DEVELOPMENT OF AN UPDATED BASE CASE AMBIENT VOC MIXURE FOR ASSESSING ATMOSPHERIC REACTIVITY

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Disclaimer

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Abstract

Volatile organic compounds (VOC) – also referred to as reactive organic gas (ROG) mixtures – are important precursors of ozone (O_3) and particulate matter (PM) pollution, and many VOC species are themselves considered as air toxics. Accurate information about VOC composition in the air is needed both to assess possible effects of pollution and to develop plans to improve air quality. One specific regulatory approach is to take the data describing the typical mixture of VOCs in an urban area and then to simulate the atmospheric chemistry and physics using specialized computer programs. Much of the data in use currently to do air pollution modeling comes from studies from late 1980s to early 1990s. In this project, data for the Los Angeles area from 2006 – 2009 plus select older data have been used to construct new "base case" ROG mixtures to characterize the air for modern air modeling software tools. Among the changes observed in the base case ROG mixture from earlier periods to more recent years is that in general, fractions of paraffins, carbonyls and biogenic hydrocarbons are higher, while anthropogenic olefins tend to be lower in updated ROG mixture profiles. This combination of changes leaves the typical ROG mixture less reactive than in the past, which predicts generally lower ozone concentrations. Maximum incremental reactivity calculates slightly higher with the new profile, particularly for alkanes, oxygenated VOCs and aromatics.

1 Executive Summary

1.1 Background

The ability to effectively and efficiently model atmospheric photochemistry is of concern to the California Air Resources Board (CARB). Development and evaluation of computationally-efficient chemical mechanisms, such as SAPRC 99 and SAPRC07, for photochemical modeling requires the use of representative, or base case, reactive organic gas (base ROG) mixtures that reflect the composition of reactive volatile organic compounds (VOC) concentrations in urban airsheds. Similarly, calculation of maximum incremental reactivity (MIR) and other VOC reactivity scales are among other air quality research and regulatory applications that require representative urban air base ROG mixtures. The base ROG mixture currently in use by the CARB was developed primarily on research from the late 1980s and early 1990s. As is described in Carter (1994),

> "The speciation for this mixture was derived by Croes (1991) based on an analysis of the EPA database (Jeffries et al 1989) for the hydrocarbons and the 1987 Southern California Air Quality Study (SCAQS) database for the oxygenates. This mixture consists of 52% (by carbon) alkanes, 15% alkenes, 27% aromatics, 1% formaldehyde, 2% higher aldehydes, 1% ketones, and 2% acetylene."

Since 1994, emissions compositions have changed due to ongoing control strategies, market-driven technology changes, and other developments. Also, analytical measurement methods have improved. Introduction of reformulated gasoline nationally, phase-out of some gasoline components, and specific programs instituted in California such as vehicle emission standards and inspection/maintenance programs, off-road vehicle standards, and stationary sources controls, have all influenced the base ROG mixture in California. However, the make-up of the base ROG mixture has not been revised.

1.2 Methods

The objective of this contract was to develop an updated ROG mixture for assessing atmospheric reactivity, using recent VOC data collected from Photochemical Assessment Monitoring Stations (PAMS) and estimated from urban emission inventories. Specific steps taken in this project included: (1) compiling recent speciated VOC measurements from various urban areas; (2) compiling recent estimates of speciated VOC emissions from various urban areas, based on emission rates and source specific VOC composition profiles; (3) analyzing ambient and emissions data for representative ROG mixtures; (4) using a box model on mixtures to assess the sensitivity of maximum incremental reactivities (MIR) to base case composition.

1.3 Results

Compared with 20 years ago, the updated ROG mixtures are lower in absolute concentrations and have significantly different profiles. In general, fractions of paraffin, carbonyls and biogenic hydrocarbons are higher, while that of anthropogenic olefins is lower in updated ROG mixture profiles. In particular, the maximum incremental reactivity (MIR) of n-hexane has doubled in the past 20 years while concurrent, significant changes of MIRs of propene and m-xylene have not

been found to occur; emission estimates of organic halogen compounds such as 1,3-dichloropropene were analyzed together with PAMS compounds.

1.4 Conclusion

The PAMS observations from 2006 – 2009 were augmented with SCOS97 observation and emission inventory in Los Angeles counties to develop new profile. In general, there has been a significant decrease in ambient concentrations over the past 10+ years. In comparison to the older profile (ARBROG), several groups of species (e.g. alkenes and aromatics with relatively large molecules) were reduced.

The ROG mixture developed in this project is dubbed the "PAMS/SCOS/Emis patched profile". This ROG mixture generated less ozone than the profile previously used. The new profile seems to lead to slightly larger (typically within 10 percent) maximum incremental reactivity for some classes of species. However, overall incremental reactivity of the ROG mixture was decreased by approximately 20 percent for all of three incremental reactivity measures.

2 Introduction

The current base case volatile organic compound (VOC) mixture used for assessing atmospheric reactivity was derived from datasets collected in the late 1980s and early 1990s. As VOC control programs have been aggressively implemented since then, the anthropogenic VOC mixture in the atmosphere has changed in both absolute and relative quantities. A recent preliminary study, funded by the U.S. EPA, showed that the make-up of the organic compounds that we breathe now differs significantly from 20 years ago.

The 20-year-old base case VOC mixture was used to derive condensed photochemical mechanisms, such as SAPRC-99 and SAPRC-07. These mechanisms have been useful for assessing atmospheric reactivity and other scientific and regulatory applications such as the State Implementation Plan. A number of VOC control measures have been implemented in California in the last two decades, resulting in a change to the relative abundance of anthropogenic versus biogenic organic compounds. More recent long-term trend observations and intensive field studies provide significantly larger datasets than 20 years ago. As a result, updating the base case VOC mixture is both necessary and feasible.

The objective of this project has been to develop representative base reactive organic gas (ROG) mixtures based on the volatile organic compound (VOC) compositions for urban air-sheds in California and other areas of the United States. At this point, however, only the Los Angeles area has sufficient data to derive a ROG profile that meets data completeness needs. The project team compiled speciated VOC measurements and estimates of speciated VOC emissions from various urban areas before making this determination. The project included statistical analysis of these data to identify several representative ROG mixtures. The project included box modeling on the recommended mixtures to assess the sensitivity of maximum incremental reactivities (MIR) to base case composition. This final report includes documentation of the data analysis and modeling methodology, and recommendations for the base ROG mixtures to be used in future photochemical modeling.

3 Methods

3.1 Introduction

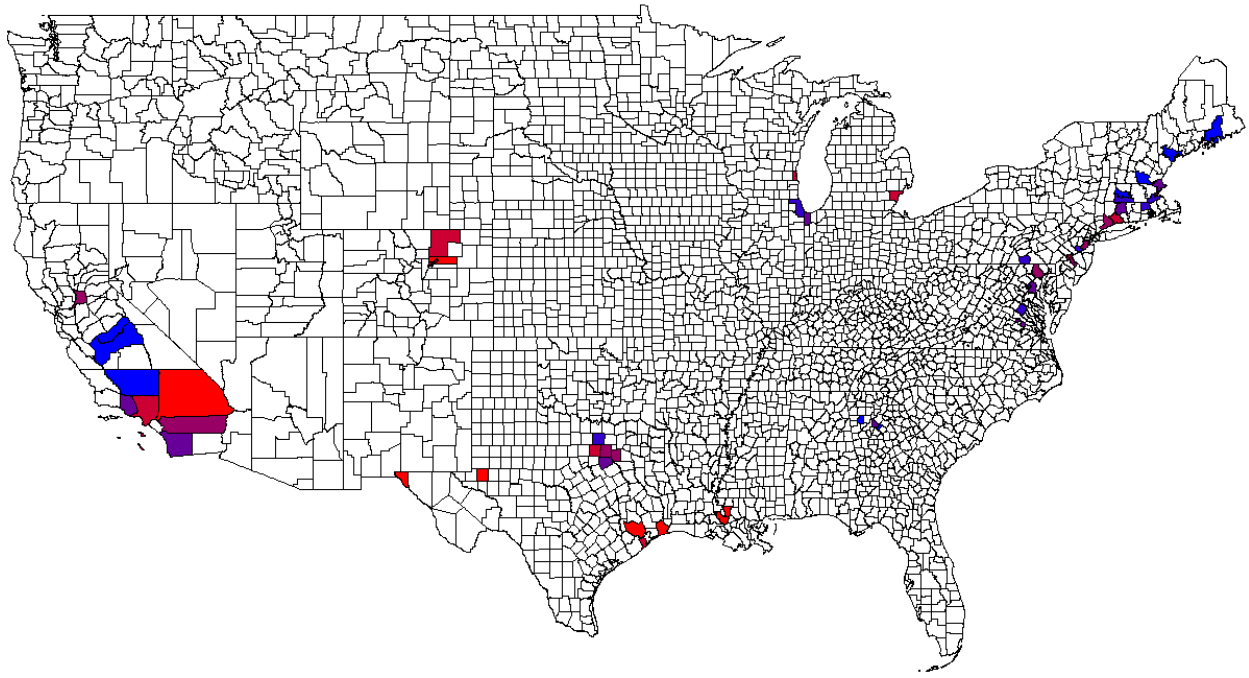
Two categories of data were collected for this study. Ambient air *measurements* were collected from a variety of sources including the EPA's Air Quality System database, the Central California Air Quality Studies Web site, and the Bay Area Air Quality Management District Technical Services Division. Emissions data *estimates* were downloaded from EPA's National Emissions Inventory Web site and from the ARB Web site.

3.2 Available Data Inventory

All of the Photochemical Assessment Monitoring Station (PAMS) data were downloaded from the U.S. EPA's Air Quality System (AQS) database for 2000 – 2009. Figure 1 shows the location of counties in America with ethylene concentration measurements in AQS for 2006. Some monitoring sites produced data from morning three-hour canister samples, while others produced data from hourly automated gas-chromatograph (auto-GC) instruments. Figure 1

mirrors the distribution of data used in McCarthy (2008), a study by Sonoma Technology, Inc. on the statistical distribution of PAMS species in 2004 – 2006.

Figure 1 Counties with data for ethylene in 2006



SAS programs were written to read the AQS download files and to extract data from particular geographic areas. Specific focus for this project has been the State of California. A table of monitor locations for California was created and used to make maps in Google Earth Pro. This same tool was used with Google Streetview to examine monitoring sites from street-side photos. Figure 2 shows the time history of available data from 30 sites with n-butane, ethylene, and benzene data in the AQS download. These three species represent three classes of hydrocarbons – alkanes, alkenes, and aromatics – so they serve as indicators for the presence of a broad suite of hydrocarbons.

Only air toxics data (benzene and 1,3-butadiene) were recovered from AQS for the San Francisco Bay area. A conference call was held with Mr. Michael Basso of the Bay Area Air Quality Management District Technical Services Division on November 12, 2009. Following the call, he emailed data not in AQS that include all the VOCs measured for air toxics purposes.

Mr. Leon Dolislager provided access to the Central California Air Quality Studies Web site from which the data from the 1997 Southern California Ozone Study (Fujita 1999) were downloaded. These included speciated VOC data for three sites in Los Angeles for 72 species.

Maps made with Google Earth Pro from an 80 kilometer look-down vantage point for the eight urban areas with the 30 sites listed in Figure 2 are shown in Figures 3 – 10.

Figure 2 Time history of data records for ethylene measurements in California in EPA's AQS database, July 2010.

