Emissions Modeling in Action: Suggestions to Improve the Process of Developing Emissions Estimates for Use in Air Quality Modeling Studies

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ABSTRACT

It is well understood that emissions estimates are a critical component to the air quality modeling process. However, even after nearly four decades, developing adequate emissions estimates for use in air quality modeling studies continues to be a difficult task. That is, though significant resources have been devoted to better understand and manage emissions data and estimates over the past four decades, the validity of emissions estimates that result from the emissions modeling process continues to be an issue for debate.

Many of the shortcomings that exist in the efforts to develop emissions estimates were highlighted in an ongoing study of regional air quality in central California for ozone episodes occurring in July 1999 and July-August 2000. Though these problem areas are not necessarily new or unique to the California modeling study, they continue to be a burden on efforts to efficiently perform the activities necessary to complete such a study on tight regulatory schedules. For example, significant wildfire emissions occurred during the July-August 2000 episode. Emissions models were applied to estimate from wildfires; however, it was shown to be impossible to verify the magnitudes of the estimates. Estimating on-road mobile source emissions proved to be just as difficult given that the process appeared to be driven as much by policy factors (e.g., conformity budgets) as it was driven by scientific and technical factors. In addition, difficulties were encountered in simply knowing the specific version of the emissions data or estimates that were used.

The emissions modeling process that was followed to estimate emissions for the California modeling study is described. Problems that occurred in this effort are discussed, and specific recommendations to mitigate the issues are described. Finally, where possible, specific local, state, and federal activities or policies that attempt to provide solutions to the problems are identified.

INTRODUCTION

The Bay Area Air Quality Management District (BAAQMD) is responsible for monitoring ambient air quality within the nine San Francisco Bay Area counties (SFBA). The BAAQMD is also responsible for developing and enforcing emissions control plans to mitigate violations of the National Ambient Air Quality Standards (NAAQS) and the California Ambient Air Quality Standards (CAAQS) within the SFBA. In the past, the U.S. Environmental Protection Agency (EPA) has designated the SFBA as non-attainment for the federal 1-hour ozone NAAQS. In response to the designation, the BAAQMD has developed and submitted implementation plans over the years, which serve as the cornerstone to reduce adverse ozone levels in SFBA.

As a result of implementing the plans, violations of the 1-hour ozone NAAQS have been reduced to levels such that on April 22, 2004, the EPA determined that the SFBA attained the 1-hour ozone NAAQS[1]. Shortly thereafter, the 1-hour ozone NAAQS was replaced by the new, stricter 8-hour ozone

NAAQS[2]. Based on SFBA ozone levels from 2001-2003, EPA has designated the SFBA as a marginal non-attainment area of the 8-hour NAAQS[3].

In an on-going study of air quality in the SFBA, in conjunction with the Central California Ozone Study (CCOS)[4], the BAAQMD developed inputs to an air quality modeling system for two episodes: 9-13 July, 1999; and 29 July through 02 August, 2000[5]. The choice of these episodes was based on the analysis of 1-hour ozone exceedances in the Bay Area from 1995 through September 2002[5], though there is supporting evidence that indicates the July 11 and 12, 1999 period will also be suitable for use in photochemical modeling of 8-hour ozone.

A core component of the BAAQMD air quality modeling system is the emissions modeling system. The emissions modeling system in use by BAAQMD is comprised of the following components:

- Emissions Modeling System of 1995 (EMS-95) for stationary and area sources emissions estimates[6];
- Biogenic Emissions Inventory – Geographic Information System (BEIGIS) for biogenic emissions estimates[7-9]; and
- California on-road EMissions FACtor model for 2002 (EMFAC2002)[10] coupled with the California Integrated Transportation Network (ITN)[11] and the Direct Travel Impact Model (DTIM)[12] for on-road mobile source emissions estimates.

