchloroethylene, elemental carbon, hexavalent chromium and particulate emissions from diesel-fueled internal combustion engines). As seen in Figure 5-2, concentration levels vary throughout the Basin with higher concentrations generally seen close to their emission sources. For mobile source compounds such as benzene, 1-3 butadiene, and particulates associated with diesel fuels, higher concentration levels are seen along freeways and freeway junctions. In addition, higher concentrations of benzene and 1,3 butadiene are estimated in and around major airports. In particular, benzene and 1,3 butadiene tend to be higher around the Los Angeles International Airport area and in the south central portions of Los Angeles County. In addition, from Figure V-11 in Appendix V, it can be seen that particulate levels tend to be higher in the south central portions of Los Angeles County and offshore of San Pedro and Long Beach.

For perchloroethylene, higher concentrations are predicted in the Anaheim area as well as in the San Fernando Valley compared to other areas in the modeling domain. In addition to the higher perchloroethylene levels at Anaheim, high concentration levels of styrene are observed in November 1998 (see Appendix V). However, measured styrene levels during the other months are much lower. As seen in the spatial concentration field for styrene, (shown in Appendix V), model estimated annual values (located six to eight km from the Anaheim site) could be as high as the levels measured at the Anaheim location. This implies that the Anaheim monitoring site may be generally upwind of the sources of styrene.

5.4 Risk Assessment Calculations

Based on the spatial concentration fields estimated by the simulation models, risk estimates can be calculated for each grid cell of the modeling domain. There are two approaches for calculating risk [one is weighed by population, the other is using the model estimated concentrations and simply multiplying by the compound's unit risk factor (URF)]. The population weighted risk calculation is more appropriate. The annual average concentration for the risk calculations are based on outdoor concentrations. (The annual average exposure to individuals from volatile chemicals may be higher if there are indoor chemical sources. For particulates, the indoor concentrations may be somewhat less. People may spend a large percentage of their time indoors.) The second approach does not assume any population in the calculation and is more appropriate when comparing with monitored concentrations. As such, both sets of numbers are provided in this Chapter.