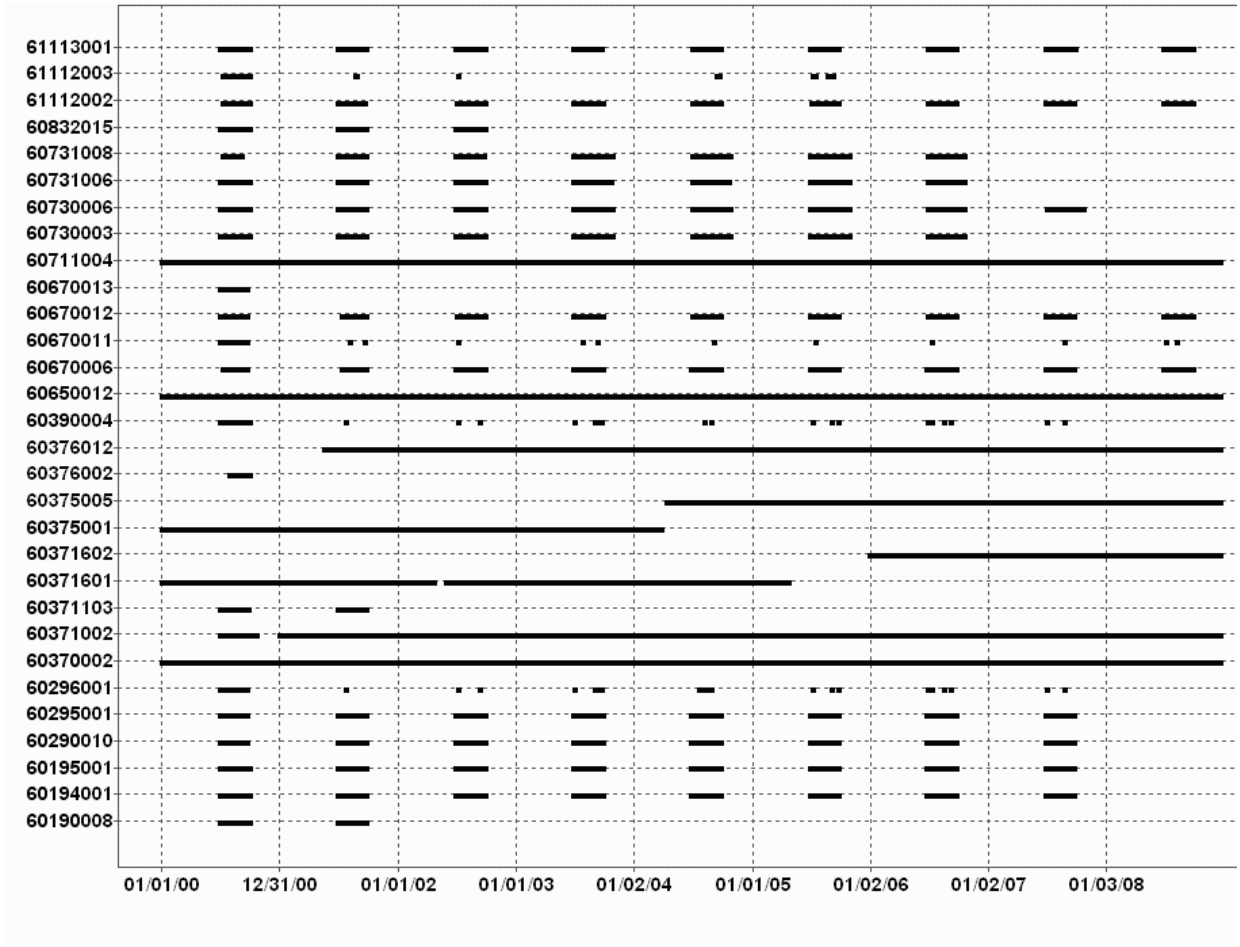


Figure 3 Four VOC sampling locations near Sacramento

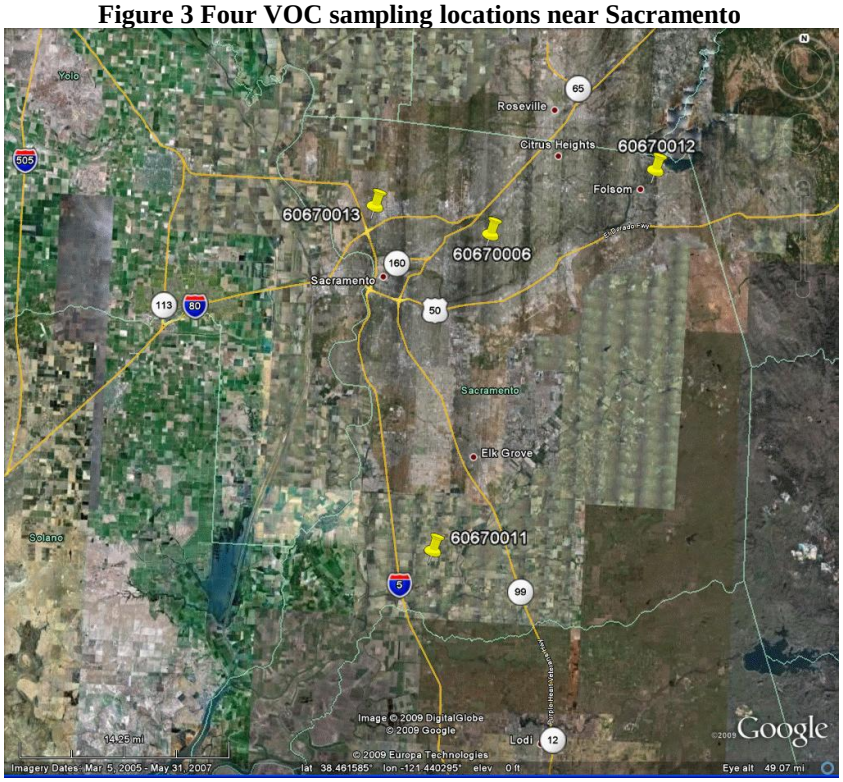


Figure 4 Four VOC sampling locations near Fresno

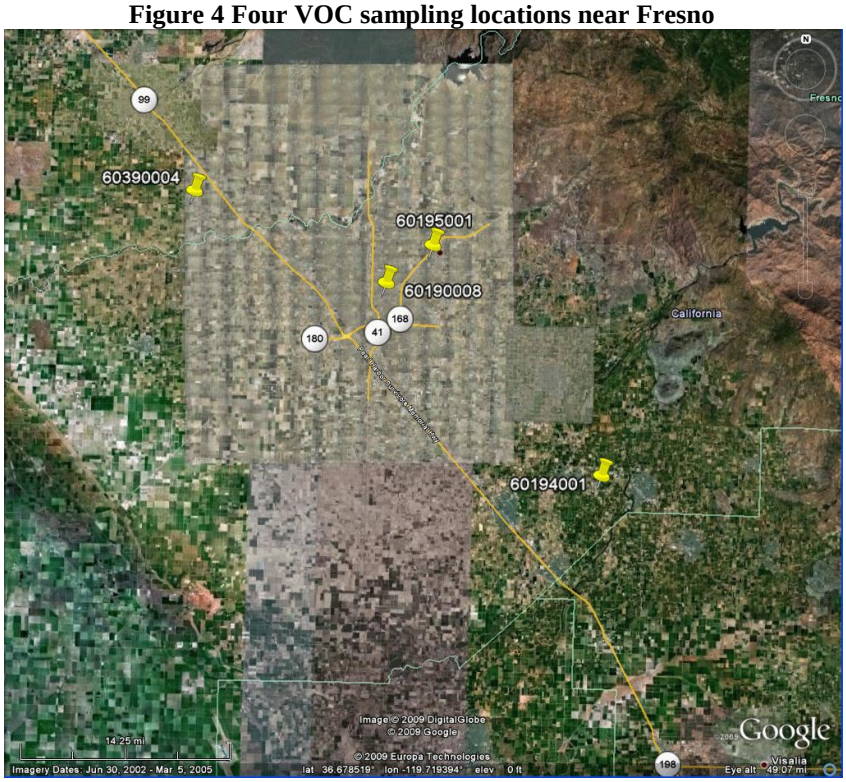


Figure 5 Three VOC sampling locations near Bakersfield

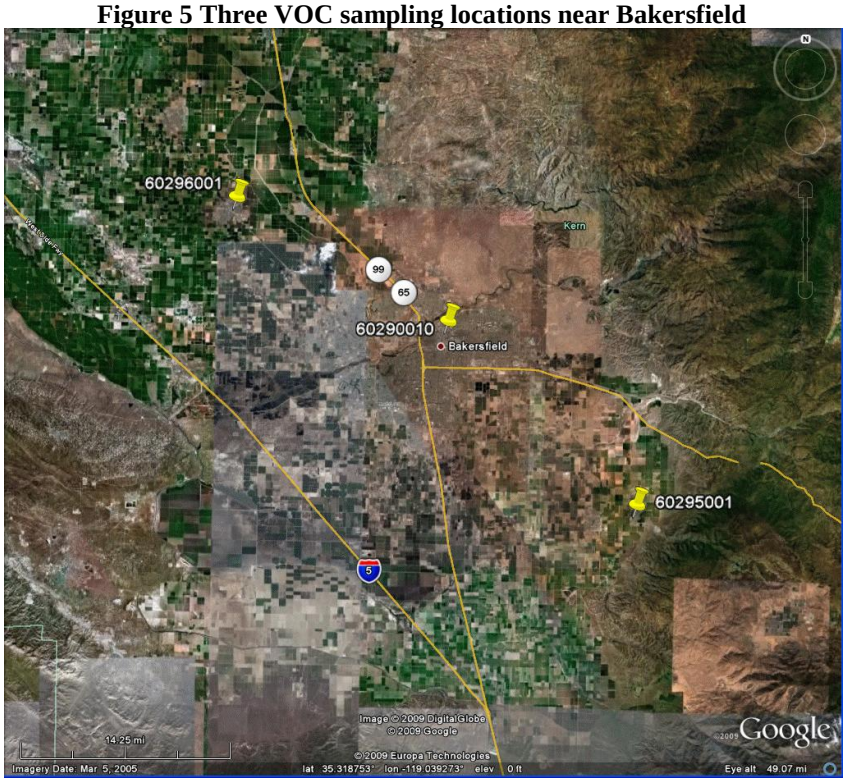


Figure 6 One VOC sampling location near Santa Barbara

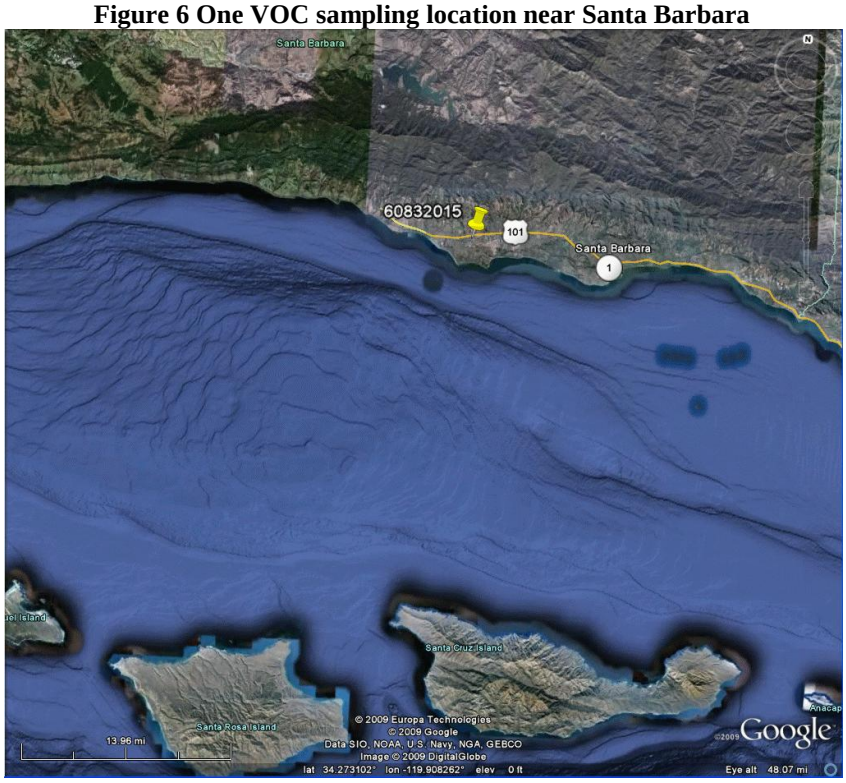


Figure 7 Six VOC sampling locations West LA region

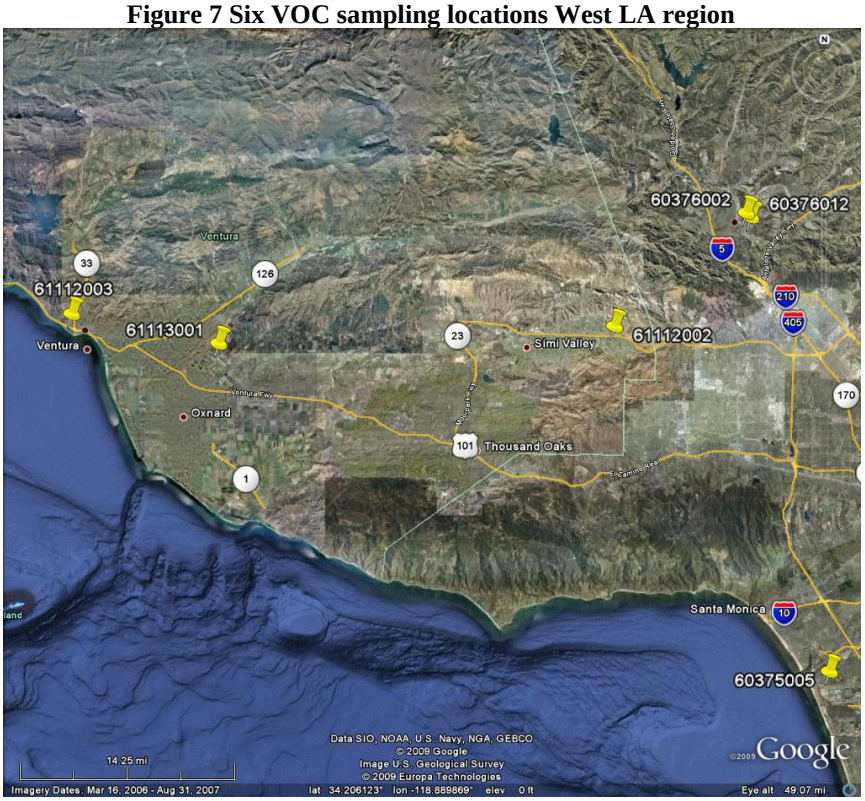


Figure 8 Seven VOC sampling locations East LA region

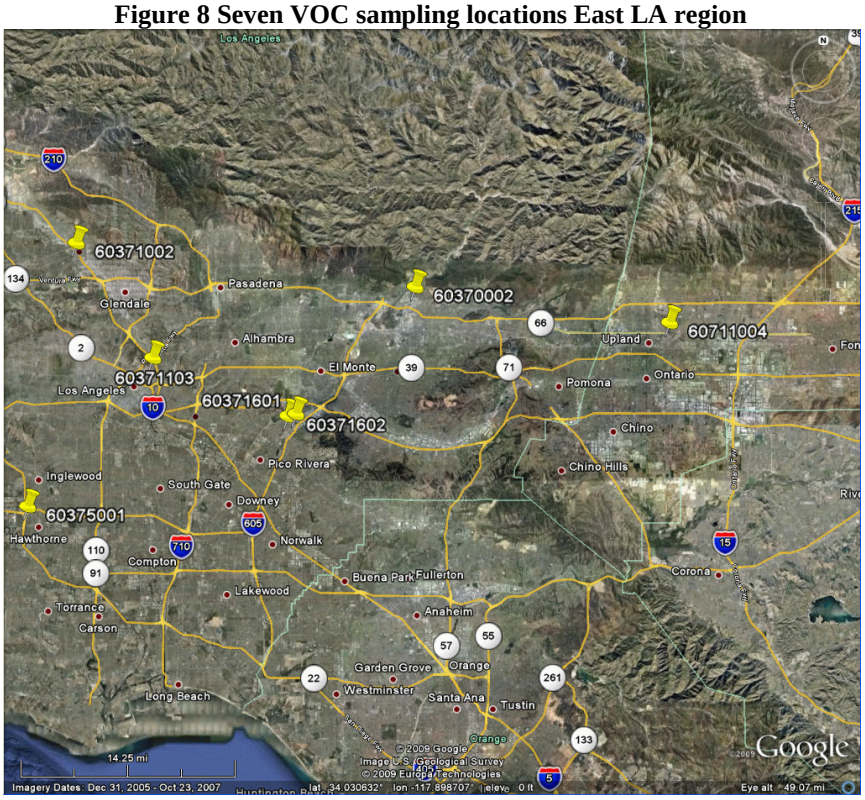


Figure 9 One VOC sampling site San Bernardino area

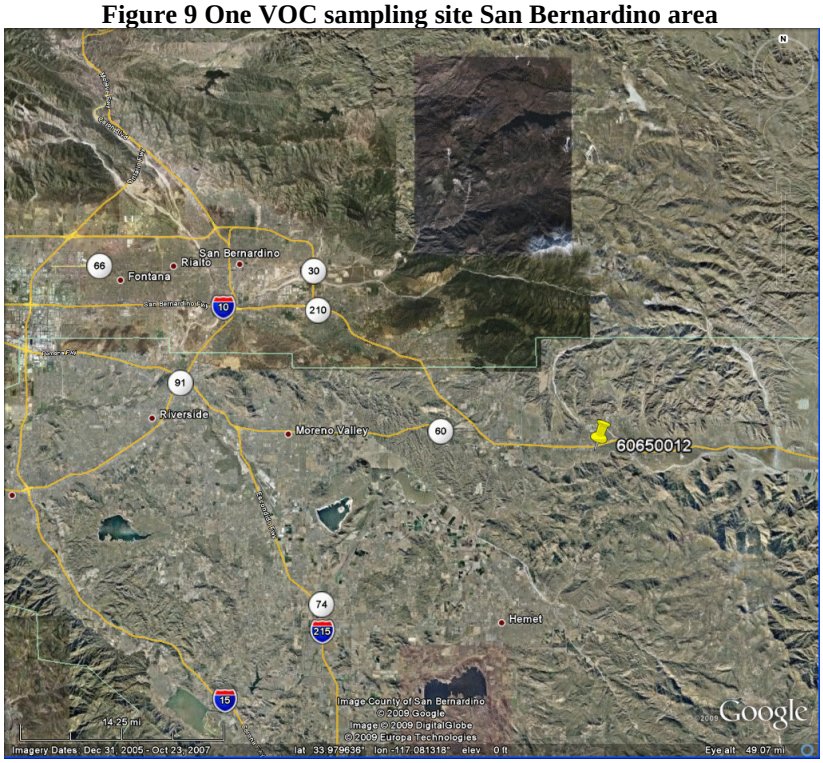
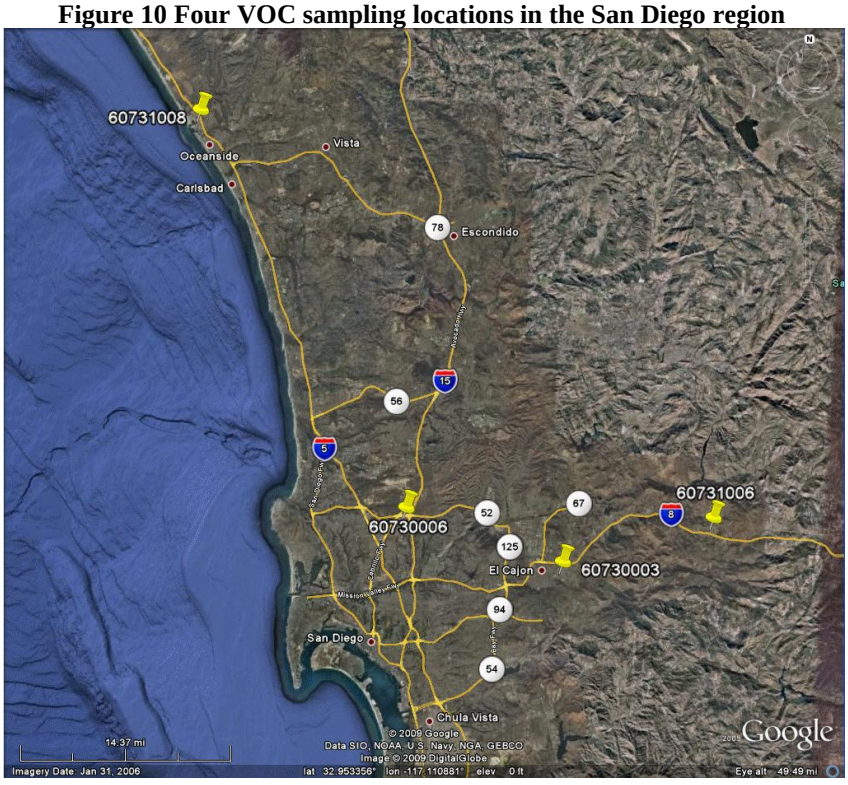


Figure 10 Four VOC sampling locations in the San Diego region



3.3 Emissions Inventory Data

EPA's 2005 National Emissions Inventory database was downloaded from http://www.epa.gov/ttnchie1/net/2005inventory.html, and the California data was extracted into a SAS dataset. This downloaded database was posted on the Web site under the heading of Tier Summaries, with the following descriptive text: *Tier summaries contain only criteria pollutants. The 42 category summaries contain both criteria and HAPS. Both the tier summaries and the 42 category summaries contain data from all data categories (point, nonpoint and mobile).* The data extracted were "42 category summaries" for individual counties in California.

Some exploratory analyses were performed on these data, and some simple comparisons were made with the Texas data. A principal component analysis suggests three factors explain most of the variability in the relative ratios of emitted species among California counties. Principal component analysis (PCA) can be used to combine a large number of variables into a smaller set of factors based on how well variables are correlated with each other. Finer manipulations (called "rotations") can improve the interpretability of the results. The rotated correlations reflecting the factors found with PCA appears in the appendix to this report in Table 1. Most species have their "weight" in factor 1, meaning that the highlighted species all tend to be higher-than-average or lower-than-average together in the same counties. A handful of species have highest weight in factor 2, while only two (Methyl Bromide and 1,3-Dichloropropene) have maximum weight in factor 3. The factor scoring for each county for the three factors appears in Figures 11, 12, and 13. Some notes for geographic characterization for each factor is listed with the figures.

The UT team working this project has held informal talks on the quality of the NEI and the level of detail and quality of data needed for the box modeling in Task 4. UT and Air Resources Board staff have exchanged emails regarding using other emission inventories. The purpose of the PCA with the NEI is simply to highlight some of the differences to be expected in the likely ambient mixtures in, say, agricultural vs. urban vs. undeveloped parts of the state.

A more detailed and more accurate emissions inventory was provided by CARB staff. The annual organic gas emission inventories for 2008 for Los Angeles County and for the State of California were both provided. Both EIs are reported by source categories (3,377 categories for the State, 2,465 categories for LA County), along with the speciation profile of each source expressed as mass fraction by Storage and Retrieval of Aerometric Data (SAROAD) code. Annual emissions from the two geographic regions were speciated first into SAROAD code, after which each resulting profile was processed by the emitdb.xls tools (Carter, 2010b).

Table 1 Rotated principal component scores for NEI data from California counties

Rotation Correlations (Structure)

Variable	RT1_2	RT2_2	RT3_2
Toluene	0.92	0.35	0.10
Formaldehyde	0.74	0.60	0.21
Benzene	0.76	0.51	0.39
Methyl_Chloroform	0.93	0.13	0.03
__2_4_Trimethylpentane	0.95	0.29	0.07
m_Xylene	0.94	0.31	0.06
Methanol	0.95	0.27	0.06
Hexane	0.94	0.30	0.13
Methylene_Chloride	0.87	0.31	0.05
Acetaldehyde	0.83	0.51	0.15
o_Xylene	0.94	0.32	0.06
Ethyl_Benzene	0.95	0.31	0.06
Methyl_Ethyl_Ketone	0.94	0.28	0.09
Tetrachloroethylene	0.95	0.28	0.07
Methyl_Bromide	0.07	0.14	0.98
Ethylene_Glycol	0.87	0.33	0.10
Xylenes__Mixture_of_o__m__and_p_	0.89	0.42	0.10
Methyl_Tert_Butyl_Ether	0.95	0.26	0.10
__3_Butadiene	0.69	0.70	0.10
Propionaldehyde	0.60	0.66	-0.05
Methyl_Isobutyl_Ketone	0.92	0.31	0.08
Styrene	0.80	-0.01	0.03
Acrolein	0.10	0.88	0.32
Glycol_Ethers	0.94	0.24	0.04
__3_Dichloropropene	0.06	0.14	0.99
Naphthalene	0.94	0.31	0.09
__4_Dichlorobenzene	0.96	0.26	0.06
p_Xylene	0.95	0.28	0.08
Trichloroethylene	0.95	0.26	0.13

Figure 11 Color-coded scores on rotated PCA factor 1 by county (strongly urban)

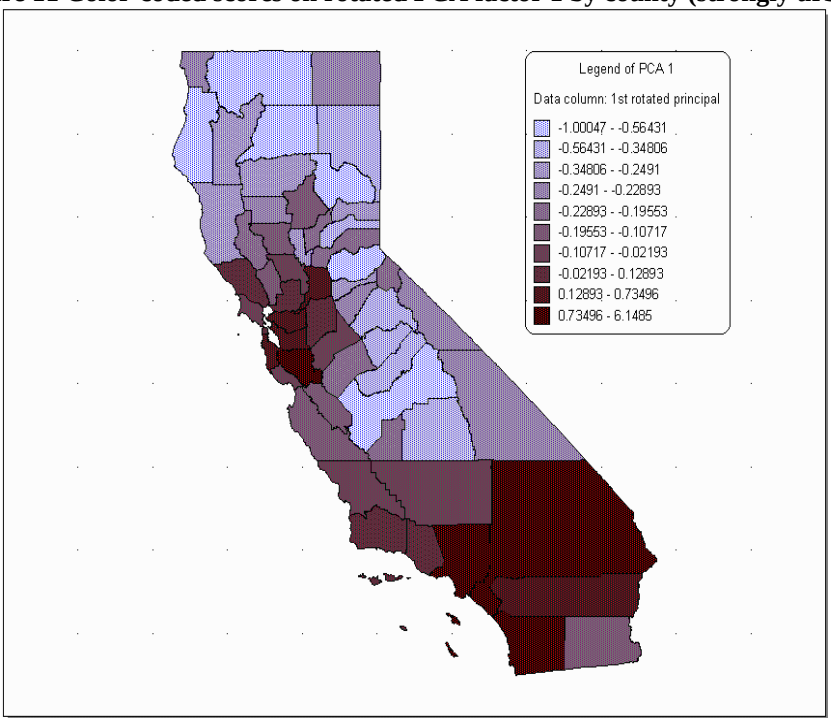


Figure 12 Color-coded scores on rotated PCA factor 2 by county (strong on Fresno, Shasta, Humboldt, Siskiyou counties)