This system of emissions modeling tools was used to prepare emissions estimates for carbon monoxide (CO), total organic gases (TOG), and oxides of nitrogen (NOx) that were suitable for input to the CAMx air quality model[13]. The emissions data were derived from a variety of sources. The California Air Resources Board (ARB) prepared stationary source and county-wide area source emissions estimates for representative episode days[14]. Estimates of temporally and spatially resolved biogenic organic gas emissions estimates were developed using BEIGIS[7-9]. Spatially and temporally resolved soil NOx emissions were estimated using the methods of Williams et al.[15] with landuse data based on version three of the Biogenic Emissions Landcover Database (BELD3)[16,17] and soil NOx emissions factors from version three of the Biogenic Emissions Inventory System (BEIS3)[18,19]. County-wide on-road mobile source emissions of NOx, CO, and TOG were estimated using EMFAC2002 and were spatially and temporally allocated using surrogates developed through the application of DTIM over the ITN[11]. For the July-August 2000 episode, the base emissions estimates were supplemented with day-specific emissions estimates from wildfires[14], refineries[5], sixty-seven other large stationary sources[14], agricultural burns[14], and commercial marine shipping[5]. For the July 1999 episode, only day-specific emissions estimates for commercial marine shipping were developed since data for the other day-specific source were unavailable in a timely manner. All emissions estimates were then chemically speciated for both Carbon Bond IV and SAPRC99 chemical mechanisms, and reformatted for use in CAMx using EMS-95[5].

In this paper, we summarize the overarching process to develop the CAMx-ready emissions estimates and discuss the technical shortcomings. These shortcomings resulted in the study team revising the following emissions source categories more than once during the study: stationary sources, area sources, biogenics, on-road mobile sources, wildfire emissions, and refinery emissions. Finally, we provide suggestions on how to improve the process to estimate air quality model ready emissions.

DISCUSSION

Base Stationary and Area Source Emissions

During the initial stages of the study, ARB supplied base emissions estimates for the CCOS modeling domain (Figure 1), which is the same domain used for the BAAQMD photochemical modeling. The base emissions included estimates for stationary and area sources. Though it is well known that emissions undergo constant revision, especially during the course of an air quality modeling study as air quality modeling results indicate potential errors in the estimates, the base stationary and area source emissions underwent no less than thirteen revisions during the course of the study. These revisions to the base estimates resulted in various changes to the overall NOx and TOG emissions that ranged on the order of a few tons per day to over two hundred tons per day. Each time a revision was made to the base stationary and area source emissions, they were reprocessed through the emissions modeling system in order to prepare a new set of CAMx-ready emissions data sets.