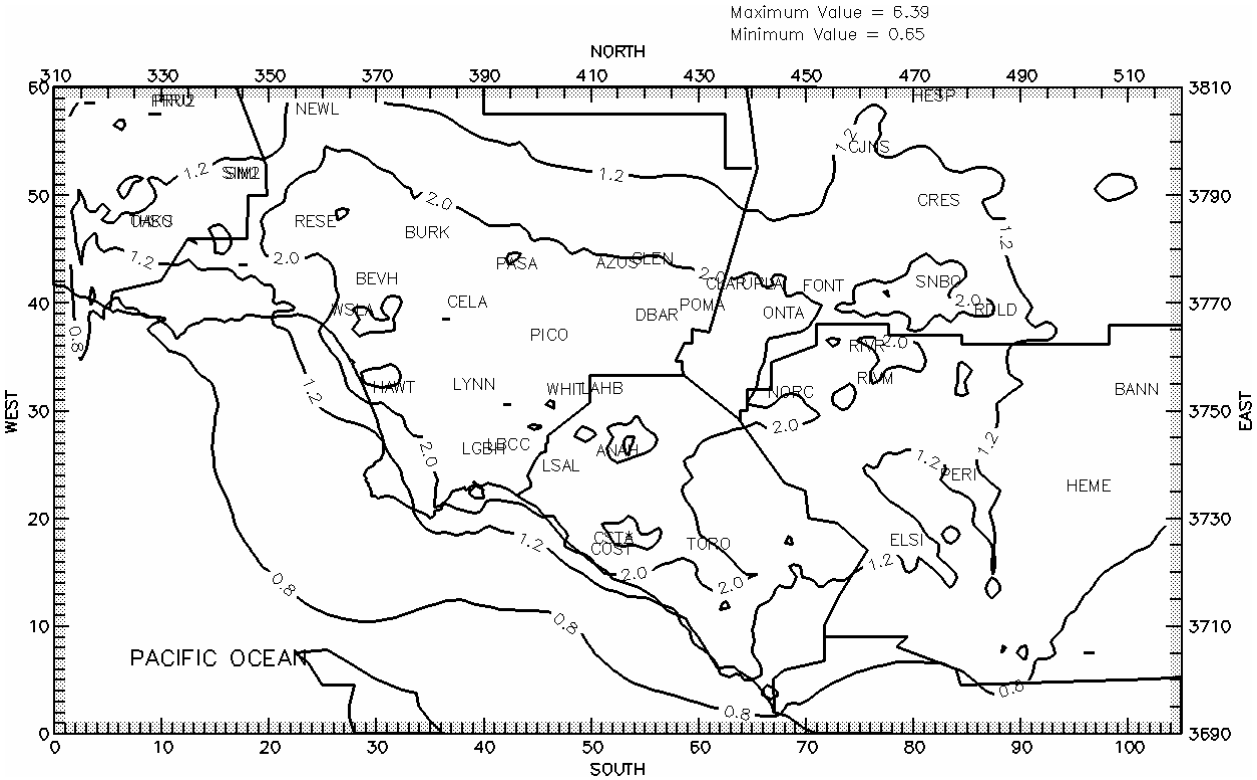

Figure 5-2a. Annual average benzene concentrations simulated for the Basin.

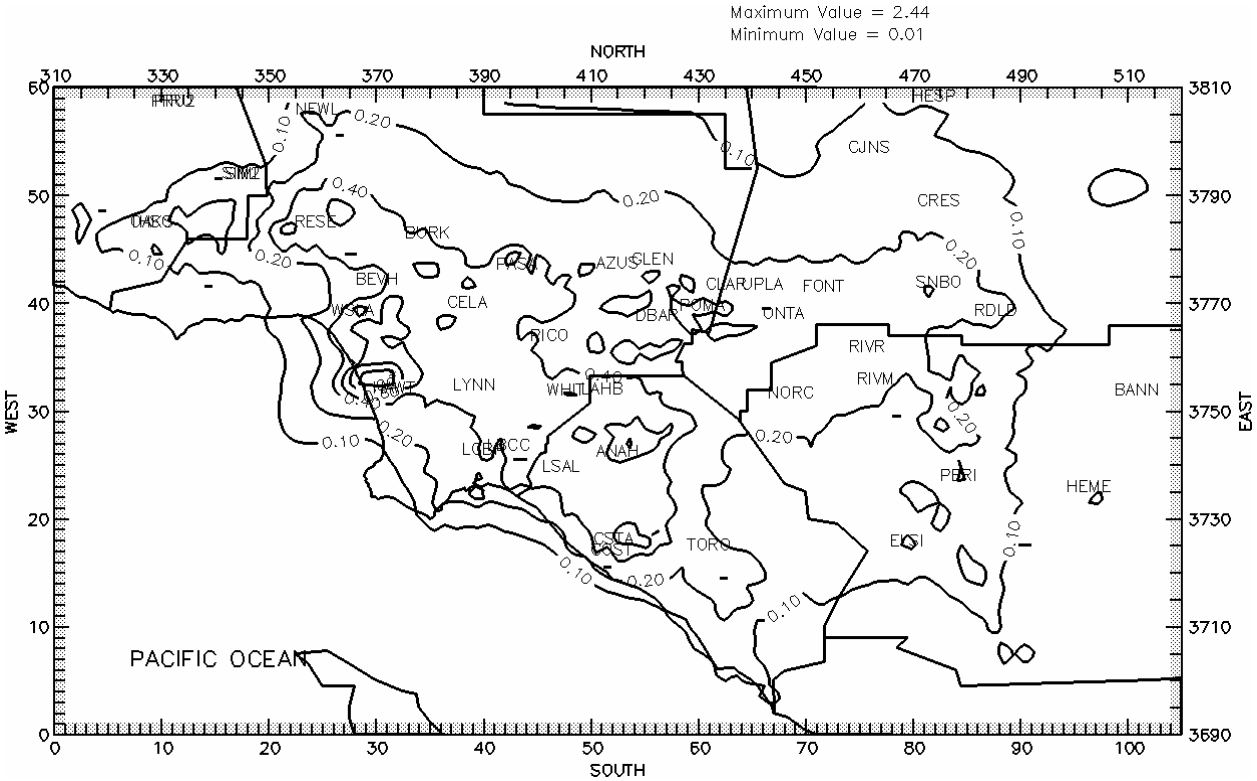

Figure 5-2b. Annual average 1,3 butadiene concentrations simulated for the Basin.