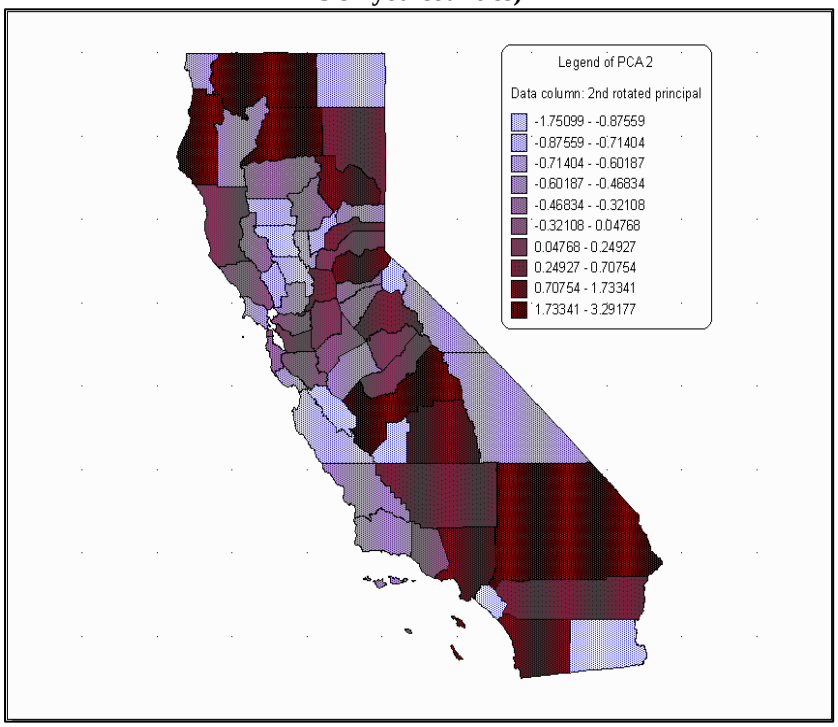
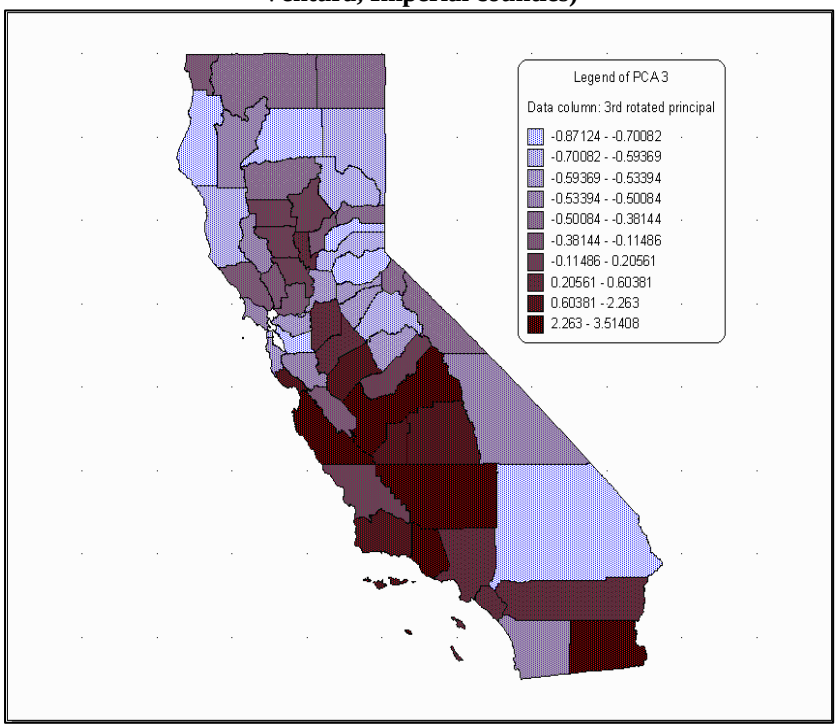


Figure 13 Color-coded scores on rotated PCA factor 3 by county (strong on Fresno, Monterey, Kern, Ventura, Imperial counties)



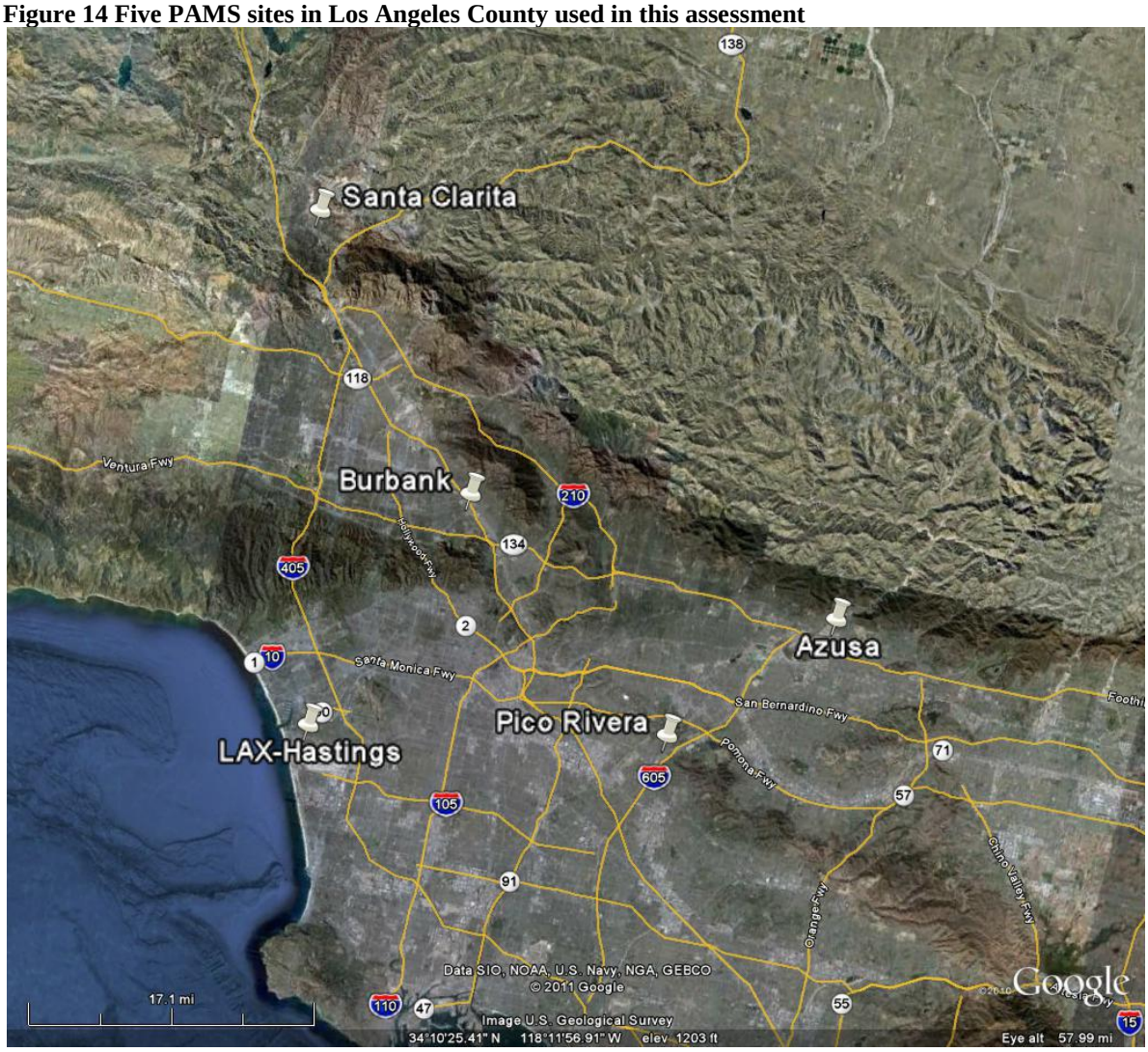
3.4 An Examination of Los Angeles County Hydrocarbon Data

Using the Photochemical Assessment Monitoring Station (PAMS) data downloaded from the EPA's Air Quality System (AQS) database in 2009 and 2010, several forms of exploratory analyses have been performed. The EPA AQS Web site http://www.epa.gov/ttn/airs/airsaqs/detaildata/downloadaqsdata.htm allows bulk downloads of AQS data in compressed ASCII text files for which SAS programs were written to input and analyze the data. For the State of California, some 2.9 million records from 84 sites are contained in the data sets. The most common parameters in the data sets are total nonmethane hydrocarbon concentrations and "Sum of PAMS Target Compounds," the most common concentration units are in parts per billion carbon (ppbC), and the most common sample duration is three hours. Los Angeles County has the largest share of data by county. In selecting only 3-hour sample speciated data in ppbC units, some 1.7 million records are available. By further restricting the data to summer (months July, August, September) and the county of Los Angeles, some 0.9 million records are available. These data have been further restricted to the period from 2006 through 2009, for which the yield is 335,587 observations from five monitor sites. Only one site (Pico Rivera #2) was found to have 2009 data in the downloaded data set. Later AQS database was accessed and queried and 2009 data for the other four sites plus data for a new sixth site were recovered. However, for the characterization analysis described in this section for the report, only the aforementioned 335,587 observation, 5 site dataset is discussed. This data set was transposed to provide multivariate samples by site, date, and time, which produced 6300 records from which to assess the mixture of hydrocarbons in Los Angeles air. The five monitoring sites with data during this period used in the assessment are shown in Figure 14, and detailed information about each is available by appending the PDF file name in the Web Site column to the link at the bottom of the table in Table 2. The full 2009 data set and the sixth PAMS site are used in later portions of this report.

Table 2 Five PAMS sites in Los Angeles County used in this analysis

name	AQS	Site Address	latitude	longitude	elevation (m)	Web Site
Azusa	060370002	803 N. Loren Av, Azusa	34.136	-117.924	187	Azusa.pdf
Burbank	060371002	228 W Palm Ave, Burbank	34.176	-118.317	171	Burbank.pdf
Pico Rivera #2	060371602	4144 San Gabriel River Pkwy, Pico Rivera	34.010	-118.069	58	PicoRivera.pdf
LAX - Hastings	060375005	7201 W Westchester Pkwy, Los Angeles	33.955	-118.430	37	LAXHastings.pdf
Santa Clarita-Placerita	060376012	22224 Placerita Canyon Rd, Santa Clarita	34.383	-118.528	386	SantaClarita.pdf
http://www.aqmd.gov/tao/AQ-Reports/AQMonitoringNetworkPlan/						

Figure 14 Five PAMS sites in Los Angeles County used in this assessment



Using the data from these five sites, the diurnal patterns for various species and the overall morning mean hydrocarbon mixture can be calculated. As this is only an initial exploratory analysis, no conclusions are offered. However, Figures 15 and 16 show the estimated mean concentrations of 54 hydrocarbon species in two manners. Figure 15 shows the mean concentrations in stacked bar charts in ppbC units. This shows a range in total hydrocarbons between 100 and 400 ppbC among the five sites. Figure 16 shows a stacked bar chart in approximate percentage mass terms. This shows the variability in composition among species. Toluene concentrations at Burbank appear to be notable. As is explained in the Appendix to this report, data from the Burbank site for the year 2007 have been excluded.

Figures 17 – 21 show the median diurnal patterns for 54 hydrocarbon species at all the five sites. The median was used to reduce the effect of outliers. Isoprene peaks late in the day, at concentrations not observable in the figure because of scale, the exception being Figure 21 for the less urban Santa Clarita site. The species with highest ppbC concentration are propane, ethane, isopentane, toluene, and n-butane. Tables of the median diurnal pattern data appear at the

below in Tables 4 – 8. The columns in these tables do not sum to equal the total nonmethane organic median owing to the contribution of other unclassified species.

Figure 15 Mean concentrations of 54 hydrocarbon species 2006 to 2008 or 2009 in July – Sept., 5:00-7:59 PST, Los Angeles County

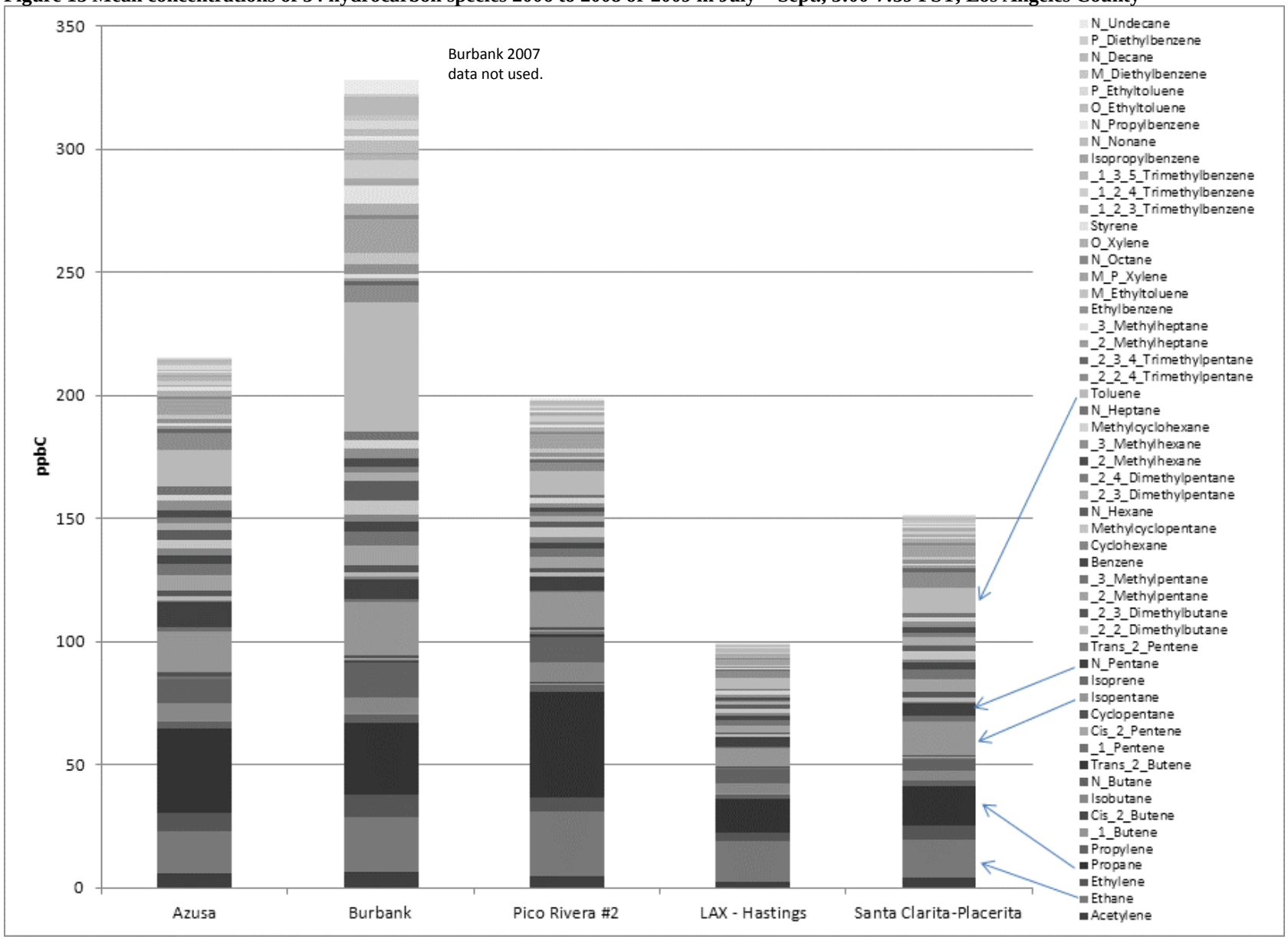


Figure 16 Mean percentage compositions of 54 hydrocarbon species 2006 to 2008 or 2009 in July – Sept., 5:00-7:59 PST, Los Angeles County

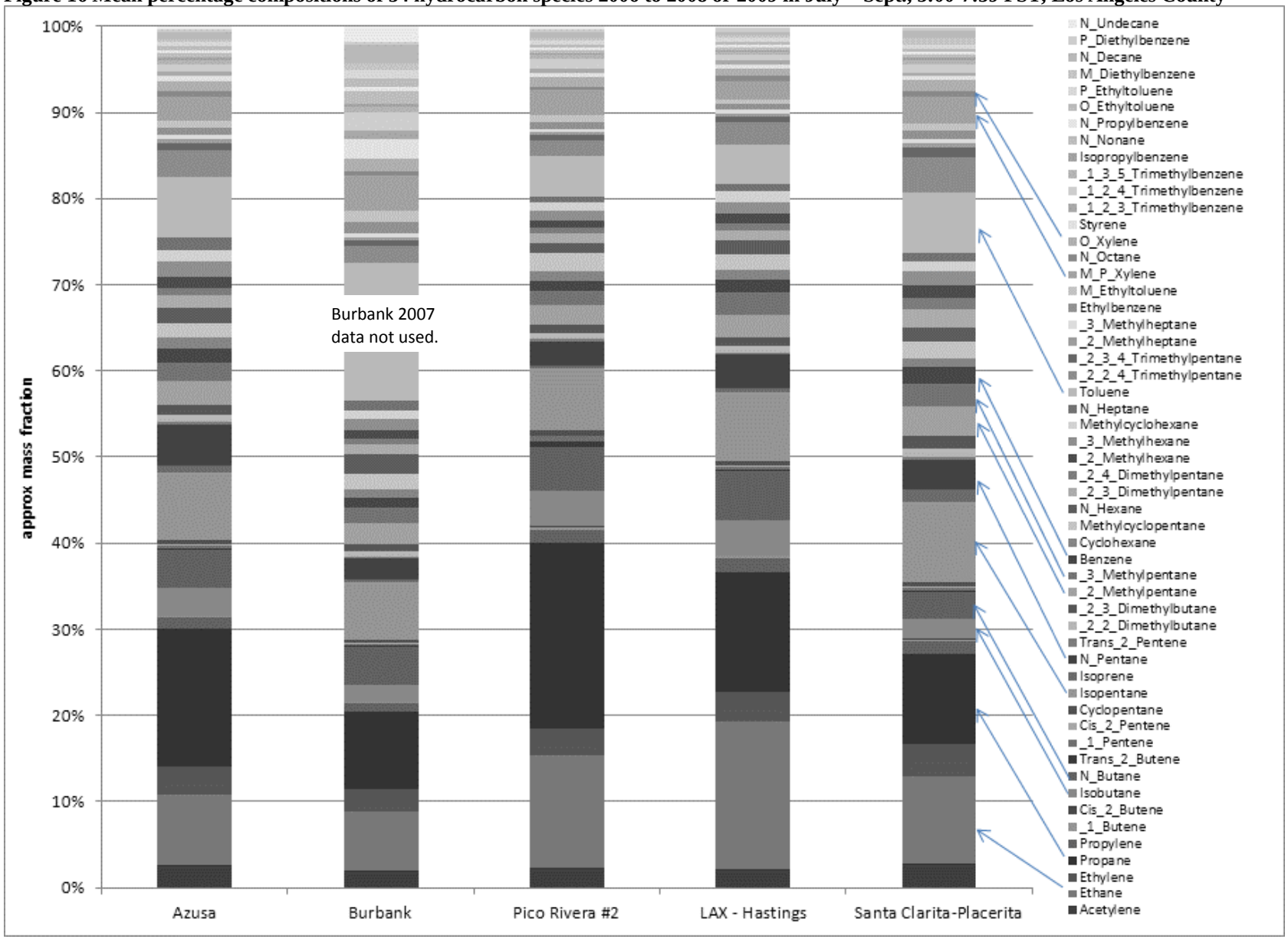


Table 3 Mean concentrations of 54 hydrocarbon species 2006 to 2008 or 2009 in July – Sept., 5:00-7:59 PST, (early-mid morning) Los Angeles County

Carbons	Species	Azusa	Burbank*	Pico Rivera #2	LAX - Hastings	Santa Clarita-Placerita
2	**Acetylene**	5.56	6.63	4.58	2.14	4.13
2	**Ethane**	**17.59**	**22.22**	**26.15**	**16.98**	**15.48**
2	**Ethylene**	7.17	8.86	6.09	3.33	5.68
3	**Propane**	**34.59**	**29.19**	**42.89**	**13.83**	**15.76**
3	**Propylene**	2.86	3.31	2.74	1.49	2.24
4	**1-Butene**	0.31	0.57	0.61	0.32	0.31
4	**Cis-2-Butene**	0.15	0.26	0.34	0.09	0.14
4	**Isobutane**	**6.95**	**6.17**	**8.16**	**4.09**	**3.54**
4	**N-Butane**	**9.62**	**14.56**	**10.04**	**5.65**	**4.73**
4	**Trans-2-Butene**	0.12	0.37	1.58	0.08	0.14
5	**1-Pentene**	0.67	0.58	1.00	0.40	0.55
5	**Cis-2-Pentene**	0.36	0.45	0.28	0.11	0.25
5	**Cyclopentane**	1.31	1.15	1.28	0.54	0.76
5	**Isopentane**	**16.77**	**21.96**	**14.24**	**7.88**	**13.94**
5	**Isoprene**	1.67	0.97	0.66	0.37	2.36
5	**N-Pentane**	**10.39**	**8.16**	**5.50**	**3.89**	**5.19**
5	**Trans-2-Pentene**	0.59	0.88	0.45	0.23	0.51
6	**2,2-Dimethylbutane**	1.92	1.92	1.41	0.79	1.55
6	**2,3-Dimethylbutane**	2.24	2.73	1.97	0.98	2.14
6	**2-Methylpentane**	6.00	7.98	4.54	2.63	5.11
6	**3-Methylpentane**	4.79	5.94	3.21	2.50	4.02
6	**Benzene**	3.39	3.87	2.47	1.46	3.01
6	**Cyclohexane**	2.83	2.86	2.06	1.11	1.37
6	**Methylcyclopentane**	3.67	5.96	4.15	1.88	2.99
6	**N-Hexane**	3.65	7.49	2.33	1.56	2.55
7	**2,3-Dimethylpentane**	3.21	3.83	2.37	1.20	3.28
7	**2,4-Dimethylpentane**	1.84	2.32	1.31	0.80	1.95
7	**2-Methylhexane**	2.93	3.19	1.73	1.06	2.16
7	**3-Methylhexane**	3.92	4.20	2.05	1.23	2.42
7	**Methylcyclohexane**	2.73	3.26	2.11	1.29	1.86
7	**N-Heptane**	3.07	3.53	1.22	0.86	1.49
7	**Toluene**	**15.15**	**52.67**	**9.52**	**4.59**	**10.48**
8	**2,2,4-Trimethylpentane**	6.67	6.65	3.57	2.49	6.18
8	**2,3,4-Trimethylpentane**	1.82	2.06	1.17	0.64	1.71
8	**2-Methylheptane**	1.01	0.94	0.69	0.40	0.76
8	**3-Methylheptane**	1.00	1.41	0.73	0.39	0.81
8	**Ethylbenzene**	1.91	4.29	1.71	0.66	1.54
8	**M-Ethyltoluene**	1.76	4.49	1.45	0.55	1.12