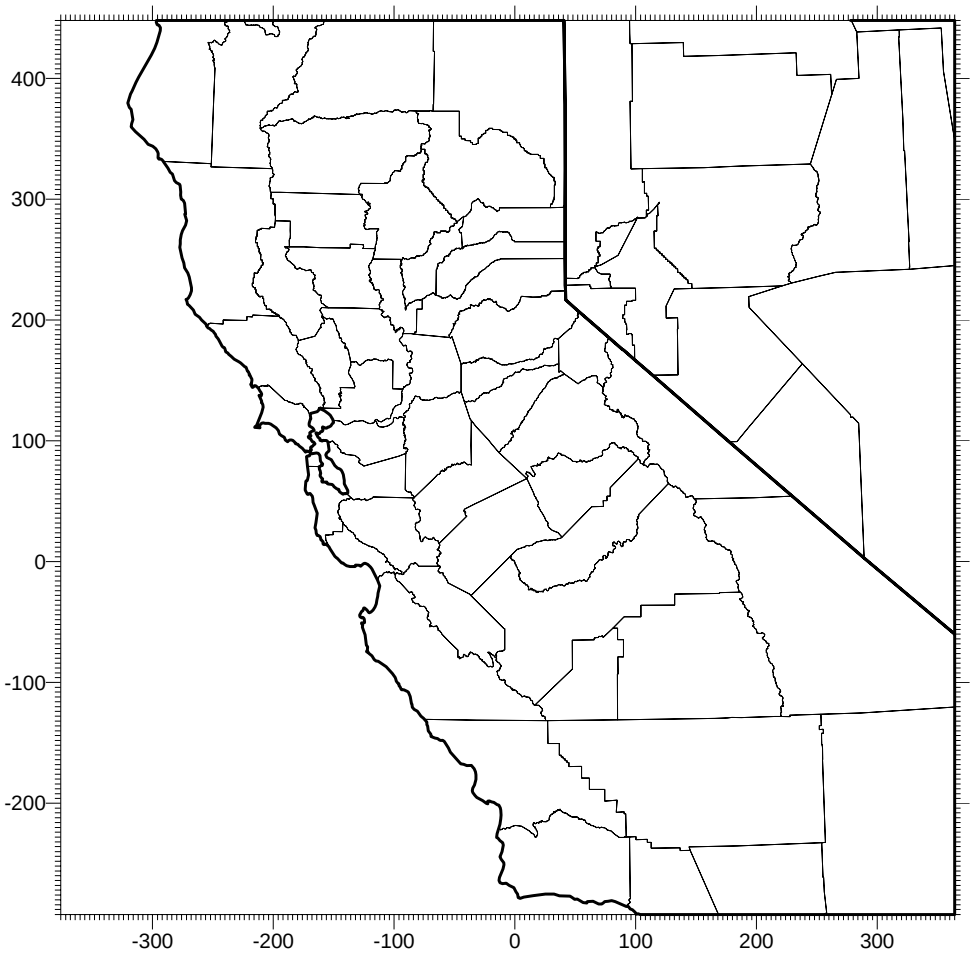

Figure 1. CCOS air quality modeling domain.

In order to track the changes to the base stationary and area source emissions, a file naming scheme was adopted that identified the version of base emissions as delivered by ARB directly in the CAMx-ready emissions files[20]. Further, an Excel spreadsheet was prepared to maintain a specific list of revisions to the base stationary and area source emissions cross-referenced to the ARB version

number[20]. Though this worked early in the process, the shear number of changes to the base stationary and area source emissions coupled with changes to emissions in the other emissions source categories resulted in difficulties in tracking which were the most recent CAMx-ready emissions files. As one can imagine, this occasionally resulted in the use of out-of-date CAMx-ready emissions estimates.

Refinery Emissions

Based on work performed by the BAAQMD, refinery NOx emissions, specifically from flaring operations, were increased from 0.1 tons per day (tpd), as they existed in the ARB emissions inventory, to 13 tpd[5]. However, early in the study, it became clear that these revised emissions estimates were not included in the base stationary source emissions estimates that were delivered by ARB for EMS-95 processing. Further, there was evidence to suggest that other refinery-related emissions were also underestimated (e.g. upset events, pressure relief valves), which might affect TOG emissions as well. In an effort to better characterize emissions from refinery operations, the BAAQMD undertook another effort to develop day-specific emissions estimates for refinery operations within the District's jurisdiction. These day-specific emissions estimates were used in lieu of the previous standard BAAQMD/CARB estimates for the July/August 2000 base case air quality modeling[5]. Hence, the study team revisited the issue of revised refinery emissions at least twice during the course of the study.

As noted previously, no such additional effort was performed for the July 1999 base case episode[5]. Instead, the standard ARB area source emissions estimates for refineries, revised to account for the factor of one hundred increase initially determined by BAAQMD, were used for July 1999.

Wildfire Emissions

Emissions from the July/August 2000 episode were characterized by a heavy contribution from forest fire smoke. The smoke plumes from this and other large regional fires in Oregon and Nevada were detected aloft on several days by multiple aircraft and ozonesonde samples taken throughout central California[5]. Further, air quality modeling experiments demonstrated that emissions from wildfires had significant impact on air quality modeling predictions throughout the CCOS domain, possibly even in the SFBA[5]. The University of California at Berkeley's Center for the Assessment and Monitoring of Forest and Environmental Resources (CAMFER) laboratory estimated day-specific temporally and spatially resolved emissions for two of the largest wildfires, the Manter fire in Tulare County and the Plaskett fire in Monterey County, using a modified version of the USDA Forest Service First Order Fire Effects Model (FOFEM)[21], called the Emissions Estimation System (EES)[14]. For a number of smaller wildfires throughout the domain, emissions were calculated based on the number of acres of three vegetation types (i.e., chaparral, grass, and timber) coupled with U.S. Forest Service fuel loading and emission factors[14]. The number of acres, vegetation type, fire duration, and location information were taken from California Department of Forestry (CDF) fire incident reports and newspaper articles[14].

The July 1999 episode was not nearly affected by forest fire smoke, as fire activity levels were more representative of a "typical" ozone day. Therefore, the emission inventory for July 1999 contained standard season day fire estimates.

Two issues arose with the use of these estimates. First, the emissions estimated by the modeling systems were not verifiable. Further, no efforts were (or have been) expended to determine the magnitude of the uncertainty in the emissions estimates. Second, it was well known that these emissions estimates had to be distributed in the vertical as the smoke plumes were observed to penetrate through the atmosphere. Given the unverifiable nature of the estimates, the magnitude of the emissions was

deemed fixed; and hence, were not revisited during the course of the study. However, the distribution of the wildfire emissions estimates were discussed extensively, and ultimately, three revisions to the emissions estimates were made to account for alternative vertical distributions of the wildfire emissions estimates.