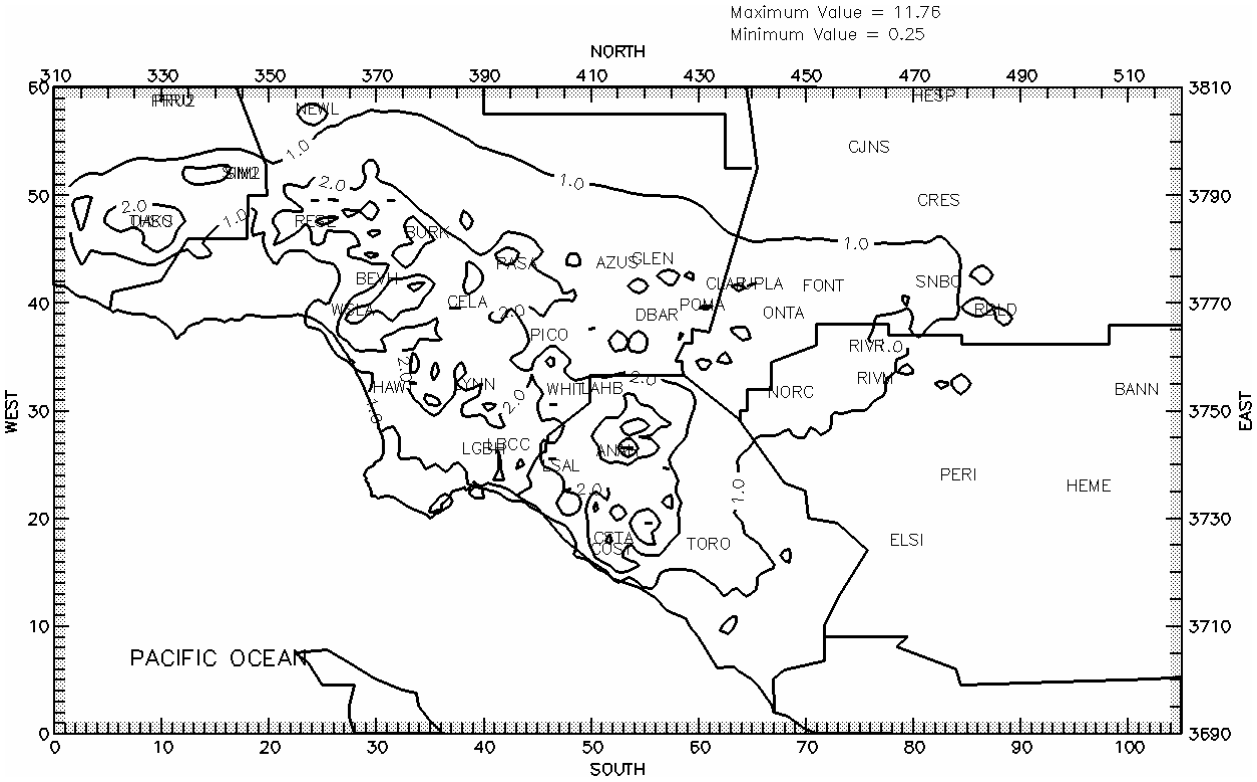

Figure 5-2c. Annual average perchloroethylene concentrations simulated for the Basin.