Carbons	Species	Azusa	Burbank*	Pico Rivera #2	LAX - Hastings	Santa Clarita-Placerita
8	**M/P-Xylene**	6.07	13.59	5.84	2.15	4.88
8	**N-Octane**	1.29	1.66	0.82	0.53	0.91
8	**O-Xylene**	2.56	4.80	2.24	0.91	2.05
8	**Styrene**	1.22	7.56	0.79	0.37	0.54
9	**1,2,3-Trimethylbenzene**	1.00	2.96	0.96	0.48	0.72
9	**1,2,4-Trimethylbenzene**	1.77	7.02	2.43	0.65	1.46
9	**1,3,5-Trimethylbenzene**	1.36	2.35	0.80	0.33	0.55
9	**Isopropylbenzene**	0.47	0.78	0.36	0.20	0.67
9	**N-Nonane**	1.31	4.82	0.70	0.31	0.44
9	**N-Propylbenzene**	0.64	1.77	0.62	0.29	0.41
9	**O-Ethyltoluene**	0.80	3.24	0.81	0.37	0.50
9	**P-Ethyltoluene**	1.16	3.07	0.97	0.43	0.84
10	**M-Diethylbenzene**	0.72	2.62	0.51	0.40	1.29
10	**N-Decane**	1.80	7.27	1.40	0.35	1.18
10	**P-Diethylbenzene**	0.67	1.10	0.49	0.39	0.49
11	**N-Undecane**	0.81	5.75	0.84	0.24	0.28

‘* Data from 2007 not used for Burbank

Figure 17 Median diurnal pattern at Azusa, 2006 – 2008, 54 hydrocarbon species

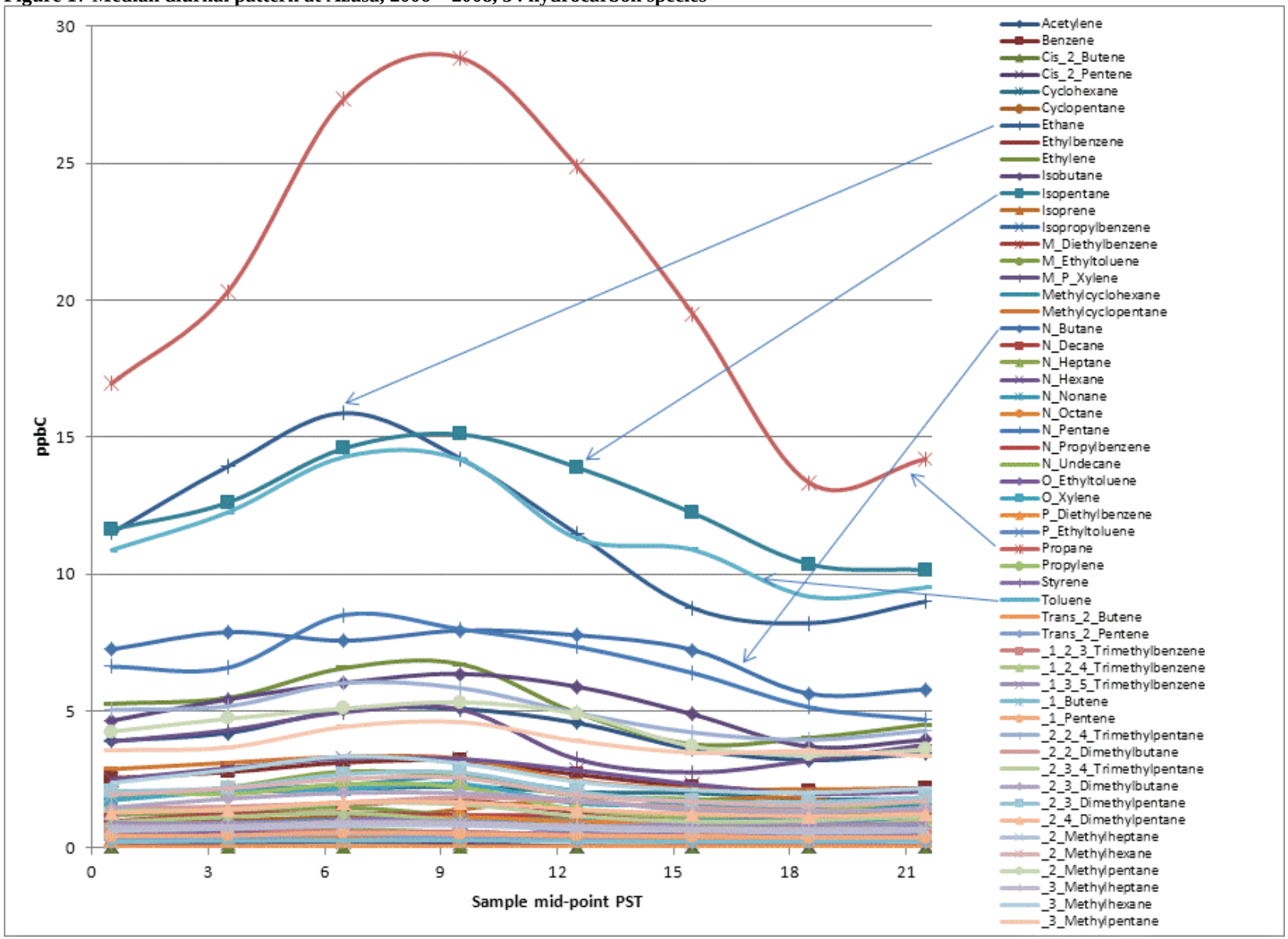


Figure 18 Median diurnal pattern at Burbank, 2006 – 2008, 54 hydrocarbon species

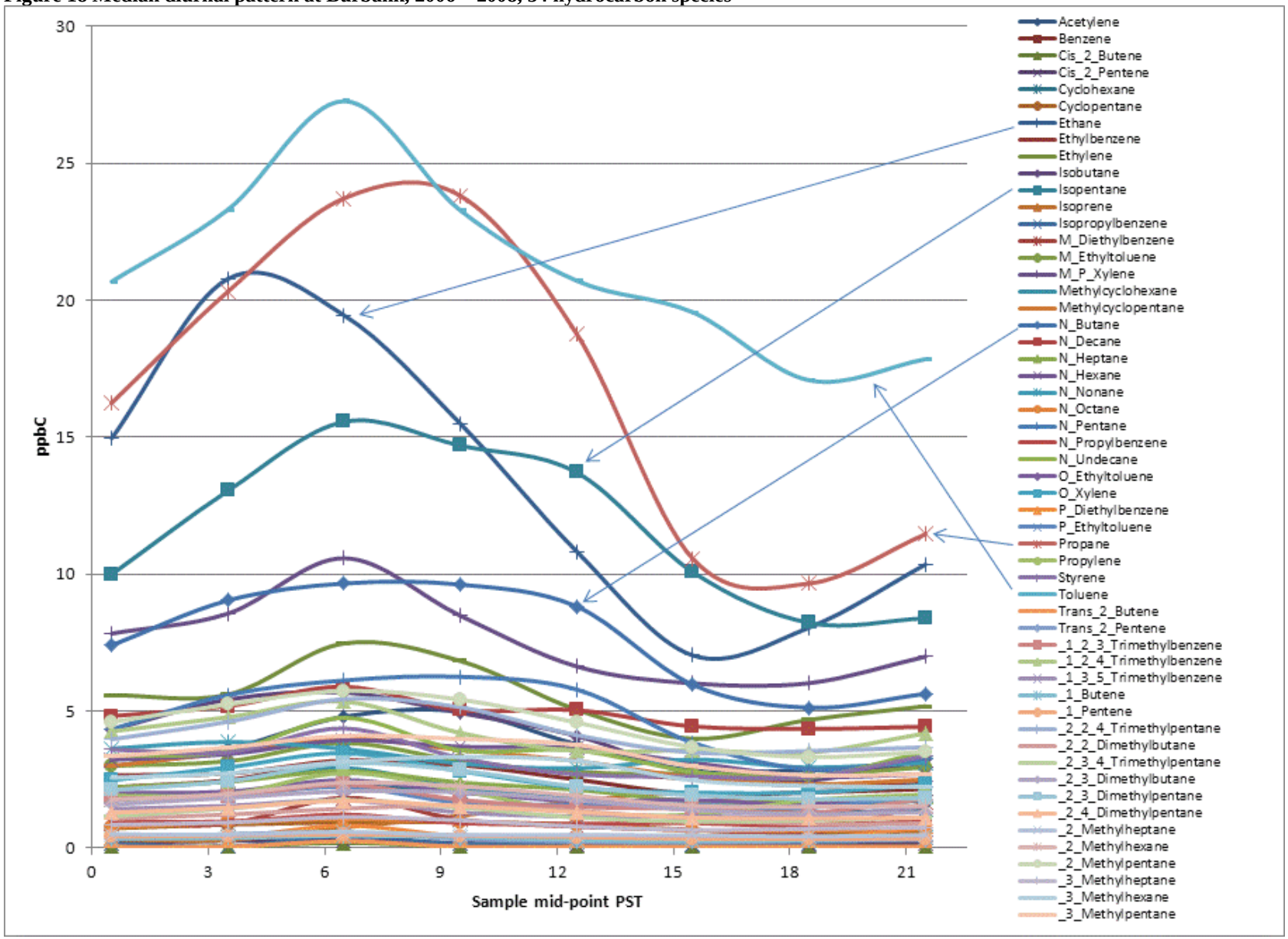


Figure 19 Median diurnal pattern at Pico, 2006 – 2008, 54 hydrocarbon species

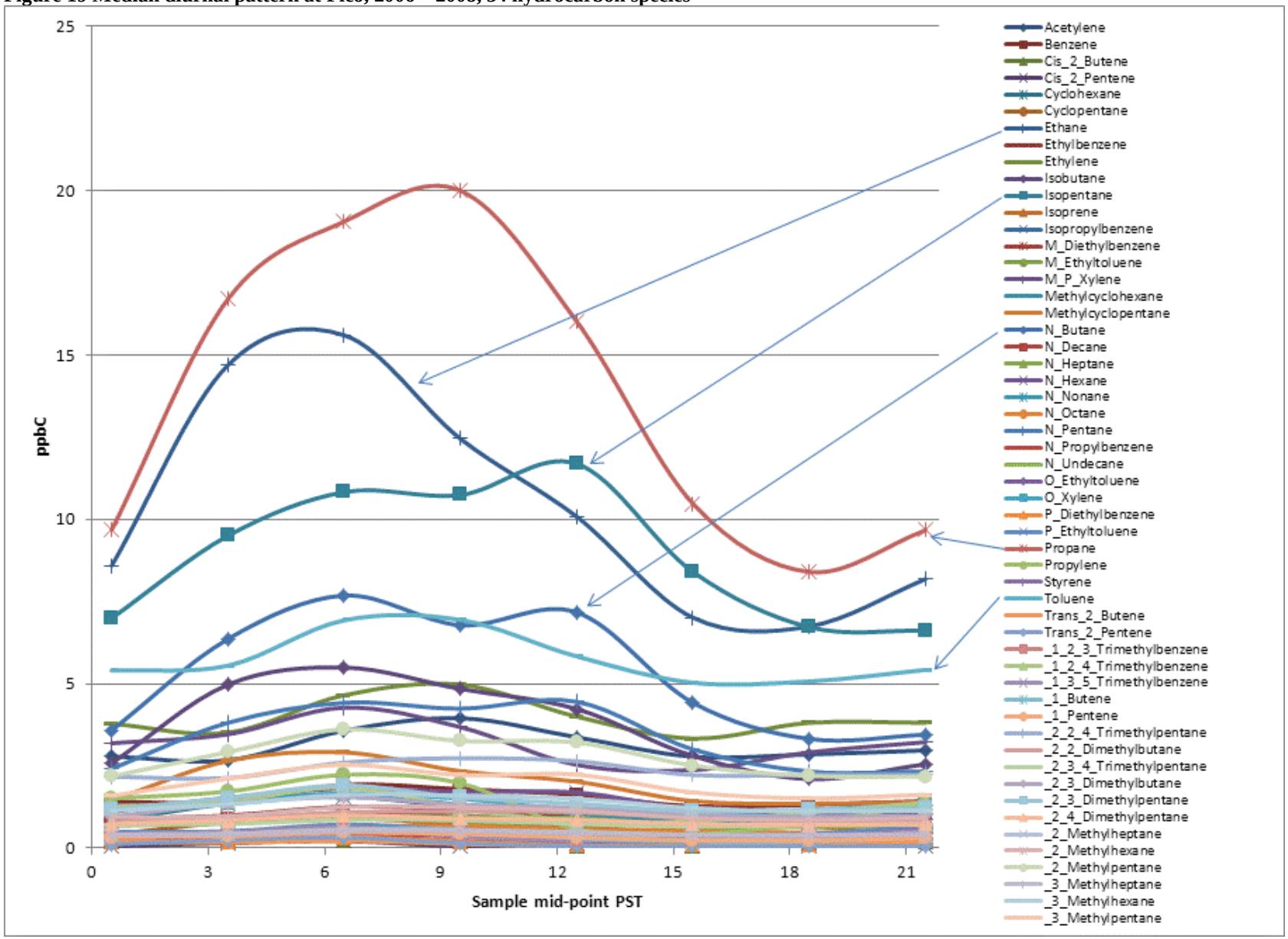


Figure 20 Median diurnal pattern at LAX, 2006 – 2008, 54 hydrocarbon species

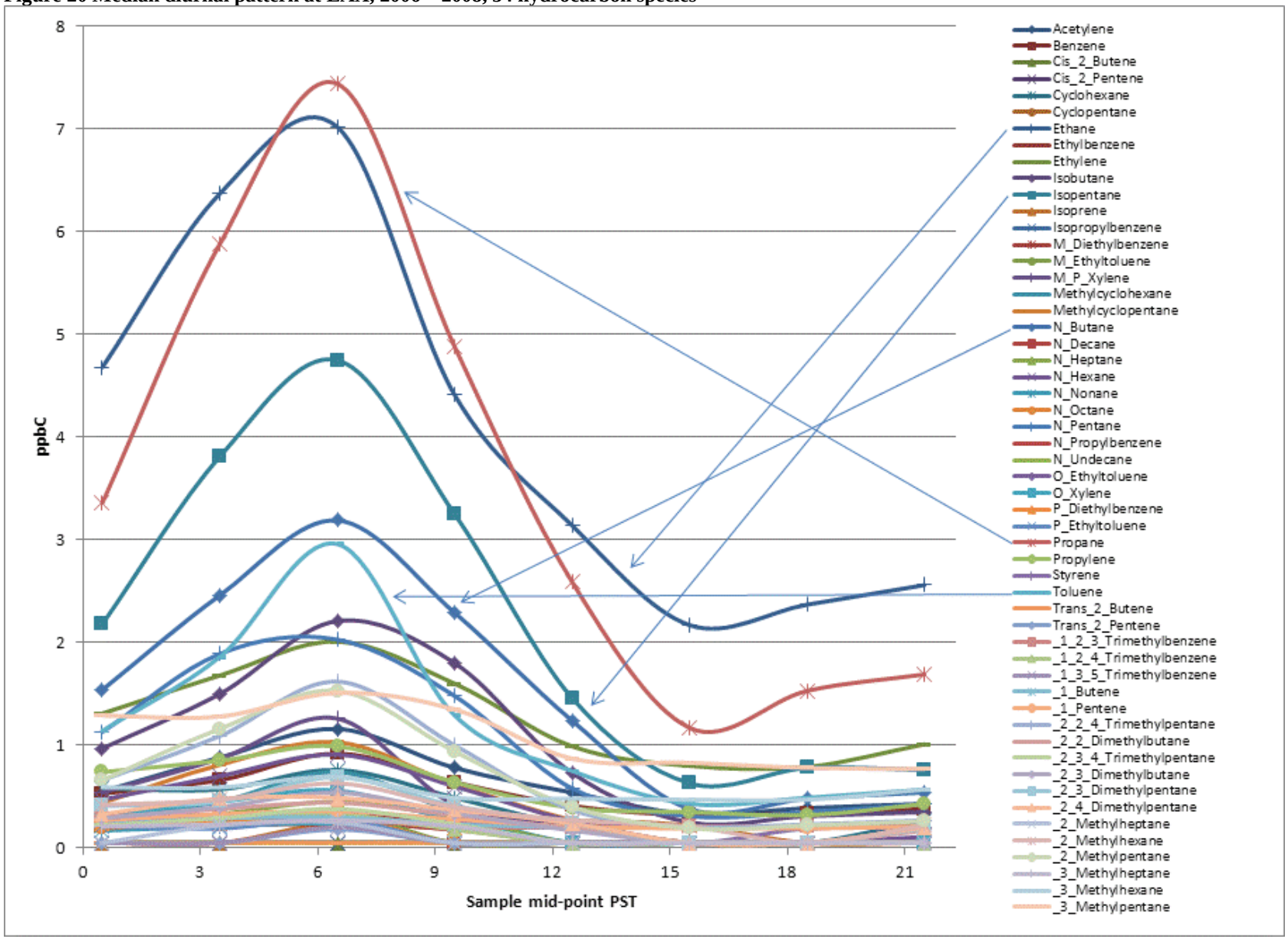


Figure 21 Median diurnal pattern at Santa Clarita, 2006 – 2008, 54 hydrocarbon species