On-road Mobile Sources

The modeling process for on-road mobile sources was very complex involving three models other than EMS-95. Day-specific, county-wide on-road mobile sources emissions for both episodes were estimated using EMFAC2002[10]. These estimates were then spatially and temporally disaggregated using on-road mobile source spatial surrogates that were prepared using DTIM[12] runs which were based on data in the ITN[11]. A complete description of the methods to estimate on-road mobile source emissions are described elsewhere[11,14].

Three issues arose during the modeling of on-road mobile source emissions. First, the modeling process was dependent on spatially and temporally resolved surface level temperature and relative humidity. During the early stages of the study, these fields were in a state a flux as the meteorological modeling was incomplete. The first round temperature and relative humidity fields that were used to estimate emissions were based on preliminary meteorological modeling (using the prognostic MM5 model), but a performance evaluation had not yet been undertaken. Screening evaluations later revealed that the daytime temperature fields were far too cool, while nighttime fields were too warm (a classic problem associated with MM5). Therefore, a second round of environmental fields were developed using a hybrid combination of prognostic meteorological modeling results and diagnostic techniques based on interpolation of observations[14]. As the study progressed and the meteorological observations were further scrutinized, it was discovered that significant errors existed in the observed temperatures especially for monitoring stations in the SFBA. Subsequently, a third and fourth round of meteorological fields were used to estimate new on-road mobile source emission inventories. The third round of meteorological fields was developed based solely on new interim meteorological modeling results, and the fourth round of meteorological fields was based on the hybrid approach with revised meteorological observations.

Second, during the course of the study, ARB released a new version of EMFAC which required that the on-road mobile source modeling undergo another change. Fortunately, the release of a new version of EMFAC coincided with the release of the second round of meteorological data.

Third, the source code that acted as a "wrapper" around EMFAC2002 underwent revisions to account for changes in data that impacted the EMFAC2002 results. These data changes impacted vehicle population counts in the SFBA. For the July-August 2000 episode, these source code and data changes were accounted for; however, as discovered very late in the study, these changes did not propagate through the July 1999 episode, which ultimately required yet another run of the modeling system to estimate on-road mobile source emissions. In all, the on-road mobile source modeling system was rerun on five different occasions.

Biogenics

Organic gas biogenic emissions were modeled using BEIGIS[7-9] and supplemented with soil NOx emissions estimated using other methods and data[15-19]. These estimates require both spatially and temporally resolved estimates of temperatures and photosynthetically active radiation (PAR). As with the second round of on-road mobile source emissions estimates, the biogenic emissions for the July-August 2000 episode were estimated based on temperatures that were derived based on the hybrid

approach and PAR values taken directly from the meteorological modeling[14]. However, as subsequent meteorological fields became available, no effort was made to remodel the biogenic emissions estimates. Though for the July 1999 episode, only the most recent meteorological fields were used to estimate biogenic emissions.

Meteorology

As noted with the biogenic and on-road mobile source emissions estimates, various meteorological fields were used in the modeling effort. Also, as can be deduced, no single, consistent meteorological field was used to estimate the emissions for all emissions sources. To further exacerbate the issue, none of the meteorological fields that were used to estimate emissions were truly consistent with the meteorological fields that were used in the air quality modeling efforts.

Organic Gas Speciation

A component of the emissions modeling process is to convert organic gas emissions estimates into a form that is suitable for input to the air quality model. This process is known as speciation, and the resulting mix of speciated emissions defines the overall reactivity of the organic gas estimates. As part of the study, air quality model ready emissions estimates were prepared using both the Statewide Air Pollution Research Center (SAPRC)[22] and the Carbon Bond Four (CBIV)[23] speciation profiles[14]. During the course of the study, three versions of the CBIV profiles and five versions of the SAPRC profiles were used[14]. The use of the alternative speciation profiles resulted in at least four additional revisions to the air quality model ready emissions files through the application of the emissions modeling system.