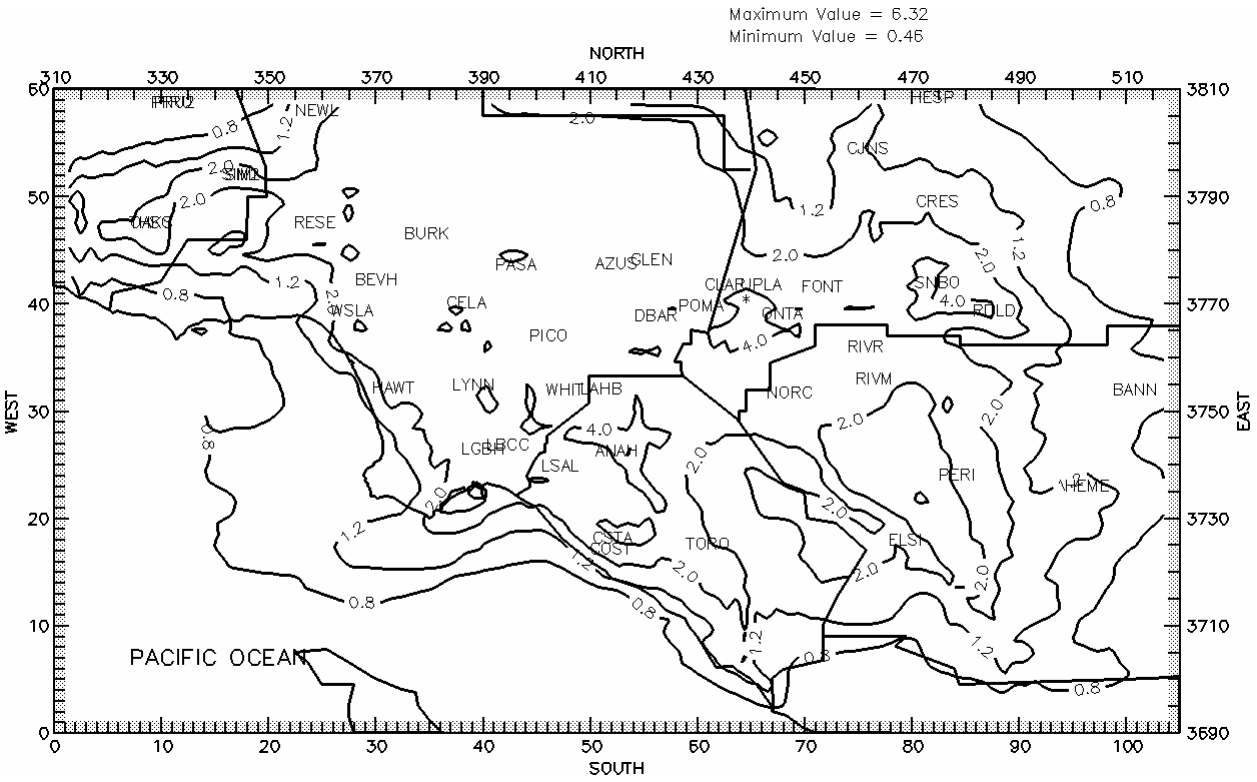

Figure 5-2d. Annual average elemental carbon concentrations simulated for the Basin.