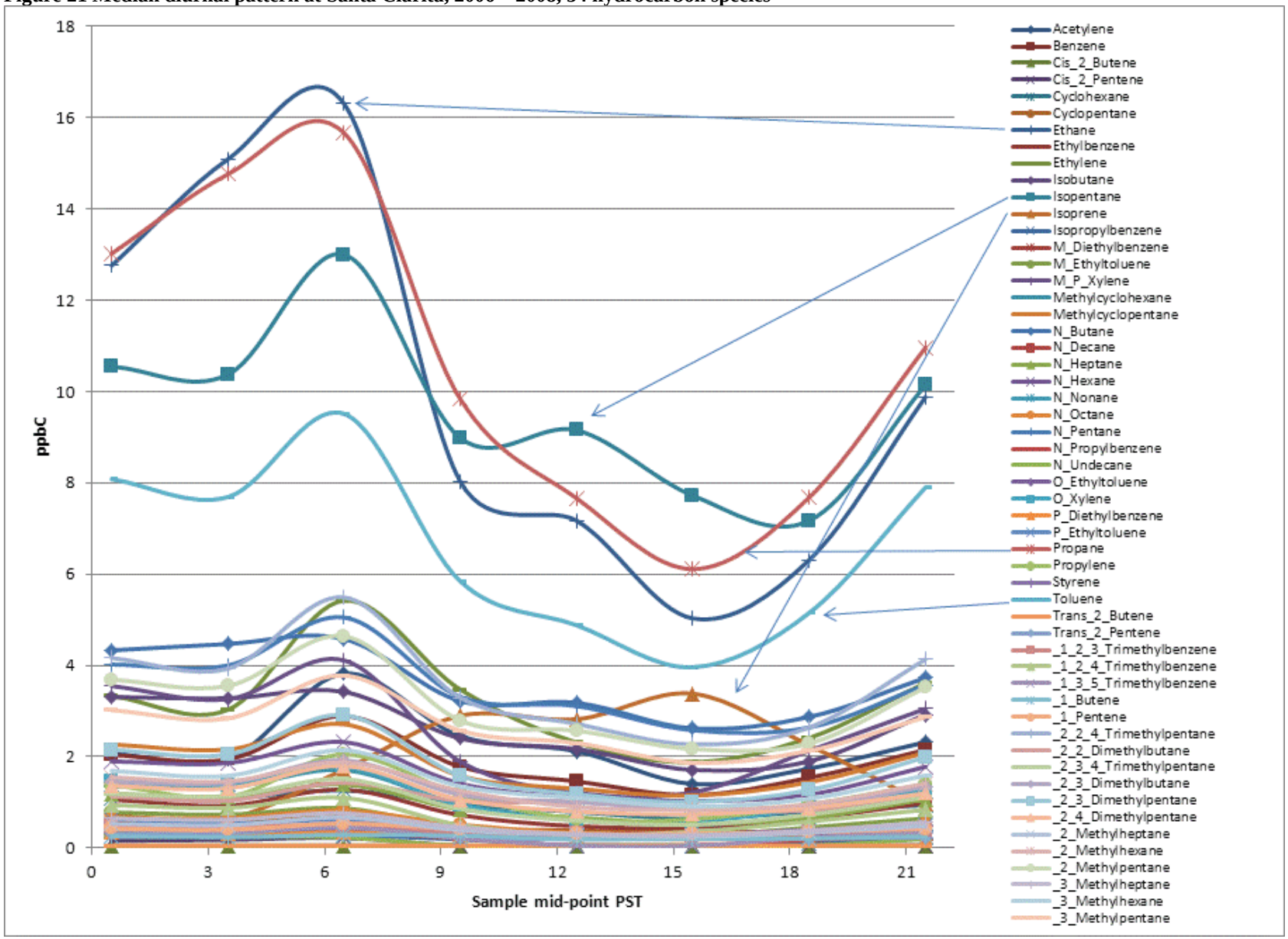


Table 4 Azusa median ppbC concentrations by sample mid-point (e.g., 23 PST time-tagged 3-hour sample from 23:00-1:59 has mid-point 0:30 PST)

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Num Obs	71	75	76	76	76	74	73	72
Acetylene	3.91	4.20	5.04	5.08	4.57	3.61	3.21	3.46
Benzene	2.55	2.77	3.12	3.18	2.68	2.25	2.09	2.19
Cis_2_Butene	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Cis_2_Pentene	0.05	0.19	0.23	0.18	0.05	0.05	0.05	0.05
Cyclohexane	2.05	2.05	2.15	2.24	2.04	2.00	1.79	1.80
Cyclopentane	0.93	1.00	1.12	1.02	0.97	0.87	0.70	0.71
Ethane	11.51	13.93	15.88	14.22	11.47	8.76	8.21	9.00
Ethylbenzene	1.23	1.40	1.57	1.74	1.31	1.05	1.09	1.18
Ethylene	5.27	5.48	6.57	6.72	4.93	3.79	4.02	4.51
Isobutane	4.65	5.43	6.03	6.36	5.89	4.88	3.70	3.95
Isopentane	11.63	12.61	14.59	15.09	13.90	12.23	10.36	10.14
Isoprene	0.71	0.78	0.97	1.41	1.80	1.76	1.80	1.03
Isopropylbenzene	0.33	0.38	0.41	0.42	0.39	0.34	0.33	0.34
M_Diethylbenzene	0.36	0.39	0.53	0.49	0.46	0.38	0.36	0.36
M_Ethyltoluene	1.21	1.32	1.48	1.19	1.05	1.02	1.21	1.19
M_P_Xylene	3.89	4.30	4.96	5.06	3.24	2.76	3.19	3.77
Methylcyclohexane	1.85	2.13	2.29	2.61	2.08	1.57	1.46	1.53
Methylcyclopentane	2.88	3.11	3.33	3.27	2.46	2.17	2.14	2.18
N_Butane	7.25	7.88	7.57	7.94	7.77	7.23	5.63	5.79
N_Decane	0.98	1.25	1.28	1.20	1.19	1.21	1.07	1.02
N_Heptane	1.75	2.21	2.79	2.60	1.91	1.79	1.57	1.69
N_Hexane	2.49	2.92	3.27	3.25	2.84	2.33	1.98	2.06
N_Nonane	0.77	0.87	1.05	1.07	1.00	1.01	1.03	0.96
N_Octane	0.76	0.82	0.91	1.13	0.96	0.95	0.84	0.92
N_Pentane	6.62	6.58	8.51	7.99	7.35	6.39	5.14	4.68
N_Propylbenzene	0.45	0.50	0.54	0.57	0.49	0.47	0.48	0.44
N_Undecane	0.43	0.49	0.67	0.55	0.44	0.50	0.52	0.42
O_Ethyltoluene	0.51	0.58	0.61	0.57	0.48	0.44	0.47	0.48
O_Xylene	1.75	2.06	2.14	2.34	1.63	1.58	1.50	1.75
P_Diethylbenzene	0.35	0.39	0.44	0.43	0.33	0.34	0.37	0.36
P_Ethyltoluene	0.83	0.93	0.97	0.92	0.81	0.80	0.90	0.83
Propane	16.96	20.32	27.35	28.85	24.90	19.50	13.34	14.20
Propylene	2.09	1.97	2.33	2.22	1.40	1.16	1.34	1.78
Styrene	0.60	0.69	1.04	1.00	0.57	0.49	0.50	0.49
Toluene	10.88	12.26	14.28	14.18	11.31	10.89	9.18	9.51

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Trans_2_Butene	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Trans_2_Pentene	0.27	0.38	0.49	0.36	0.28	0.23	0.23	0.24
_1_2_3_Trimethylbenzene	0.61	0.70	0.61	0.60	0.47	0.47	0.71	0.65
_1_2_4_Trimethylbenzene	0.95	1.14	1.28	1.00	0.70	0.77	0.70	1.06
_1_3_5_Trimethylbenzene	0.91	0.90	0.96	0.97	0.80	0.88	0.85	0.89
_1_Butene	0.23	0.26	0.27	0.28	0.25	0.24	0.25	0.28
_1_Pentene	0.45	0.46	0.56	0.52	0.46	0.43	0.39	0.40
_2_2_4_Trimethylpentane	5.04	5.18	6.02	5.84	4.93	4.22	3.95	4.28
_2_2_Dimethylbutane	1.46	1.51	1.66	1.85	1.70	1.47	1.36	1.36
_2_3_4_Trimethylpentane	1.37	1.38	1.63	1.59	1.17	0.97	1.00	1.17
_2_3_Dimethylbutane	1.48	1.80	2.01	2.00	1.76	1.36	1.30	1.46
_2_3_Dimethylpentane	2.06	2.20	2.69	2.75	2.05	1.70	1.67	1.85
_2_4_Dimethylpentane	1.29	1.41	1.67	1.67	1.41	1.24	1.16	1.24
_2_Methylheptane	0.63	0.71	0.81	0.82	0.68	0.64	0.56	0.62
_2_Methylhexane	1.94	2.17	2.52	2.56	1.93	1.68	1.55	1.71
_2_Methylpentane	4.25	4.72	5.09	5.32	4.90	3.71	3.40	3.59
_3_Methylheptane	0.77	0.80	0.94	0.92	0.81	0.69	0.68	0.71
_3_Methylhexane	2.38	2.85	3.34	3.09	2.42	2.11	2.02	2.18
_3_Methylpentane	3.57	3.67	4.42	4.60	3.91	3.48	3.54	3.37
Total_Nmoc	257.6	293.5	356.7	359.1	313.9	294.5	254.9	249.8

Table 5 Burbank median ppbC concentrations by sample mid-point (e.g., 23 PST time-tagged 3-hour sample from 23:00-1:59 has mid-point 0:30 PST). Data from 2007 not used in this table.

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Num Obs	141	139	137	144	148	149	149	145
Acetylene	2.98	3.61	4.8	4.98	3.79	2.83	2.84	2.95
Benzene	2.22	2.48	3.19	3.03	2.5	1.97	2.03	2.15
Cis_2_Butene	0.05	0.05	0.19	0.05	0.05	0.05	0.05	0.05
Cis_2_Pentene	0.19	0.27	0.28	0.18	0.12	0.11	0.14	0.18
Cyclohexane	1.77	1.99	2.26	2.05	1.84	1.44	1.28	1.4
Cyclopentane	0.72	0.86	0.94	0.95	0.86	0.66	0.53	0.58
Ethane	14.96	20.78	19.45	15.49	10.83	7.03	8.05	10.35
Ethylbenzene	2.66	2.72	3.2	3.03	2.78	2.53	2.27	2.34
Ethylene	5.58	5.6	7.47	6.83	5.05	3.99	4.68	5.18
Isobutane	4.32	5.42	5.68	4.93	4.1	2.71	2.47	3.26
Isopentane	9.99	13.04	15.56	14.69	13.71	10.07	8.22	8.39
Isoprene	0.31	0.29	0.75	1.18	1.71	1.98	1.14	0.46
Isopropylbenzene	0.16	0.05	0.44	0.15	0.2	0.12	0.18	0.37
M_Diethylbenzene	0.91	0.89	1.84	1.04	0.78	0.66	0.53	1.64
M_Ethyltoluene	3	3.17	3.83	3.18	2.76	2.72	2.65	2.96
M_P_Xylene	7.83	8.56	10.58	8.48	6.63	6.01	6.02	6.99
Methylcyclohexane	2.17	2.43	2.92	2.2	1.86	1.48	1.5	1.74
Methylcyclopentane	3	3.48	4	3.58	3.18	2.58	2.33	2.5
N_Butane	7.4	9.04	9.66	9.62	8.82	5.96	5.12	5.63
N_Decane	4.82	5.18	5.89	5.04	5.03	4.44	4.35	4.43
N_Heptane	2.21	2.42	2.81	2.39	2.13	1.71	1.73	1.87
N_Hexane	3.22	3.43	3.93	3.7	3.65	3.12	2.61	2.7
N_Nonane	3.63	3.87	3.62	3.08	2.91	3.23	2.94	3.12
N_Octane	0.75	0.94	1.06	0.95	0.83	0.64	0.64	0.7
N_Pentane	4.33	5.59	6.12	6.25	5.79	3.84	2.88	3.27
N_Propylbenzene	0.97	0.97	1.22	0.91	0.88	0.91	0.79	1.03
N_Undecane	3.37	3.52	4.75	3.57	3.57	2.79	2.58	3.52
O_Ethyltoluene	2.01	2.06	2.48	2.03	1.72	1.75	1.6	1.94
O_Xylene	2.48	2.94	3.46	2.81	2.21	2.02	2.03	2.31
P_Diethylbenzene	0.36	0.38	0.82	0.43	0.39	0.32	0.34	0.77
P_Ethyltoluene	1.78	1.91	2.23	1.65	1.58	1.58	1.47	1.96
Propane	16.25	20.32	23.72	23.81	18.77	10.56	9.66	11.46
Propylene	1.91	1.96	2.74	2.1	1.31	1.22	1.75	1.95
Styrene	3.6	3.49	4.37	3.28	2.69	2.61	2.6	3.36
Toluene	20.68	23.31	27.27	23.28	20.71	19.56	17.08	17.85

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Trans_2_Butene	0.05	0.05	0.25	0.05	0.05	0.05	0.05	0.05
Trans_2_Pentene	0.32	0.51	0.56	0.33	0.23	0.21	0.26	0.3
_1_2_3_Trimethylbenzene	1.8	1.88	2.31	1.76	1.5	1.43	1.29	1.8
_1_2_4_Trimethylbenzene	4.26	4.78	5.35	4.2	3.54	3.57	3.49	4.19
_1_3_5_Trimethylbenzene	1.43	1.54	1.75	1.3	1.15	1.16	1.15	1.52
_1_Butene	0.34	0.36	0.45	0.4	0.29	0.25	0.3	0.37
_1_Pentene	0.42	0.45	0.5	0.45	0.4	0.34	0.33	0.35
_2_2_4_Trimethylpentane	3.97	4.61	5.44	5.14	4.12	3.49	3.54	3.68
_2_2_Dimethylbutane	1.07	1.22	1.44	1.54	1.35	1.06	0.88	0.9
_2_3_4_Trimethylpentane	1.15	1.44	1.75	1.48	1.11	0.96	1.01	1.11
_2_3_Dimethylbutane	1.59	1.83	2.07	2.04	1.75	1.39	1.23	1.31
_2_3_Dimethylpentane	2.12	2.44	3.09	2.83	2.24	1.92	1.79	1.82
_2_4_Dimethylpentane	1.29	1.47	1.72	1.53	1.31	1.11	1.08	1.11
_2_Methylheptane	0.5	0.49	0.59	0.47	0.48	0.46	0.42	0.47
_2_Methylhexane	1.77	1.97	2.39	2.25	1.91	1.54	1.51	1.53
_2_Methylpentane	4.6	5.24	5.74	5.42	4.58	3.68	3.32	3.51
_3_Methylheptane	0.85	0.93	1.13	1.01	0.79	0.66	0.7	0.75
_3_Methylhexane	2.57	2.73	3.15	3.33	3.18	2.47	2.27	2.23
_3_Methylpentane	3.35	3.67	4.1	3.98	3.77	2.99	2.66	2.7
Total_Nmoc	341.87	356.46	461.76	401.87	356.36	294.44	260.48	281.70

Table 6 Pico Rivera #2 median ppbC concentrations by sample mid-point (e.g., 23 PST time-tagged 3-hour sample from 23:00-1:59 has mid-point 0:30 PST)

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Num Obs	271	271	274	294	295	300	292	284
Acetylene	2.79	2.67	3.57	3.95	3.37	2.78	2.85	2.97
Benzene	1.41	1.40	1.92	1.79	1.62	1.27	1.32	1.43
Cis_2_Butene	0.22	0.18	0.24	0.18	0.05	0.05	0.18	0.20
Cis_2_Pentene	0.05	0.15	0.21	0.05	0.05	0.05	0.05	0.05
Cyclohexane	0.82	1.35	1.57	1.25	1.05	0.78	0.75	0.83
Cyclopentane	0.41	0.78	0.89	0.76	0.64	0.46	0.37	0.39
Ethane	8.59	14.69	15.60	12.45	10.08	7.01	6.74	8.18
Ethylbenzene	0.88	0.99	1.26	1.16	0.94	0.84	0.83	0.92
Ethylene	3.78	3.51	4.65	4.97	4.00	3.33	3.81	3.81
Isobutane	2.58	4.97	5.49	4.84	4.23	2.80	2.10	2.55
Isopentane	6.99	9.50	10.83	10.74	11.69	8.40	6.72	6.61
Isoprene	0.27	0.26	0.49	0.83	0.93	0.97	0.68	0.30
Isopropylbenzene	0.17	0.19	0.31	0.20	0.16	0.12	0.13	0.27
M_Diethylbenzene	0.20	0.20	0.42	0.19	0.14	0.12	0.14	0.35
M_Ethyltoluene	0.83	0.85	1.06	0.82	0.57	0.55	0.71	0.91
M_P_Xylene	3.19	3.46	4.27	3.68	2.53	2.37	2.91	3.22
Methylcyclohexane	0.88	1.39	1.65	1.32	1.04	0.80	0.82	0.87
Methylcyclopentane	1.44	2.65	2.91	2.34	2.02	1.43	1.35	1.40
N_Butane	3.58	6.36	7.68	6.78	7.17	4.42	3.32	3.45
N_Decane	0.80	0.87	1.03	0.99	0.76	0.67	0.69	0.83
N_Heptane	0.68	0.76	0.95	0.95	0.91	0.68	0.64	0.68
N_Hexane	1.10	1.53	1.81	1.70	1.69	1.17	1.02	1.09
N_Nonane	0.42	0.46	0.53	0.54	0.48	0.44	0.42	0.45
N_Octane	0.47	0.48	0.65	0.67	0.57	0.51	0.47	0.48
N_Pentane	2.41	3.81	4.42	4.24	4.45	3.00	2.33	2.33
N_Propylbenzene	0.29	0.31	0.48	0.35	0.31	0.26	0.26	0.39
N_Undecane	0.37	0.46	0.61	0.41	0.37	0.32	0.34	0.48
O_Ethyltoluene	0.38	0.44	0.61	0.46	0.34	0.30	0.33	0.46
O_Xylene	1.26	1.34	1.66	1.50	1.16	1.06	1.16	1.34
P_Diethylbenzene	0.20	0.19	0.33	0.20	0.11	0.10	0.12	0.29
P_Ethyltoluene	0.49	0.51	0.72	0.54	0.40	0.37	0.43	0.66
Propane	9.68	16.70	19.06	20.00	16.02	10.48	8.40	9.67
Propylene	1.51	1.72	2.23	1.97	0.57	0.42	0.76	1.35
Styrene	0.46	0.40	0.62	0.37	0.20	0.24	0.32	0.58
Toluene	5.40	5.55	6.93	6.94	5.83	5.03	5.07	5.42

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Trans_2_Butene	0.19	0.17	0.22	0.12	0.05	0.05	0.15	0.18
Trans_2_Pentene	0.11	0.25	0.32	0.15	0.05	0.05	0.05	0.05
_1_2_3_Trimethylbenzene	0.42	0.47	0.64	0.40	0.25	0.25	0.32	0.50
_1_2_4_Trimethylbenzene	1.26	1.42	1.84	1.23	0.78	0.81	1.09	1.38
_1_3_5_Trimethylbenzene	0.44	0.48	0.62	0.36	0.24	0.23	0.36	0.52
_1_Butene	0.37	0.42	0.57	0.57	0.30	0.20	0.21	0.33
_1_Pentene	0.33	0.36	0.47	0.43	0.33	0.24	0.24	0.32
_2_2_4_Trimethylpentane	2.17	2.13	2.60	2.73	2.64	2.22	2.23	2.22
_2_2_Dimethylbutane	0.78	0.90	1.09	1.11	1.09	0.91	0.81	0.80
_2_3_4_Trimethylpentane	0.71	0.73	0.86	0.84	0.73	0.65	0.69	0.71
_2_3_Dimethylbutane	0.96	1.35	1.55	1.32	1.23	1.03	0.95	0.98
_2_3_Dimethylpentane	1.17	1.53	1.91	1.54	1.35	1.13	1.17	1.20
_2_4_Dimethylpentane	0.73	0.84	0.99	0.90	0.86	0.73	0.71	0.73
_2_Methylheptane	0.41	0.43	0.53	0.54	0.49	0.40	0.39	0.42
_2_Methylhexane	0.93	0.97	1.25	1.24	1.13	0.91	0.85	0.92
_2_Methylpentane	2.18	2.92	3.61	3.26	3.21	2.51	2.19	2.17
_3_Methylheptane	0.40	0.42	0.56	0.53	0.45	0.39	0.39	0.42
_3_Methylhexane	1.14	1.33	1.62	1.59	1.50	1.22	1.11	1.14
_3_Methylpentane	1.59	2.11	2.53	2.22	2.23	1.69	1.51	1.62
Total_Nmoc	104.3	147.4	178.4	163.3	144.7	111.0	98.7	105.0

Table 7 LAX-Hastings median ppbC concentrations by sample mid-point (e.g., 23 PST time-tagged 3-hour sample from 23:00-1:59 has mid-point 0:30 PST)