Studies performed by Tesche et al.[24], Vizuete et al.[25], and Emery and Tai[26] indicated that a possible explanation for persistent photochemical model under-predictions of ozone at key monitoring stations was due to the lack of reactivity in the organic gas emissions. It was well known that the CBIV speciation profiles used by ARB and EPA were different, and that the use of each set of speciation profiles would produce an inventory with different overall reactivity. This was tested by mapping the ARB emissions source categories to the EPA CBIV speciation profiles for just the stationary and area source emissions categories and running the EMS-95 speciation processors

Table 1 shows the results of the speciated emissions estimates based on the EPA CBIV speciation profiles. Table 2 shows the results of the speciated emissions estimates based on the ARB CBIV speciation profiles. *PAR* indicates the paraffinic portion of the emissions estimates. *REACTIVE* indicates the sum of the remaining CB-IV components of the emissions estimates (i.e., higher molecular weight aldehydes [ALD2], ethylene [ETH], formaldehyde [FORM], methanol [MEOH], ethanol [ETOH], isoprene [ISOP], olefins [OLE], toluene [TOL], and xylenes [XYL]). Representative days for each episode are also shown: J-WE is a July weekend day; J-WD is a July weekday; and A-WD is an August weekday. The emissions source categories are as follows: *EGU* is electric generating utilities; *Other* is stationary sources other than EGU; *Area* is area sources; *Ship* is commercial marine shipping; *Off-road* is non-road mobile sources; *On-road* is on-road mobile sources; and *Bio* is biogenics. Though alternative speciated emissions were estimated for the entire domain, only the emissions estimates for the SFBA are shown.

Table 3 shows the difference between the two model-ready inventories (EPA minus CARB). For both episodes, PAR and REACTIVE emissions increase using the EPA speciation profiles in SFBA for *EGU, Other,* and *Area* for both weekend day and weekday. Interesting differences include the following: *Off-road* REACTIVE emissions for both episodes show a sign flip from weekend day to

weekday; *Area* and *Other* PAR emissions in July 1999 are about 10% greater than those in July/August 2000; and *Area* REACTIVE emissions in July 1999 are double those of July/August 2000. Given that the underlying criteria pollutant emissions estimates are similar between the two episodes, it is unclear why this is occurring. That is, one would expect similar changes in the speciated emissions from one episode to the next. It is possible that the inclusion of day-specific emissions estimates in the July/August 2000 episode may have some impact; however, due to limited resources for this experiment, an explanation as to why this has occurred was not definitely determined.

Table 1. Speciated organic gas emissions estimates based on EPA CBIV speciation profiles (tons per day).

Bay Area	PAR					REACTIVE				
	July-August 2000			Jul-99		July-August 2000			Jul-99	
	J-WE	J-WD	A-WD	J-WE	J-WD	J-WE	J-WD	A-WD	J-WE	J-WD
EGU	6	6	7	5	5	4	4	5	4	4
Other	73	88	90	70	88	63	77	78	61	78
Area	104	106	106	126	128	44	46	46	53	55
Ship	-	-	-	-	-	-	1	1	1	-
Off-road	84	43	43	73	37	73	45	45	65	41
On-road	115	136	136	123	144	57	65	65	52	60
Bio	44	55	54	85	96	270	366	325	478	545
Total	426	434	436	482	498	511	604	565	714	783

Table 2. Speciated organic gas emissions estimates based on ARB CBIV speciation profiles (tons per day).

Bay Area	PAR					REACTIVE				
	July-August 2000			Jul-99		July-August 2000			Jul-99	
	J-WE	J-WD	A-WD	J-WE	J-WD	J-WE	J-WD	A-WD	J-WE	J-WD
EGU	2	2	3	1	1	-	1	1	-	-
Other	45	58	59	38	54	14	22	23	13	24
Area	72	75	75	89	91	41	43	43	46	49
Ship	-	-	-	-	-	-	1	1	1	1
Off-road	80	42	42	69	37	80	44	44	70	39
On-road	115	136	136	123	144	57	65	65	52	60
Bio	44	55	54	85	96	270	366	325	478	545
Total	358	368	369	405	423	462	542	502	660	718

Table 3. Difference (EPA minus ARB) in speciated organic gas emissions estimates based on EPA and ARB CBIV speciation profiles (tons per day).

Bay Area	PAR					REACTIVE				
	July-August 2000			Jul-99		July-August 2000			Jul-99	
	J-WE	J-WD	A-WD	J-WE	J-WD	J-WE	J-WD	A-WD	J-WE	J-WD
EGU	4	4	4	4	4	4	3	4	4	4
Other	28	30	31	32	34	49	55	55	48	54
Area	32	31	31	37	37	3	3	3	7	6
Ship	-	-	-	-	-	-	-	-	-	(1)
Off-road	4	1	1	4	-	(7)	1	1	(5)	2
On-road	-	-	-	-	-	-	-	-	-	-
Bio	-	-	-	-	-	-	-	-	-	-
Total	68	66	67	77	75	49	62	63	54	65