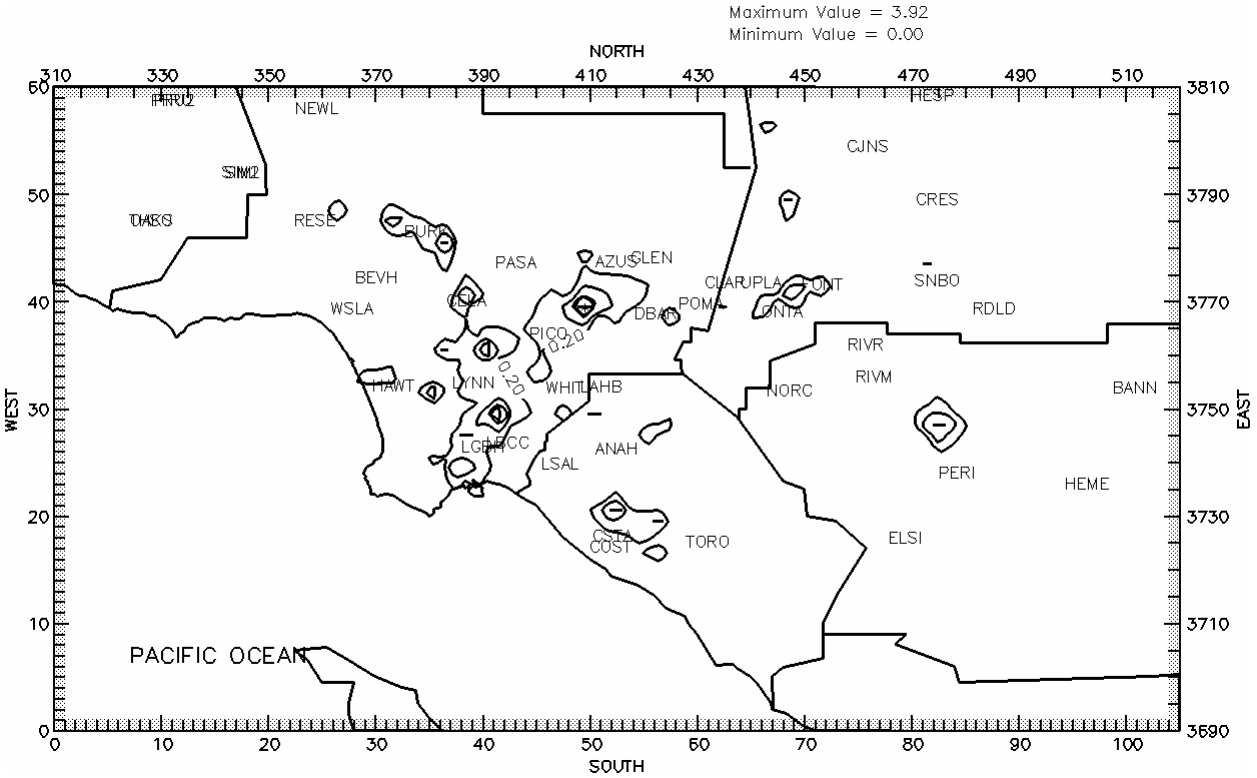

Figure 5-2e. Annual average hexavalent chromium concentrations simulated for the Basin.