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Num Obs	83	79	80	79	78	78	78	78
Acetylene	0.55	0.88	1.16	0.78	0.54	0.33	0.39	0.43
Benzene	0.53	0.66	0.92	0.64	0.41	0.32	0.34	0.38
Cis_2_Butene	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Cis_2_Pentene	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Cyclohexane	0.58	0.57	0.76	0.49	0.21	0.05	0.05	0.27
Cyclopentane	0.19	0.27	0.31	0.21	0.05	0.05	0.05	0.05
Ethane	4.68	6.37	7.02	4.41	3.14	2.17	2.37	2.56
Ethylbenzene	0.23	0.29	0.34	0.21	0.05	0.05	0.05	0.05
Ethylene	1.31	1.68	2.01	1.60	0.99	0.80	0.79	1.01
Isobutane	0.97	1.50	2.21	1.80	0.73	0.25	0.31	0.35
Isopentane	2.18	3.81	4.75	3.25	1.46	0.63	0.78	0.76
Isoprene	0.05	0.05	0.25	0.19	0.26	0.22	0.05	0.05
Isopropylbenzene	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
M_Diethylbenzene	0.25	0.24	0.25	0.18	0.05	0.05	0.05	0.05
M_Ethyltoluene	0.27	0.25	0.36	0.05	0.05	0.05	0.05	0.05
M_P_Xylene	0.54	0.87	1.26	0.42	0.24	0.20	0.21	0.26
Methylcyclohexane	0.29	0.45	0.74	0.35	0.05	0.05	0.05	0.05
Methylcyclopentane	0.44	0.81	1.03	0.62	0.27	0.05	0.05	0.20
N_Butane	1.54	2.46	3.19	2.29	1.24	0.38	0.48	0.54
N_Decane	0.21	0.22	0.22	0.05	0.05	0.05	0.05	0.05
N_Heptane	0.22	0.33	0.45	0.30	0.05	0.05	0.05	0.05
N_Hexane	0.47	0.70	0.91	0.60	0.26	0.05	0.05	0.11
N_Nonane	0.17	0.21	0.23	0.05	0.05	0.05	0.05	0.05
N_Octane	0.19	0.25	0.31	0.05	0.05	0.05	0.05	0.05
N_Pentane	1.13	1.89	2.03	1.48	0.58	0.31	0.35	0.43
N_Propylbenzene	0.05	0.05	0.19	0.05	0.05	0.05	0.05	0.05
N_Undecane	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
O_Ethyltoluene	0.24	0.23	0.27	0.19	0.05	0.05	0.05	0.05
O_Xylene	0.32	0.45	0.56	0.26	0.05	0.05	0.05	0.05
P_Diethylbenzene	0.24	0.24	0.28	0.19	0.05	0.05	0.05	0.05
P_Ethyltoluene	0.21	0.19	0.28	0.05	0.05	0.05	0.05	0.05
Propane	3.36	5.88	7.44	4.88	2.59	1.17	1.53	1.69
Propylene	0.74	0.85	0.99	0.64	0.39	0.35	0.32	0.43
Styrene	0.29	0.32	0.27	0.24	0.20	0.05	0.19	0.19
Toluene	1.14	1.86	2.96	1.29	0.75	0.43	0.49	0.57

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Trans_2_Butene	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Trans_2_Pentene	0.05	0.05	0.18	0.05	0.05	0.05	0.05	0.05
_1_2_3_Trimethylbenzene	0.32	0.30	0.32	0.21	0.20	0.21	0.21	0.21
_1_2_4_Trimethylbenzene	0.28	0.30	0.33	0.18	0.05	0.05	0.05	0.05
_1_3_5_Trimethylbenzene	0.05	0.05	0.20	0.05	0.05	0.05	0.05	0.05
_1_Butene	0.26	0.29	0.30	0.23	0.19	0.05	0.05	0.20
_1_Pentene	0.27	0.33	0.36	0.28	0.21	0.19	0.19	0.21
_2_2_4_Trimethylpentane	0.66	1.09	1.62	1.00	0.37	0.21	0.23	0.27
_2_2_Dimethylbutane	0.29	0.38	0.44	0.32	0.19	0.05	0.05	0.17
_2_3_4_Trimethylpentane	0.22	0.29	0.38	0.23	0.05	0.05	0.05	0.05
_2_3_Dimethylbutane	0.29	0.40	0.54	0.34	0.17	0.05	0.05	0.05
_2_3_Dimethylpentane	0.41	0.45	0.69	0.41	0.24	0.05	0.05	0.19
_2_4_Dimethylpentane	0.33	0.48	0.49	0.37	0.24	0.05	0.05	0.20
_2_Methylheptane	0.05	0.22	0.25	0.05	0.05	0.05	0.05	0.05
_2_Methylhexane	0.42	0.47	0.63	0.40	0.27	0.21	0.05	0.22
_2_Methylpentane	0.66	1.16	1.53	0.94	0.40	0.19	0.22	0.26
_3_Methylheptane	0.21	0.23	0.27	0.21	0.05	0.05	0.05	0.05
_3_Methylhexane	0.59	0.59	0.69	0.49	0.48	0.47	0.47	0.57
_3_Methylpentane	1.29	1.28	1.51	1.35	0.87	0.83	0.78	0.77
Total_Nmoc	74.1	95.3	102.0	75.4	53.6	43.6	42.9	46.5

Table 8 Santa Clarita median ppbC concentrations by sample mid-point (e.g., 23 PST time-tagged 3-hour sample from 23:00-1:59 has mid-point 0:30 PST)

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Num Obs	91	92	92	92	91	92	92	92
Acetylene	2.08	1.94	3.82	2.45	2.12	1.40	1.74	2.32
Benzene	2.04	1.94	2.89	1.78	1.46	1.16	1.54	2.15
Cis_2_Butene	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Cis_2_Pentene	0.16	0.18	0.22	0.05	0.05	0.05	0.05	0.05
Cyclohexane	1.09	1.09	1.26	0.96	0.79	0.64	0.80	0.94
Cyclopentane	0.57	0.56	0.69	0.42	0.39	0.35	0.38	0.51
Ethane	12.76	15.09	16.30	8.02	7.17	5.03	6.31	9.88
Ethylbenzene	1.06	0.93	1.28	0.72	0.48	0.45	0.65	0.99
Ethylene	3.33	3.03	5.42	3.47	2.31	1.88	2.41	3.62
Isobutane	3.31	3.28	3.42	2.40	2.17	1.71	1.90	2.92
Isopentane	10.55	10.37	13.00	8.98	9.15	7.72	7.17	10.14
Isoprene	0.72	0.64	1.72	2.90	2.82	3.38	2.25	0.97
Isopropylbenzene	0.26	0.23	0.27	0.19	0.05	0.05	0.10	0.22
M_Diethylbenzene	0.47	0.39	0.38	0.34	0.31	0.32	0.34	0.33
M_Ethyltoluene	0.78	0.73	0.87	0.41	0.25	0.25	0.45	0.65
M_P_Xylene	3.55	3.26	4.11	1.89	1.21	1.22	2.13	3.05
Methylcyclohexane	1.35	1.33	1.71	0.95	0.64	0.51	0.72	1.16
Methylcyclopentane	2.27	2.16	2.71	1.58	1.30	1.15	1.44	2.09
N_Butane	4.33	4.47	4.58	3.22	3.18	2.62	2.87	3.73
N_Decane	0.40	0.43	0.43	0.28	0.29	0.25	0.27	0.37
N_Heptane	1.19	1.11	1.39	0.85	0.67	0.53	0.66	1.07
N_Hexane	1.90	1.86	2.32	1.41	1.12	1.03	1.17	1.78
N_Nonane	0.35	0.35	0.37	0.26	0.26	0.21	0.26	0.34
N_Octane	0.65	0.66	0.82	0.51	0.33	0.29	0.39	0.52
N_Pentane	4.02	4.00	5.05	3.31	3.11	2.58	2.64	3.57
N_Propylbenzene	0.35	0.30	0.35	0.21	0.05	0.05	0.18	0.26
N_Undecane	0.26	0.25	0.23	0.05	0.05	0.05	0.05	0.20
O_Ethyltoluene	0.41	0.33	0.40	0.29	0.21	0.21	0.26	0.33
O_Xylene	1.46	1.38	1.78	0.94	0.61	0.58	0.88	1.26
P_Diethylbenzene	0.36	0.33	0.35	0.28	0.25	0.19	0.23	0.26
P_Ethyltoluene	0.63	0.54	0.61	0.38	0.27	0.27	0.39	0.49
Propane	13.02	14.76	15.66	9.83	7.66	6.11	7.68	10.96
Propylene	1.38	1.12	2.05	1.17	0.63	0.63	0.95	1.40
Styrene	0.44	0.36	0.44	0.35	0.28	0.29	0.39	0.38
Toluene	8.08	7.69	9.51	5.84	4.88	3.96	5.15	7.90

Hour →	0.5	3.5	6.5	9.5	12.5	15.5	18.5	21.5
Trans_2_Butene	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Trans_2_Pentene	0.32	0.33	0.46	0.22	0.19	0.21	0.21	0.23
_1_2_3_Trimethylbenzene	0.48	0.48	0.48	0.33	0.31	0.26	0.34	0.39
_1_2_4_Trimethylbenzene	0.94	0.88	1.10	0.50	0.29	0.36	0.58	0.84
_1_3_5_Trimethylbenzene	0.42	0.37	0.47	0.21	0.05	0.05	0.23	0.36
_1_Butene	0.26	0.24	0.29	0.27	0.19	0.20	0.21	0.26
_1_Pentene	0.43	0.40	0.54	0.41	0.31	0.31	0.35	0.42
_2_2_4_Trimethylpentane	4.16	3.93	5.49	3.29	2.72	2.27	2.64	4.13
_2_2_Dimethylbutane	1.13	1.04	1.43	1.03	1.01	0.84	0.82	1.13
_2_3_4_Trimethylpentane	1.18	1.14	1.51	0.86	0.60	0.51	0.73	1.11
_2_3_Dimethylbutane	1.45	1.43	1.92	1.17	1.01	0.85	0.89	1.35
_2_3_Dimethylpentane	2.15	2.05	2.91	1.58	1.18	1.01	1.27	1.99
_2_4_Dimethylpentane	1.36	1.31	1.80	1.06	0.80	0.74	0.88	1.20
_2_Methylheptane	0.53	0.50	0.67	0.39	0.29	0.25	0.34	0.48
_2_Methylhexane	1.55	1.46	1.88	1.25	0.90	0.84	0.96	1.41
_2_Methylpentane	3.69	3.55	4.64	2.79	2.57	2.17	2.29	3.52
_3_Methylheptane	0.65	0.62	0.76	0.45	0.30	0.28	0.38	0.57
_3_Methylhexane	1.69	1.58	2.14	1.35	1.10	0.91	1.08	1.59
_3_Methylpentane	3.02	2.84	3.78	2.57	2.30	1.87	2.13	2.87
Total_Nmoc	191.4	198.3	230.1	180.1	135.6	133.3	138.8	185.9

3.5 Box Modeling

3.5.1 Development of Profiles for Box Modeling

Given the ambient VOC compositions described in previous section (Table 3), the ozone forming potential has been evaluated using a box model that has been used in a series of studies for ROG reactivity assessment (Carter 1994, 2000, 2003, 2008, 2010a).

The modeling approach is built on 39 single-day "base case" EKMA box model scenarios (EPA, 1984) originally derived by the EPA for assessing the impacts of various ROG and NOx control strategies in different urban region in the U.S. It has been a basis for the "maximum incremental reactivity" scale which was last updated by Carter (2010a). In brief, the model is a one-cell box model representing the planetary boundary layer. The model implements, in addition to photochemistry, the emission of precursor species, entrainment of aloft species, and dry deposition. The environmental condition for the modeling was that of "Average condition", which is derived from conditions for 39 different U.S. cities. In addition to this single day scenario, the five day scenario (Carter, 2010c) was used in order to examine evolution of oxidation products while varying ROG to NOx ratio from 3.85 to 70.4.

The current base case VOC file (arbrog.cmp) and maximum incremental reactivity table (scales07.xls) were downloaded from http://www.cert.ucr.edu/~carter/SAPRC/. (Carter, 2010a).

The annual organic gas emission inventories (EI) for 2008 for Los Angeles County and for the State of California were provided by CARB staff. Both EIs are reported by source categories (3,377 categories for the State, 2,465 categories for LA County), along with the speciation profile of each source expressed as mass fraction by Storage and Retrieval of Aerometric Data (SAROAD) code. Annual emissions from the two geographic regions were speciated first into SAROAD code, after which each resulting profile was processed by the emitdb.xls tools (Carter, 2010b). Dr. Carter's tools speciate the SAROAD species that represent mixtures of species into single compounds or groups of similar compounds such as isomers. The results provided molar fractions of each species within the emission inventory. This profile was expressed as ppbC, assuming that the emissions were mixed into air to give total ROG concentration of 233.7 ppbC, as was done for the rest of chemical profiles.

Table 9 compares six ROG compositions, all relevant to Los Angeles County:

- the ROG mixture value that has been used in Carter's reactivity calculations (labeled "ARBROG") (2010a),
- estimations based on emission inventory (labeled "Emission LA"),
- the average of three monitoring sites from SCOS97 studies (labeled "SCOS97 LA County"),

- average of Photochemical Assessment Monitoring Station (PAMS) observations of six monitoring sites located in Los Angeles county, 2006 - 2008 (labeled "PAMS LA County"),
- two more profiles derived from PAMS profile in conjunction of the three other profiles mentioned above (labeled "PAMS/SCOS patched" and "PAMS/SCOS/Emis patched").

The rest of this section discusses how these different profiles were derived.

As was noted above, each profile has been normalized to have total mass of ROG equal to 234.4 ppbC, which is the average value derived from the PAMS observations. In order to compare the contribution of different kinds of ROG species, the species were binned by the SAPRC07 mechanism's classifications systems. For example, species having double bonds were grouped in OLE1 and OLE2, grouping lower and higher reactivity species within olefins. Figure 22 shows the contribution of different groups for the six profiles in ppbC. In order to evaluate the contribution to ozone formation, the maximum incremental reactivity (MIR) values are multiplied with each ROG species and shown in Figure 23. Table 10 lists species concentration profiles from Table 9 corresponding to rotate principal components in Table 1, factors 2 and 3. Table 11 compares the sum of MIR across all species within each of six profiles.

Table 9 Species concentration profiles derived from ambient data and original ARB ROG mixture (All profiles are normalized have total of 234.446 ppbC, the morning observed average for Los Angeles County).

Species	CAS Number	Carter SDB ID [a]	#C	Carter Emis-sion Group [a]	S07 Spec. Group [a]	ARBROG profile [b]	Emission LA [c]	SCOS97 LA Average [c]	PAMS LA Average [c]	PAMS / SCOS patch [c]	PAMS / SCOS / Emis patch [d]
ethane	74-84-0	C74-84-0	2	ETHA	ALK1	7.902	5.064	11.015	19.686	18.708	7.902
propane	74-98-6	C74-98-6	3	PROP	ALK2	9.940	4.030	15.066	27.250	25.897	9.940
2,2-dimethylpropane	463-82-1	C463-82-1	5	ALK2	ALK2	n/a	0.002	n/a	n/a	n/a	n/a
2-methylpropane; isobutane	75-28-5	C75-28-5	4	ALK3	ALK3	7.387	3.095	4.083	5.781	5.494	7.387
n-butane	106-97-8	C106-97-8	4	ALK3	ALK3	16.947	5.749	6.840	8.918	8.476	16.947
2,2-dimethylbutane	75-83-2	C75-83-2	6	ALK3	ALK3	0.649	1.058	1.569	1.517	1.442	0.649
3,3-dimethylpentane	562-49-2	C562-49-2	7	ALK3	ALK3	n/a	0.131	n/a	n/a	n/a	n/a
2,2-dimethylpentane	590-35-2	C590-35-2	7	ALK3	ALK3	n/a	0.026	n/a	n/a	n/a	n/a
2,2,4-trimethylpentane	540-84-1	C540-84-1	8	ALK3	ALK3	n/a	4.671	5.501	5.112	4.859	n/a
cyclopentane	287-92-3	C287-92-3	5	ALK4	ALK4	0.828	0.729	1.180	1.010	0.959	0.828
2-methyl-butane	78-78-4	C78-78-4	5	ALK4	ALK4	17.774	19.226	20.922	14.958	14.215	17.774
n-pentane	109-66-0	C109-66-0	5	ALK4	ALK4	7.186	6.237	9.858	6.625	6.296	7.186
2,3-dimethylbutane	79-29-8	C79-29-8	6	ALK4	ALK4	1.343	1.688	2.264	2.014	1.914	1.343
2-methylpentane	107-83-5	C107-83-5	6	ALK4	ALK4	4.992	5.374	7.426	5.252	4.991	4.992
3-methylpentane	96-14-0	C96-14-0	6	ALK4	ALK4	3.559	3.053	4.425	4.092	3.889	3.559
n-hexane	110-54-3	C110-54-3	6	ALK4	ALK4	1.858	2.842	4.068	3.517	3.342	1.858
methylcyclopentane	96-37-7	C96-37-7	6	ALK4	ALK4	2.261	3.179	4.867	3.730	3.545	2.261
Branched C6 Alkanes	n/a	SM-BR-C6	6	ALK4	ALK4	0.336	n/a	n/a	n/a	n/a	0.336
2,4-dimethylpentane	108-08-7	C108-08-7	7	ALK4	ALK4	0.985	1.503	1.819	1.643	1.562	0.985
n-heptane	142-82-5	C142-82-5	7	ALK4	ALK4	1.970	2.544	2.432	2.033	1.932	1.970
Branched C7 Alkanes	n/a	SM-BR-C7	7	ALK4	ALK4	3.425	n/a	n/a	n/a	n/a	3.425
2,2,3-trimethylbutane	464-06-2	C464-06-2	7	ALK4	ALK4	n/a	0.080	n/a	n/a	n/a	n/a
1,1-dimethylcyclopentane	1638-26-2	C1638-26-2	7	ALK4	ALK4	n/a	0.071	n/a	n/a	n/a	n/a
2,3,4-trimethylpentane	565-75-3	C565-75-3	8	ALK4	ALK4	n/a	1.311	1.850	1.483	1.409	n/a
2,2-dimethylhexane	590-73-8	C590-73-8	8	ALK4	ALK4	n/a	0.143	n/a	n/a	n/a	n/a
2,3,3-trimethylpentane	560-21-4	C560-21-4	8	ALK4	ALK4	n/a	0.593	n/a	n/a	n/a	n/a
2,2,3-trimethylpentane	564-02-3	C564-02-3	8	ALK4	ALK4	n/a	0.074	n/a	n/a	n/a	n/a
1,1,3-trimethylcyclopentane	4516-69-2	C4516-69-2	8	ALK4	ALK4	n/a	0.105	n/a	n/a	n/a	n/a
1,1,2-trimethylcyclopentane	4259-00-1	C4259-00-1	8	ALK4	ALK4	n/a	0.045	n/a	n/a	n/a	n/a