RECOMMENDATIONS/CONCLUSIONS

In all, there were twenty-four reruns of various aspects of the emissions modeling system to account for changes in emissions data and estimates. The complexity of the emissions modeling system coupled with the volume of changes resulted in numerous stops-and-starts of the overall air quality modeling process. This significantly impacted not only the project schedule, but also significantly stressed project resources. One overriding problem that continued to occur was the difficulty in knowing which set of air quality model ready emissions estimates were most current. Though a file naming convention was used to distinguish among the various air quality model ready emissions files, it became clear early in the project that the shear number of files and the rapidity of their change would confuse users as to their content. Further, though it was possible to couple the contents of an Excel spreadsheet with components of the air quality model ready emissions file name to determine which emissions data and estimates were changed, again because of the shear number of files present and the rapidity of change, it was simply difficult to ascertain what was changed. Finally, though it could be discerned what emissions source categories were changed in each air quality model ready emissions data set, the magnitudes of the changes were not adequately maintained.

In order to ameliorate these problems in the future, there are at least two approaches that can be followed. First, all source code related to the emissions modeling system needs to be placed under a central version control system. Users can then download either the most recent production release, or opt to download a release candidate. Given the ubiquitous nature of the World Wide Web in the sciences, it seems particularly natural for model developers to provide a central site to deploy software. Emissions modeling systems can be deployed by developers through their own websites. Or sites such as sourceforge.net can provide capabilities to manage Open Source projects. By centralizing source code deployment, modelers will ideally not be beholden to more than one source for emissions model code. Such an effort to centralize emissions modeling source code, of course, will require some effort by the developers of EMS-95, DTIM, EMFAC, EMFAC-wrapper, ITN, BEIGIS, BELD3, BEIS3 and the like to setup and maintain such central repositories. Of note, EMFAC[10], BEIS3[19], and BELD3[16] currently have central release points though only BEIS3 is provided in its FORTRAN source form. That is, only a Windows-compatible executable is provided for EMFAC, and BELD3 is a suite of ASCII data that requires other software to manipulate for use in BEIS3.

Second, it is time to begin housing all emissions related data and estimates under a true data base management system. In this study, emissions data and estimates were maintained in SAS data sets, ASCII files, Excel spreadsheets, UNIX binary files, and PC binary files. By housing the emissions data and estimates under a true data base platform, the emissions data and estimates can be "tagged" with an appropriate identifier as to their context. Such a "tag" can be carried through to the air quality model ready emissions estimates. Use of the "tag" can be used to determine not only the emissions source categories that had changed from "tag" to "tag," but it can also be used to track such things as the magnitude of the change and the date of the change.

Efforts are now well underway to deploy the CONsolidated Community Emissions Processing Tool (CONCEPT)[27]. In many ways, CONCEPT codifies these two recommendations. CONCEPT currently has emissions modeling capabilities for stationary sources, area sources, biogenics, on-road mobiles sources, and non-road mobile sources. CONCEPT is an open source emissions modeling system based on the open source PostgreSQL[28] Structured Query Language (SQL) data management system.

It was clear from the start of the study that changes were to be expected to the emissions data and estimates as the study was to progress. It was not clear just how numerous these changes were to be. Nor was it clear just how significant these changes were to detrimentally impact project resources. It is

possible that better planning may have mitigated some of the problems that occurred during the emissions modeling component of the study. Regardless, the shear number of the emissions models employed, coupled with the complexity of operating the models and the number of groups involved in operating them, contributed to the problematic aspects that were encountered. Though emissions estimates suitable for input to CAMx were developed and much modeling has been performed by several California regulatory agencies, the emissions data and estimates are still suspect. Indeed, on-going review of both the air quality model results and of the emissions estimates have shown: (1) that the temporal distribution of emissions from heavy-duty diesel vehicles, a key contributor to NOx, is incorrect for both episodes; (2) that VOC reactivity and/or total VOC emission rates are too low in key areas of the domain; and (3) that there are suspected over estimates of the biogenic OVOC and monoterpene emissions in the July 1999 episode. Given the suspect nature of the emissions inventory, it is remiss to conclude that the current emissions estimates are truly suitable for use in SIP-related air quality planning efforts. Hence, they are currently being used as a place holder in on-going air quality modeling analyses.

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KEYWORD

Emissions Inventory
Emissions Modeling
Ozone
Air Quality Modeling
Data Base