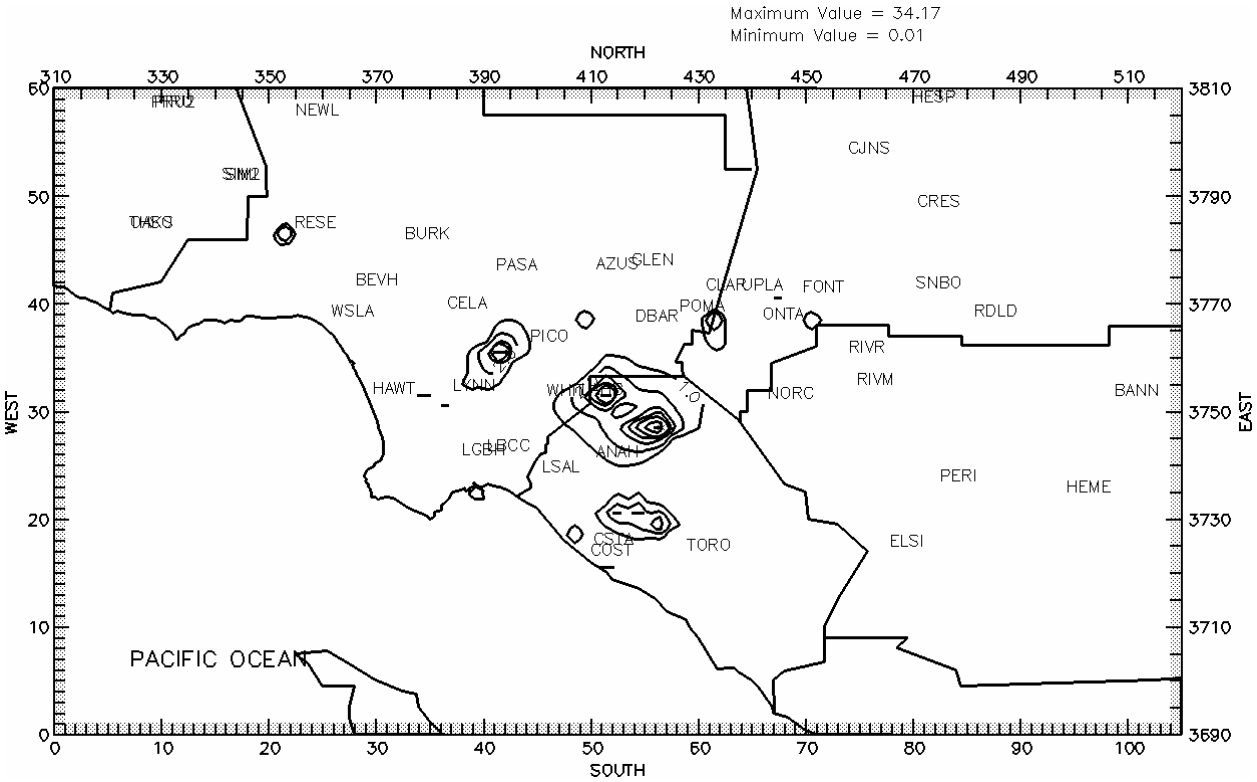

Figure 5-2f. Annual average styrene concentrations simulated for the Basin.

Table 5-2 shows the risk for the four counties in the South Coast Air Basin. The average risk levels ranges from 619 to about 1048 in one million with an overall Basin average of about 981 in one million. As seen from Table 5-2, Los Angeles County has the highest risk levels followed by Orange and San Bernardino counties. The lowest average risk is estimated in Riverside County.

Table 5-2. South Coast Air Basin Modeled Risk and Expected Excess Cancer Cases

	Population	Average Risk (per million)
Los Angeles County	9,305,726	1048
Orange County	2,579,974	940
Riverside County	1,249,554	619
San Bernardino County	1,269,919	926
Basin Total	14,404,993	981

To compare with the network average risk calculated based on concentrations measured at the ten MATES-II sites, modeled concentrations in the grid cells of each of the ten sites are multiplied by their associated URFs (see Table 5-3). Table 5-3 presents the model estimated average risk over the ten sites. For comparison purposes to the monitored values an eight-site average is provided also (there were no measured elemental carbon at Compton or Wilmington). The overall average of the ten locations is about 1200 in one million (see Table 5-3) compared to the network average value of 1400 in one million based on measured concentrations. This analysis also indicates that the average basin risk may be 16% lower than the average risk based on the actual monitoring sites (i.e., 1180 in a million, rather than 1400 in a million).

5.5 Conclusion

Overall, the UAM and UAM-TOX model perform within ±50 to 60 percent of measured annual values. However, the model performance varies significantly on short-term averaged concentrations. In addition, given that mobile source emissions are most likely underestimated with the current ARB mobile source emission factor models, the model performance would improve somewhat with the latest versions of the mobile source models.

The spatial concentration fields show that higher concentrations generally occur near their emission sources. Higher concentrations of compounds that are emitted primarily from stationary and area sources tend to be highest within a few kilometers from the source location. Mobile source related compounds such as benzene and 1,3 butadiene tend to be generally high throughout the Basin. However, the models estimate spatial variations with higher concentrations occurring along freeway corridors and junctions. In addition, higher levels of mobile source related compounds are estimated near major mobile source activities such as airports and other areas with major industrial activities such as south central Los Angeles County, and the industrial areas of Orange, Riverside, and San Bernardino counties.