Species	CAS Number	Carter SDB ID [a]	#C	Carter Emis-sion Group [a]	S07 Spec. Group [a]	ARBROG profile [b]	Emission LA [c]	SCOS97 LA Average [c]	PAMS LA Average [c]	PAMS / SCOS patch [c]	PAMS / SCOS / Emis patch [d]
3,3-dimethylhexane	563-16-6	C563-16-6	8	ALK4	ALK4	n/a	0.032	n/a	n/a	n/a	n/a
3,3-dimethylheptane	4032-86-4	C4032-86-4	9	ALK4	ALK4	n/a	0.068	n/a	n/a	n/a	n/a
2,2,4-trimethylhexane	16747-26-5	C16747-26-5	9	ALK4	ALK4	n/a	0.076	0.964	n/a	0.695	n/a
2,4,4-trimethylhexane	16747-30-1	C16747-30-1	9	ALK4	ALK4	n/a	0.012	n/a	n/a	n/a	n/a
2,2,5-trimethylhexane	3522-94-9	C3522-94-9	9	ALK4	ALK4	n/a	0.663	n/a	n/a	n/a	n/a
2,2-dimethylheptane	1071-26-7	C1071-26-7	9	ALK4	ALK4	n/a	0.011	n/a	n/a	n/a	n/a
4,4-dimethylheptane	1068-19-5	C1068-19-5	9	ALK4	ALK4	n/a	0.014	n/a	n/a	n/a	n/a
cyclohexane	110-82-7	C110-82-7	6	ALK5	ALK5	0.963	0.966	2.600	2.046	1.945	0.963
2-methylhexane	591-76-4	C591-76-4	7	ALK5	ALK5	n/a	1.707	2.639	2.213	2.103	n/a
2,3-dimethylpentane	565-59-3	C565-59-3	7	ALK5	ALK5	1.836	2.872	3.321	2.777	2.639	1.836
3-methylhexane	589-34-4	C589-34-4	7	ALK5	ALK5	2.082	2.347	3.506	2.764	2.627	2.082
methylcyclohexane	108-87-2	C108-87-2	7	ALK5	ALK5	1.119	2.725	3.305	2.249	2.138	1.119
c7 cycloparaffins	n/a	S0-43115	7	ALK5	ALK5	0.201	0.327	n/a	n/a	n/a	0.201
3-ethylpentane	617-78-7	C617-78-7	7	ALK5	ALK5	n/a	0.404	n/a	n/a	n/a	n/a
1,2-dimethylcyclopentane	2452-99-5	C2452-99-5	7	ALK5	ALK5	n/a	0.236	n/a	n/a	n/a	n/a
ethylcyclopentane	1640-89-7	C1640-89-7	7	ALK5	ALK5	n/a	0.363	n/a	n/a	n/a	n/a
1,3-dimethylcyclopentane	2453-00-1	C2453-00-1	7	ALK5	ALK5	n/a	0.996	n/a	n/a	n/a	n/a
2-methylheptane	592-27-8	C592-27-8	8	ALK5	ALK5	n/a	1.017	1.115	0.758	0.720	n/a
3-methylheptane	589-81-1	C589-81-1	8	ALK5	ALK5	n/a	1.092	n/a	0.866	0.823	n/a
n-octane	111-65-9	C111-65-9	8	ALK5	ALK5	1.388	1.191	1.279	1.042	0.991	1.388
ethylcyclohexane	1678-91-7	C1678-91-7	8	ALK5	ALK5	0.336	0.266	n/a	n/a	n/a	0.336
Branched C8 Alkanes	n/a	SM-BR-C8	8	ALK5	ALK5	7.566	0.146	n/a	n/a	n/a	7.566
2-methyl-3-ethylpentane	609-26-7	C609-26-7	8	ALK5	ALK5	n/a	0.080	n/a	n/a	n/a	n/a
2,5-dimethylhexane	592-13-2	C592-13-2	8	ALK5	ALK5	n/a	0.630	1.223	n/a	1.020	n/a
c8 cycloparaffins	n/a	S0-43116	8	ALK5	ALK5	n/a	0.859	n/a	n/a	n/a	n/a
1,1-dimethylcyclohexane	590-66-9	C590-66-9	8	ALK5	ALK5	n/a	0.062	n/a	n/a	n/a	n/a
1,4-dimethylcyclohexane	589-90-2	C589-90-2	8	ALK5	ALK5	n/a	0.238	n/a	n/a	n/a	n/a
1,3-Dimethyl Cyclohexane	591-21-9	C591-21-9	8	ALK5	ALK5	n/a	0.852	n/a	n/a	n/a	n/a
2,4-dimethylhexane	589-43-5	C589-43-5	8	ALK5	ALK5	n/a	1.069	1.103	n/a	0.920	n/a
4-methylheptane	589-53-7	C589-53-7	8	ALK5	ALK5	n/a	0.403	n/a	n/a	n/a	n/a
2,3-dimethylhexane	584-94-1	C584-94-1	8	ALK5	ALK5	n/a	0.566	0.646	n/a	0.539	n/a
3,4-dimethylhexane	583-48-2	C583-48-2	8	ALK5	ALK5	n/a	0.060	n/a	n/a	n/a	n/a

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propylcyclopentane	2040-96-2	C2040-96-2	8	ALK5	ALK5	n/a	0.032	n/a	n/a	n/a	n/a
1,2-dimethylcyclohexane	583-57-3	C583-57-3	8	ALK5	ALK5	n/a	0.044	n/a	n/a	n/a	n/a
C8 Bicycloalkanes	n/a	SM-BCYC-C8	8	ALK5	ALK5	n/a	0.010	n/a	n/a	n/a	n/a
3-(chloromethyl)-heptane	123-04-6	C123-04-6	8	ALK5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
3-ethylhexane	619-99-8	C619-99-8	8	ALK5	ALK5	n/a	n/a	1.233	n/a	1.029	n/a
n-nonane	111-84-2	C111-84-2	9	ALK5	ALK5	1.567	0.635	0.923	1.516	1.440	1.567
Branched C9 Alkanes	n/a	SM-BR-C9	9	ALK5	ALK5	3.604	0.168	n/a	n/a	n/a	3.604
2-methyloctane	3221-61-2	C3221-61-2	9	ALK5	ALK5	n/a	0.253	n/a	n/a	n/a	n/a
2,3-dimethylheptane	3074-71-3	C3074-71-3	9	ALK5	ALK5	n/a	0.094	n/a	n/a	n/a	n/a
4-methyloctane	2216-34-4	C2216-34-4	9	ALK5	ALK5	n/a	0.376	n/a	n/a	n/a	n/a
3-methyloctane	2216-33-3	C2216-33-3	9	ALK5	ALK5	n/a	0.517	n/a	n/a	n/a	n/a
C9 cycloalkanes	n/a	DMS-CYC-C9	9	ALK5	ALK5	n/a	0.234	n/a	n/a	n/a	n/a
1,1,3-trimethylcyclohexane	3073-66-3	C3073-66-3	9	ALK5	ALK5	n/a	0.255	n/a	n/a	n/a	n/a
1,2,3-trimethylcyclohexane	1678-97-3	C1678-97-3	9	ALK5	ALK5	n/a	0.509	n/a	n/a	n/a	n/a
propylcyclohexane	1678-92-8	C1678-92-8	9	ALK5	ALK5	n/a	0.087	n/a	n/a	n/a	n/a
2,6-dimethylheptane	1072-05-5	C1072-05-5	9	ALK5	ALK5	n/a	0.276	n/a	n/a	n/a	n/a
1,3,5-trimethylcyclohexane	1839-63-0	C1839-63-0	9	ALK5	ALK5	n/a	0.287	n/a	n/a	n/a	n/a
2,5-dimethylheptane	2216-30-0	C2216-30-0	9	ALK5	ALK5	n/a	0.138	n/a	n/a	n/a	n/a
2,4-dimethylheptane	2213-23-2	C2213-23-2	9	ALK5	ALK5	n/a	0.125	n/a	n/a	n/a	n/a
3-ethylheptane	15869-80-4	C15869-80-4	9	ALK5	ALK5	n/a	0.048	n/a	n/a	n/a	n/a
3,4-dimethylheptane	922-28-1	C922-28-1	9	ALK5	ALK5	n/a	0.073	n/a	n/a	n/a	n/a
3,5-dimethylheptane	926-82-9	C926-82-9	9	ALK5	ALK5	n/a	0.140	n/a	n/a	n/a	n/a
2,3,5-trimethylhexane	1069-53-0	C1069-53-0	9	ALK5	ALK5	n/a	0.070	n/a	n/a	n/a	n/a
trans 1-methyl-4-ethylcyclohexane	6236-88-0	C6236-88-0	9	ALK6	ALK5	n/a	0.253	n/a	n/a	n/a	n/a
cis-bicyclo[4.3.0]nonane	4551-51-3	C4551-51-3	9	ALK6	ALK5	n/a	0.027	n/a	n/a	n/a	n/a
n-decane	124-18-5	C124-18-5	10	ALK5	ALK5	4.321	1.006	1.553	2.400	2.281	4.321
Branched C10 Alkanes	n/a	SM-BR-C10	10	ALK5	ALK5	3.649	0.441	n/a	n/a	n/a	3.649
4-Propyl Heptane	3178-29-8	C3178-29-8	10	ALK5	ALK5	n/a	0.057	n/a	n/a	n/a	n/a
3,4-Diethyl Hexane	19398-77-7	C19398-77-7	10	ALK5	ALK5	n/a	0.057	n/a	n/a	n/a	n/a
2,5-dimethyloctane	15869-89-3	C15869-89-3	10	ALK5	ALK5	n/a	0.106	n/a	n/a	n/a	n/a
2,2,4-trimethylheptane	14720-74-2	C14720-74-2	10	ALK5	ALK5	n/a	0.102	n/a	n/a	n/a	n/a

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4-methylnonane	17301-94-9	C17301-94-9	10	ALK5	ALK5	n/a	0.146	n/a	n/a	n/a	n/a
2-methylnonane	871-83-0	C871-83-0	10	ALK5	ALK5	n/a	0.291	n/a	n/a	n/a	n/a
2,6-dimethyloctane	2051-30-1	C2051-30-1	10	ALK5	ALK5	n/a	0.130	n/a	n/a	n/a	n/a
2,3-dimethyloctane	7146-60-3	C7146-60-3	10	ALK5	ALK5	n/a	0.101	n/a	n/a	n/a	n/a
3-methylnonane	5911-04-6	C5911-04-6	10	ALK5	ALK5	n/a	0.069	n/a	n/a	n/a	n/a
3-ethyl-2-methylheptane	14676-29-0	C14676-29-0	10	ALK5	ALK5	n/a	0.030	n/a	n/a	n/a	n/a
2,4-dimethyloctane	4032-94-4	C4032-94-4	10	ALK5	ALK5	n/a	0.176	n/a	n/a	n/a	n/a
2,2-dimethyloctane	15869-87-1	C15869-87-1	10	ALK5	ALK5	n/a	0.018	n/a	n/a	n/a	n/a
3,3-dimethyloctane	4110-44-5	C4110-44-5	10	ALK5	ALK5	n/a	0.049	n/a	n/a	n/a	n/a
C10 Bicycloalkanes	n/a	SM-BCYC-C10	10	ALK6	ALK5	n/a	0.022	n/a	n/a	n/a	n/a
butylcyclohexane	1678-93-9	C1678-93-9	10	ALK6	ALK5	n/a	0.133	n/a	n/a	n/a	n/a
1,4-Diethyl-Cyclohexane	1679-00-1	C1679-00-1	10	ALK6	ALK5	n/a	0.028	n/a	n/a	n/a	n/a
1-Methyl-3-Isopropyl Cyclohexane	16580-24-8	C16580-24-8	10	ALK6	ALK5	n/a	0.013	n/a	n/a	n/a	n/a
C10 Cycloalkanes	n/a	SM-CYC-C10	10	ALK6	ALK5	n/a	0.535	n/a	n/a	n/a	n/a
isobutylcyclohexane (2-methylpropyl cyclohexane)	1678-98-4	C1678-98-4	10	ALK6	ALK5	n/a	0.047	n/a	n/a	n/a	n/a
1,3-Diethyl-Cyclohexane	1678-99-5	C1678-99-5	10	ALK6	ALK5	n/a	0.023	n/a	n/a	n/a	n/a
sec-butylcyclohexane	7058-01-7	C7058-01-7	10	ALK6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
n-undecane	1120-21-4	C1120-21-4	11	ALK5	ALK5	0.425	0.895	n/a	1.583	1.505	0.425
Branched C11 alkanes	n/a	SM-BR-C11	11	ALK5	ALK5	0.425	0.637	n/a	n/a	n/a	0.425
4-methyldecane	2847-72-5	C2847-72-5	11	ALK5	ALK5	n/a	0.130	n/a	n/a	n/a	n/a
2,6-dimethylnonane	17302-28-2	C17302-28-2	11	ALK5	ALK5	n/a	0.233	n/a	n/a	n/a	n/a
3-methyldecane	13151-34-3	C13151-34-3	11	ALK5	ALK5	n/a	0.119	n/a	n/a	n/a	n/a
C11 Bicycloalkanes	n/a	SM-BCYC-C11	11	ALK6	ALK5	n/a	0.036	n/a	n/a	n/a	n/a
c11 cycloalkanes	n/a	S2-98071	11	ALK6	ALK5	n/a	0.143	n/a	n/a	n/a	n/a
1,3-Diethyl-5-Methyl Cyclohexane	164259-42-1	C164259-42-1	11	ALK6	ALK5	n/a	0.010	n/a	n/a	n/a	n/a
1-Ethyl-2-Propyl Cyclohexane	62238-33-9	C62238-33-9	11	ALK6	ALK5	n/a	0.183	n/a	n/a	n/a	n/a
pentyl Cyclohexane	4292-92-6	C4292-92-6	11	ALK6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
n-dodecane	112-40-3	C112-40-3	12	ALK5	ALK5	0.918	0.219	n/a	n/a	n/a	0.918
Branched C12 Alkanes	n/a	SM-BR-C12	12	ALK6	ALK5	0.918	0.248	n/a	n/a	n/a	0.918
1-Methyl-4-Pentyl Cyclohexane	75736-67-3	C75736-67-3	12	ALK6	ALK5	n/a	0.015	n/a	n/a	n/a	n/a

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hexylcyclohexane	4292-75-5	C4292-75-5	12	ALK6	ALK5	n/a	0.016	n/a	n/a	n/a	n/a
1,3,5-Triethyl Cyclohexane	164259-43-2	C164259-43-2	12	ALK6	ALK5	n/a	0.013	n/a	n/a	n/a	n/a
3,6-Dimethyl Decane	17312-53-7	C17312-53-7	12	ALK6	ALK5	n/a	0.017	n/a	n/a	n/a	n/a
5-methylundecane	1632-70-8	C1632-70-8	12	ALK6	ALK5	n/a	0.025	n/a	n/a	n/a	n/a
3-methylundecane	1002-43-3	C1002-43-3	12	ALK6	ALK5	n/a	0.030	n/a	n/a	n/a	n/a
c12 cycloalkanes	n/a	S2-98072	12	ALK6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
C12 bicycloalkanes	n/a	DMS-BCYC-C12	12	ALK6	ALK5	n/a	0.008	n/a	n/a	n/a	n/a
n-tridecane	629-50-5	C629-50-5	13	ALK6	ALK5	0.045	0.073	n/a	n/a	n/a	0.045
c13 branched alkanes	n/a	S1-91013	13	ALK6	ALK5	0.045	0.121	n/a	n/a	n/a	0.045
5-Methyl Dodecane	17453-93-9	C17453-93-9	13	ALK6	ALK5	n/a	0.013	n/a	n/a	n/a	n/a
3-Methyl Dodecane	17312-57-1	C17312-57-1	13	ALK6	ALK5	n/a	0.013	n/a	n/a	n/a	n/a
3,6-Dimethyl Undecane	17301-28-9	C17301-28-9	13	ALK6	ALK5	n/a	0.016	n/a	n/a	n/a	n/a
2,4,6,8-Tetramethyl Nonane	14638-54-1	C14638-54-1	13	ALK6	ALK5	n/a	0.013	n/a	n/a	n/a	n/a
1-Methyl-2-Hexyl-Cyclohexane	92031-93-1	C92031-93-1	13	ALK6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
Heptyl Cyclohexane	5617-41-4	C5617-41-4	13	ALK6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
n-tetradecane	629-59-4	C629-59-4	14	ALK6	ALK5	n/a	0.036	n/a	n/a	n/a	n/a
3,7-Dimethyl Dodecane	82144-67-0	C82144-67-0	14	ALK6	ALK5	n/a	0.003	n/a	n/a	n/a	n/a
3-Methyl Tridecane	6418-41-3	C6418-41-3	14	ALK6	ALK5	n/a	0.003	n/a	n/a	n/a	n/a
3,8-Diethyl Decane	6224-52-8	C6224-52-8	14	ALK6	ALK5	n/a	0.003	n/a	n/a	n/a	n/a
6-Methyl Tridecane	13287-21-3	C13287-21-3	14	ALK6	ALK5	n/a	0.003	n/a	n/a	n/a	n/a
1,3-Dipropyl-5-Ethyl Cyclohexane	n/a	Sx-020	14	ALK6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
trans 1-Methyl-4-Heptyl Cyclohexane	205324-73-8	C205324-73-8	14	ALK6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
Octyl Cyclohexane	1795-15-9	C1795-15-9	14	ALK6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
n-pentadecane	629-62-9	C629-62-9	15	ALK6	ALK5	n/a	0.419	n/a	n/a	n/a	n/a
6-Methyl Tetradecane	26730-16-5	C26730-16-5	15	ALK6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
3-Methyl Tetradecane	18435-22-8	C18435-22-8	15	ALK6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
3,9-Diethyl Undecane	13286-72-1	C13286-72-1	15	ALK6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
hexadecane	544-76-3	C544-76-3	16	ALK6	ALK5	n/a	0.005	n/a	n/a	n/a	n/a
n-heptadecane	629-78-7	C629-78-7	17	ALK6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
dichloromethane {methylene chloride}	75-09-2	C75-09-2	1	OTH1	ALK1	n/a	0.581	n/a	n/a	n/a	n/a

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perchloroethylene	127-18-4	C127-18-4	2	PERC	ALK1	n/a	0.398	n/a	n/a	n/a	n/a
1,1-dichloroethane	75-34-3	C75-34-3	2	OTH1	ALK1	n/a	0.000	n/a	n/a	n/a	n/a
ethylene dichloride	107-06-2	C107-06-2	2	OTH1	ALK1	n/a	0.003	n/a	n/a	n/a	n/a
1,1,2-trichloroethane	79-00-5	C79-00-5	2	OTH1	ALK1	n/a	0.000	n/a	n/a	n/a	n/a
ethylene dibromide	106-93-4	C106-93-4	2	OTH1	ALK1	n/a	0.000	n/a	n/a	n/a	n/a
methyl formate	107-31-3	C107-31-3	2	OTH1	ALK1	n/a	0.003	n/a	n/a	n/a	n/a
ethyl chloride	75-00-3	C75-00-3	2	OTH2	ALK2	n/a	0.003	n/a	n/a	n/a	n/a
methyl acetate	79-20-9	C79-20-9	3	OTH2	ALK2	n/a	0.004	n/a	n/a	n/a	n/a
propylene oxide	75-56-9	C75-56-9	3	OTH2	ALK2	n/a	0.000	n/a	n/a	n/a	n/a
n-Propyl Bromide	106-94-5	C106-94-5	3	OTH2	ALK2	n/a	0.001	n/a	n/a	n/a	n/a
1,2-dichloropropane	78-87-5	C78-87-5	3	OTH2	ALK2	n/a	0.000	n/a	n/a	n/a	n/a
ethyl acetate	141-78-6	C141-78-6	4	OTH2	ALK2	n/a	0.207	n/a	n/a	n/a	n/a
propylene carbonate	108-32-7	C108-32-7	4	OTH2	ALK2	n/a	0.000	n/a	n/a	n/a	n/a
tert-butyl alcohol	75-65-0	C75-65-0	4	TBOH	ALK2	n/a	0.000	n/a	n/a	n/a	n/a
t-butyl acetate	540-88-5	C540-88-5	6	OTH2	ALK2	n/a	0.011	n/a	n/a	n/a	n/a
dimethyl succinate (dimethyl butaneoate)	106-65-0	C106-65-0	6	OTH2	ALK2	n/a	0.000	n/a	n/a	n/a	n/a
carbon disulfide	75-15-0	C75-15-0	1	OTH3	ALK3	n/a	0.000	n/a	n/a	n/a	n/a
trichloroethylene (tce)	79-01-6	C79-01-6	2	TCE	ALK3	n/a	0.064	n/a	n/a	n/a	n/a
methyl isothiocyanate	556-61-6	C556-61-6	2	OTH3	ALK3	n/a	0.045	n/a	n/a	n/a	n/a
dimethyl ether	115-10-6	C115-10-6	2	OTH3	ALK3	n/a	0.213	n/a	n/a	n/a	n/a
trans-1,2-dichloroethene	156-60-5	C156-60-5	2	OTH3	ALK3	n/a	0.000	n/a	n/a	n/a	n/a
ethyl alcohol	64-17-5	C64-17-5	2	ETOH	ALK3	n/a	9.894	n/a	n/a	n/a	n/a
1-chlorobutane	109-69-3	C109-69-3	4	OTH3	ALK3	n/a	0.001	n/a	n/a	n/a	n/a
1,2-epoxybutane	106-88-7	C106-88-7	4	OTH3	ALK3	n/a	0.000	n/a	n/a	n/a	n/a
methyl t-butyl ether (mtbe)	1634-04-4	C1634-04-4	5	OTH3	ALK3	n/a	0.001	10.904	n/a	0.000	n/a
propyl acetate	109-60-4	C109-60-4	5	OTH3	ALK3	n/a	0.136	n/a	n/a	n/a	n/a
isopropyl acetate	108-21-4	C108-21-4	5	OTH3	ALK3	n/a	0.004	n/a	n/a	n/a	n/a
methyl isobutyrate	547-63-7	C547-63-7	5	OTH3	ALK3	n/a	0.000	n/a	n/a	n/a	n/a
dimethoxymethane (methylal)	109-87-5	C109-87-5	3	OTH4	ALK4	n/a	0.001	n/a	n/a	n/a	n/a
n-propyl alcohol	71-23-8	C71-23-8	3	C3OH	ALK4	n/a	0.004	n/a	n/a	n/a	n/a
isopropyl alcohol	67-63-0	C67-63-0	3	C3OH	ALK4	n/a	3.172	n/a	n/a	n/a	n/a