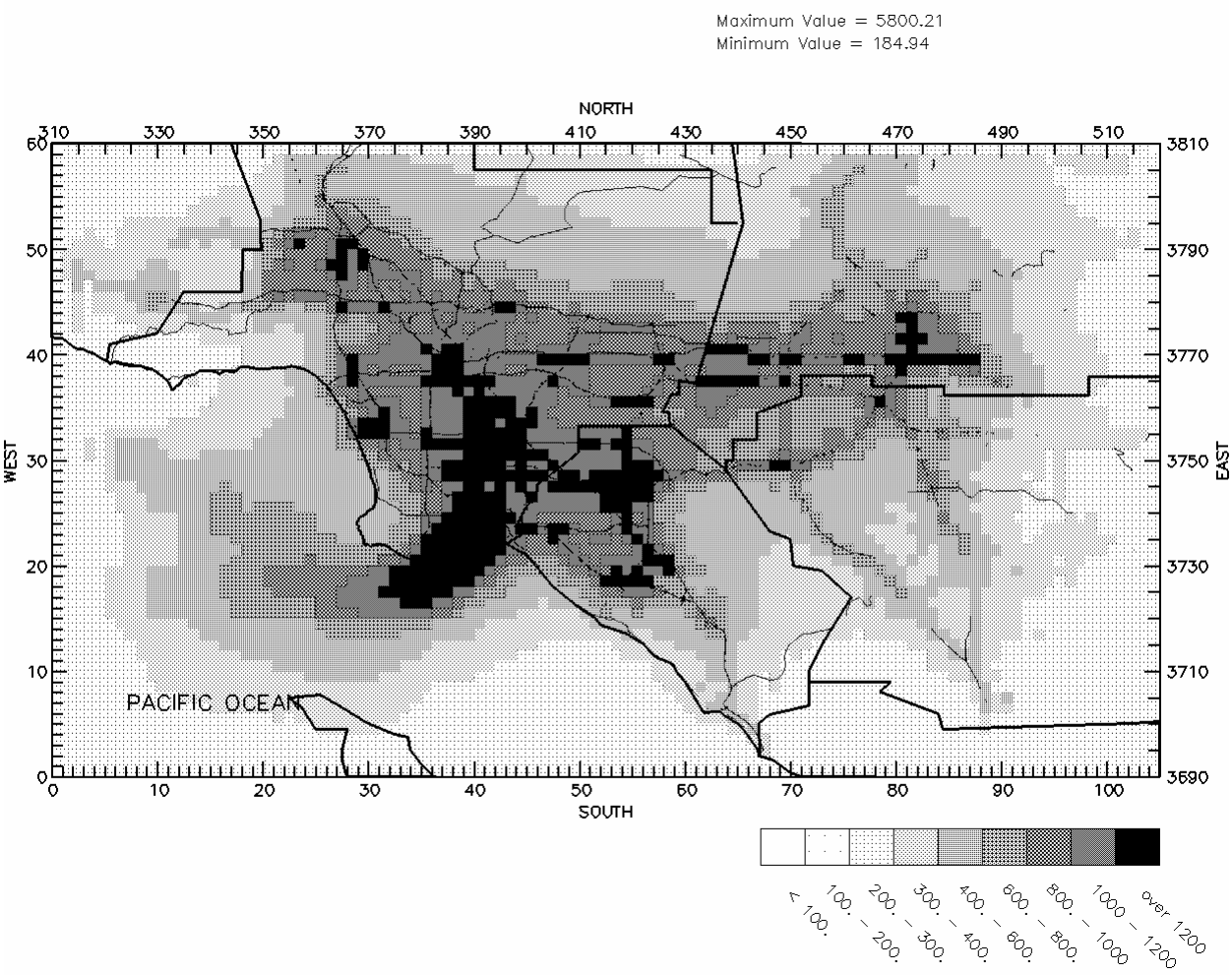

Figure 5-3a. Model estimated risk for the Basin
(Number in a million, all sources)

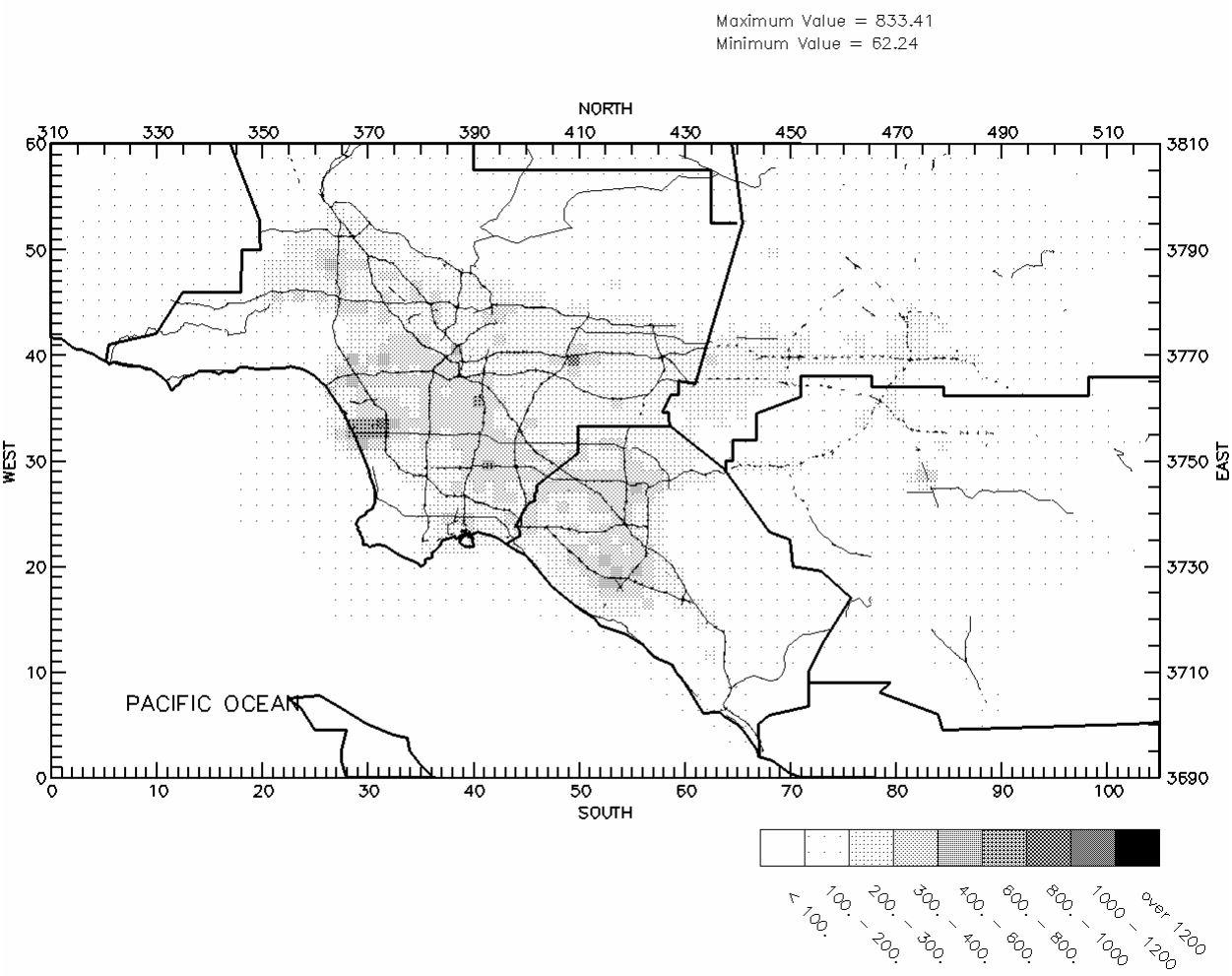

Figure 5-3b. Model estimated risk for the Basin (without diesel sources).

Table 5-3. Comparison of the Network Averaged Modeled Risk to Measured Risk at the Ten MATES-II Sites

	Benzene	1,3 Butadiene	Other	Diesel	Total
Anaheim	119	87	161	963	1330
Burbank	93	62	164	842	1161
Compton	96	65	147	994	1302
Fontana	48	19	120	752	939
Huntington Park	88	61	179	867	1195
Downtown L.A.	94	65	170	1176	1505
Long Beach	88	58	138	920	1204
Pico Rivera	77	43	142	869	1131
Rubidoux	57	26	107	797	987
Wilmington	81	46	222	1182	1531
Modeled Average	**84**	**53**	**155**	**936**	**1228**
Modeled Average*	**83**	**53**	**147**	**898**	**1182**
Monitored Average*	**92**	**118**	**187**	**1017**	**1414**

* Eight monitoring site average excluding Wilmington and Compton where elemental carbon was not measured.