Species	CAS Number	Carter SDB ID [a]	#C	Carter Emis-sion Group [a]	S07 Spec. Group [a]	ARBROG profile [b]	Emission LA [c]	SCOS97 LA Average [c]	PAMS LA Average [c]	PAMS / SCOS patch [c]	PAMS / SCOS / Emis patch [d]
Ethyl Lactate	97-64-3	C97-64-3	5	OTH4	ALK4	n/a	0.000	n/a	n/a	n/a	n/a
n-butyl acetate	123-86-4	C123-86-4	6	OTH4	ALK4	n/a	0.613	n/a	n/a	n/a	n/a
isobutyl acetate	110-19-0	C110-19-0	6	OTH4	ALK4	n/a	0.009	n/a	n/a	n/a	n/a
t-amylmethylether (tame)	994-05-8	C994-05-8	6	OTH4	ALK4	n/a	0.003	n/a	n/a	n/a	n/a
isoamyl acetate (3-methylbutyl acetate)	123-92-2	C123-92-2	7	OTH4	ALK4	n/a	0.000	n/a	n/a	n/a	n/a
pentanedioic acid, dimethyl ester (dimethyl glutarate)	1119-40-0	C1119-40-0	7	OTH4	ALK4	n/a	0.001	n/a	n/a	n/a	n/a
amyl acetate	628-63-7	C628-63-7	7	OTH4	ALK4	n/a	0.000	n/a	n/a	n/a	n/a
isobutyl isobutyrate	97-85-8	C97-85-8	8	OTH4	ALK4	n/a	0.002	n/a	n/a	n/a	n/a
ethylene glycol	107-21-1	C107-21-1	2	ETGL	ALK5	n/a	0.081	n/a	n/a	n/a	n/a
vinyl chloride	75-01-4	C75-01-4	2	OTH5	ALK5	n/a	0.004	n/a	n/a	n/a	n/a
1,1-dichloroethene {vinylidene chloride}	75-35-4	C75-35-4	2	OTH5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
ethylamine	75-04-7	C75-04-7	2	OTH6	ALK5	n/a	0.028	n/a	n/a	n/a	n/a
ethanolamine	141-43-5	C141-43-5	2	OTH6	ALK5	n/a	0.353	n/a	n/a	n/a	n/a
dimethyl sulfoxide	67-68-5	C67-68-5	2	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
2-methoxyethanol {methyl cellosolve} {egme}	109-86-4	C109-86-4	3	OTH5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
cis-1,3-dichloropropene	10061-01-5	C10061-01-5	3	OTH5	ALK5	n/a	0.014	n/a	n/a	n/a	n/a
propylene glycol	57-55-6	C57-55-6	3	OTH6	ALK5	n/a	0.127	n/a	n/a	n/a	n/a
glycerol	56-81-5	C56-81-5	3	OTH6	ALK5	n/a	0.028	n/a	n/a	n/a	n/a
trimethyl amine	75-50-3	C75-50-3	3	OTH6	ALK5	n/a	0.032	n/a	n/a	n/a	n/a
trans-1,3-dichloropropene	10061-02-6	C10061-02-6	3	OTH6	ALK5	n/a	0.014	n/a	n/a	n/a	n/a
acrylonitrile	107-13-1	C107-13-1	3	MRCT	ALK5	n/a	0.004	n/a	n/a	n/a	n/a
ethyl ether	60-29-7	C60-29-7	4	OTH5	ALK5	n/a	0.008	n/a	n/a	n/a	n/a
1,4-butanediol	110-63-4	C110-63-4	4	OTH5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
2-ethoxyethanol {cellosolve} {egee}	110-80-5	C110-80-5	4	OTH6	ALK5	n/a	0.007	n/a	n/a	n/a	n/a
propylene glycol methyl ether {1-methoxy-2-propanol}	107-98-2	C107-98-2	4	OTH6	ALK5	n/a	0.049	n/a	n/a	n/a	n/a
diethylene glycol (2,2'-	111-46-6	C111-46-6	4	OTH6	ALK5	n/a	0.019	n/a	n/a	n/a	n/a

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oxybisethanol)											
tetrahydrofuran	109-99-9	C109-99-9	4	OTH6	ALK5	n/a	0.068	n/a	n/a	n/a	n/a
diethanolamine	111-42-2	C111-42-2	4	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
1,3-butanediol	107-88-0	C107-88-0	4	OTH6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
1,4-dioxane	123-91-1	C123-91-1	4	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
1,2-butanediol	584-03-2	C584-03-2	4	OTH6	ALK5	n/a	0.054	n/a	n/a	n/a	n/a
2-methoxy-1-propanol	1589-47-5	C1589-47-5	4	OTH6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
morpholine (tetrahydro-1,4-oxazin)	110-91-8	C110-91-8	4	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
n-butyl alcohol	71-36-3	C71-36-3	4	ROH5	ALK5	n/a	0.032	n/a	n/a	n/a	n/a
isobutyl alcohol	78-83-1	C78-83-1	4	ROH5	ALK5	n/a	0.084	n/a	n/a	n/a	n/a
sec-butyl alcohol	78-92-2	C78-92-2	4	ROH5	ALK5	n/a	0.042	n/a	n/a	n/a	n/a
ethyl isopropyl ether	625-54-7	C625-54-7	5	OTH6	ALK5	n/a	0.004	n/a	n/a	n/a	n/a
1-ethoxy-2-propanol	1569-02-4	C1569-02-4	5	OTH6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
methyl carbitol {2-(2-methoxyethoxy)ethanol} {degme}	111-77-3	C111-77-3	5	OTH6	ALK5	n/a	0.047	n/a	n/a	n/a	n/a
tetrahydro-2-furanmethanol	97-99-4	C97-99-4	5	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
ethylene glycol propyl ether {2-propoxyethanol}	2807-30-9	C2807-30-9	5	OTH6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
adipic acid	124-04-9	C124-04-9	6	OTH5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
ethyl t-butyl ether	637-92-3	C637-92-3	6	OTH5	ALK5	n/a	n/a	0.240	n/a	0.000	n/a
hexylene glycol (2-methylpentane-2,4-diol)	107-41-5	C107-41-5	6	OTH6	ALK5	n/a	0.009	n/a	n/a	n/a	n/a
diisopropylene glycol; 1,1'-oxydipropan-2-ol	110-98-5	C110-98-5	6	OTH6	ALK5	n/a	0.008	n/a	n/a	n/a	n/a
propylene glycol monomethyl ether acetate {2-(1-methoxy)propyl acetate}	108-65-6	C108-65-6	6	OTH6	ALK5	n/a	0.040	n/a	n/a	n/a	n/a
2-ethoxyethyl acetate {cellosolve acetate}	111-15-9	C111-15-9	6	OTH6	ALK5	n/a	0.011	n/a	n/a	n/a	n/a
triethanolamine	102-71-6	C102-71-6	6	OTH6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
propylene glycol n-propyl ether	1569-01-3	C1569-01-3	6	OTH6	ALK5	n/a	0.003	n/a	n/a	n/a	n/a

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butyl cellosolve {2-butoxyethanol} {egbe}	111-76-2	C111-76-2	6	OTH6	ALK5	n/a	1.128	n/a	n/a	n/a	n/a
carbitol {degee} {2-(2-ethoxyethoxy)ethanol}	111-90-0	C111-90-0	6	OTH6	ALK5	n/a	0.116	n/a	n/a	n/a	n/a
3-methyl-3-methoxy-1-butanol	56539-66-3	C56539-66-3	6	OTH6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
4-methyl-2-pentanol (methyl isobutyl carbinol)	108-11-2	C108-11-2	6	ROH5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
1-hexanol (n-hexanol)	111-27-3	C111-27-3	6	ROH6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
cyclohexanol	108-93-0	C108-93-0	6	ROH6	ALK5	n/a	0.006	n/a	n/a	n/a	n/a
2-(2-methoxypropoxy)-1-propanol (dipropylene glycol methyl ether isomer)	13588-28-8	C13588-28-8	7	OTH6	ALK5	n/a	0.096	n/a	n/a	n/a	n/a
ethyl-3-ethoxypropionate	763-69-9	C763-69-9	7	OTH6	ALK5	n/a	0.005	n/a	n/a	n/a	n/a
propylene glycol butyl ether {1-butoxy-2-propanol}	5131-66-8	C5131-66-8	7	OTH6	ALK5	n/a	0.110	n/a	n/a	n/a	n/a
propyleneglycol-t-butylether{1-(1,1,-dimethylethoxy)-2-propanol}	57018-52-7	C57018-52-7	7	OTH6	ALK5	n/a	0.004	n/a	n/a	n/a	n/a
1-heptanol	111-70-6	C111-70-6	7	ROH6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
dimethyl adipate (dimethylhexanedioate)	627-93-0	C627-93-0	8	OTH5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
2-butyltetrahydrofuran	1004-29-1	C1004-29-1	8	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
dibutyl ether	142-96-1	C142-96-1	8	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
2-(2-butoxyethoxy)ethanol {butyl carbitol}	112-34-5	C112-34-5	8	OTH6	ALK5	n/a	0.103	n/a	n/a	n/a	n/a
2-ethyl-1-hexanol	104-76-7	C104-76-7	8	ROH5	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
4-Octanol	589-62-8	C589-62-8	8	ROH6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
2-Octanol	4128-31-8	C4128-31-8	8	ROH6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
3-Octanol	20296-29-1	C20296-29-1	8	ROH6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
1-octanol	111-87-5	C111-87-5	8	ROH6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
isoamyl isobutyrate	2050-01-3	C2050-01-3	9	OTH5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
glyceryl triacetate	102-76-1	C102-76-1	9	OTH5	ALK5	n/a	0.002	n/a	n/a	n/a	n/a

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Dipropylene glycol methyl ether acetate isomer #1	n/a	Sc-88917-22-0a	9	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
Dipropylene glycol methyl ether acetate isomer #2	n/a	Sc-88917-22-0b	9	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
molinate	2212-67-1	C2212-67-1	9	OTH6	ALK5	n/a	0.015	n/a	n/a	n/a	n/a
eptc {s-ethyl dipropylthiocarbamate}	759-94-4	C759-94-4	9	OTH6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
trimethylcyclohexanol	1321-60-4	C1321-60-4	9	ROH6	ALK5	n/a	0.003	n/a	n/a	n/a	n/a
pebulate	1114-71-2	C1114-71-2	10	OTH6	ALK5	n/a	0.002	n/a	n/a	n/a	n/a
diethylene glycol butyl ether acetate {2-2-(butoxyethoxy)ethylacetate}	124-17-4	C124-17-4	10	OTH6	ALK5	n/a	0.005	n/a	n/a	n/a	n/a
glycol ether dpnb {1-(2-butoxy-1-methylethoxy)-2-propanol}	29911-28-2	C29911-28-2	10	OTH6	ALK5	n/a	0.017	n/a	n/a	n/a	n/a
menthol	89-78-1	C89-78-1	10	ROH6	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	18491-15-1	C18491-15-1	12	OTH5	ALK5	n/a	0.018	n/a	n/a	n/a	n/a
diisopropyl adipate	6938-94-9	C6938-94-9	12	OTH5	ALK5	n/a	0.001	n/a	n/a	n/a	n/a
3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	77-68-9	C77-68-9	12	OTH6	ALK5	n/a	0.018	n/a	n/a	n/a	n/a
methyl dodecanoate {methyl laurate}	111-82-0	C111-82-0	13	OTH5	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
methyl myristate {methyl tetradecanoate}	124-10-7	C124-10-7	15	OTH6	ALK5	n/a	0.000	n/a	n/a	n/a	n/a
ethylene	74-85-1	C74-85-1	2	ETHE	ETHE	6.313	11.911	10.177	6.225	5.916	6.313
propylene	115-07-1	C115-07-1	3	PRPE	OLE1	2.239	4.586	4.469	2.527	2.402	2.239
acrylic acid	79-10-7	C79-10-7	3	OLE1	OLE1	n/a	0.000	n/a	n/a	n/a	n/a
vinylacetylene	689-97-4	C689-97-4	3	OLE1	OLE1	n/a	0.065	n/a	n/a	n/a	n/a
1-butene	106-98-9	C106-98-9	4	OLE1	OLE1	1.075	0.838	0.794	0.425	0.404	1.075
C4 Terminal Alkenes	n/a	SM-C4-OLE1	4	OLE1	OLE1	0.134	n/a	n/a	n/a	n/a	0.134
methyl acrylate	96-33-3	C96-33-3	4	OLE1	OLE1	n/a	0.000	n/a	n/a	n/a	n/a
vinyl acetate	108-05-4	C108-05-4	4	OLE1	OLE1	n/a	0.009	n/a	n/a	n/a	n/a

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1-pentene	109-67-1	C109-67-1	5	OLE1	OLE1	0.940	0.312	0.363	0.638	0.606	0.940
3-methyl-1-butene	563-45-1	C563-45-1	5	OLE1	OLE1	0.381	0.225	0.188	n/a	0.164	0.381
C5 Terminal Alkenes	n/a	SM-C5-OLE1	5	OLE1	OLE1	0.515	n/a	n/a	n/a	n/a	0.515
ethyl acrylate	140-88-5	C140-88-5	5	OLE1	OLE1	n/a	0.002	n/a	n/a	n/a	n/a
1-methyl-2-pyrrolidinone	872-50-4	C872-50-4	5	OLE1	OLE1	n/a	0.012	n/a	n/a	n/a	n/a
1-hexene	592-41-6	C592-41-6	6	OLE1	OLE1	0.470	0.108	0.184	n/a	0.161	0.470
C6 Terminal Alkenes	n/a	SM-C6-OLE1	6	OLE1	OLE1	3.134	n/a	n/a	n/a	n/a	3.134
3-methyl-1-pentene	760-20-3	C760-20-3	6	OLE1	OLE1	n/a	0.073	n/a	n/a	n/a	n/a
4-methyl-1-pentene	691-37-2	C691-37-2	6	OLE1	OLE1	n/a	0.048	0.195	n/a	0.170	n/a
3,3-dimethyl-1-butene	558-37-2	C558-37-2	6	OLE1	OLE1	n/a	0.601	n/a	n/a	n/a	n/a
C7 Terminal Alkenes	n/a	SM-C7-OLE1	6	OLE1	OLE1	1.948	0.005	n/a	n/a	n/a	1.948
3-methyl-1-hexene	3404-61-3	C3404-61-3	7	OLE1	OLE1	n/a	0.000	n/a	n/a	n/a	n/a
3,4-dimethyl-1-pentene	7385-78-6	C7385-78-6	7	OLE1	OLE1	n/a	0.002	n/a	n/a	n/a	n/a
3,3-dimethyl-1-pentene	3404-73-7	C3404-73-7	7	OLE1	OLE1	n/a	0.029	n/a	n/a	n/a	n/a
1-heptene	592-76-7	C592-76-7	7	OLE1	OLE1	n/a	0.022	n/a	n/a	n/a	n/a
n-butyl acrylate	141-32-2	C141-32-2	7	OLE1	OLE1	n/a	0.001	n/a	n/a	n/a	n/a
isobutyl acrylate {2-propenoic acid}	106-63-8	C106-63-8	7	OLE1	OLE1	n/a	0.000	n/a	n/a	n/a	n/a
C8 Terminal Alkenes	n/a	SM-C8-OLE1	8	OLE1	OLE1	0.448	0.003	n/a	n/a	n/a	0.448
1-octene	111-66-0	C111-66-0	8	OLE1	OLE1	n/a	0.016	n/a	n/a	n/a	n/a
C9 Terminal Alkenes	n/a	SM-C9-OLE1	9	OLE1	OLE1	1.097	0.007	n/a	n/a	n/a	1.097
1-nonene	124-11-8	C124-11-8	9	OLE1	OLE1	n/a	0.030	n/a	n/a	n/a	n/a
C10 Terminal Alkenes	n/a	SM-C10-OLE1	10	OLE1	OLE1	0.224	0.000	n/a	n/a	n/a	0.224
1-decene	872-05-9	C872-05-9	10	OLE1	OLE1	n/a	0.006	n/a	n/a	n/a	n/a
C11 Terminal Alkenes	n/a	SM-C11-OLE1	11	OLE1	OLE1	0.492	0.007	n/a	n/a	n/a	0.492
1-Dodecene	112-41-4	C112-41-4	12	OLE1	OLE1	n/a	0.000	n/a	n/a	n/a	n/a
C13 Terminal Alkenes	n/a	SM-C13-OLE1	13	OLE1	OLE1	n/a	0.001	n/a	n/a	n/a	n/a
1-Tetradecene	1120-36-1	C1120-36-1	14	OLE1	OLE1	n/a	0.000	n/a	n/a	n/a	n/a
1-propyne	74-99-7	C74-99-7	3	ALYN1	OLE1	n/a	0.317	n/a	n/a	n/a	n/a
1-butyne (ethylacetylene)	107-00-6	C107-00-6	4	ALYN1	OLE1	n/a	0.001	n/a	n/a	n/a	n/a
1,2-propadiene	463-49-0	C463-49-0	3	ALLE1	OLE1	n/a	0.303	n/a	n/a	n/a	n/a
1,2-butadiene {methylallene}	590-19-2	C590-19-2	4	ALLE1	OLE1	n/a	0.026	n/a	n/a	n/a	n/a

Species	CAS Number	Carter SDB ID [a]	#C	Carter Emis-sion Group [a]	S07 Spec. Group [a]	ARBROG profile [b]	Emission LA [c]	SCOS97 LA Average [c]	PAMS LA Average [c]	PAMS / SCOS patch [c]	PAMS / SCOS / Emis patch [d]
trans-2-butene	624-64-6	C624-64-6	4	OLE2	OLE2	1.075	0.541	0.576	0.458	0.435	1.075
cis-2-butene	590-18-1	C590-18-1	4	OLE2	OLE2	0.851	0.327	0.359	0.196	0.186	0.851
C4 Internal Alkenes	n/a	SM-C4-OLE2	4	OLE2	OLE2	0.134	n/a	n/a	n/a	n/a	0.134
2-methylpropene (isobutene)	115-11-7	C115-11-7	4	OLE2	OLE2	1.075	1.613	3.182	n/a	2.547	1.075
1,3-butadiene	106-99-0	C106-99-0	4	13BDE	OLE2	0.582	0.752	0.683	n/a	0.547	0.582
trans-2-pentene	646-04-8	C646-04-8	5	OLE2	OLE2	n/a	0.502	0.518	0.534	0.507	n/a
cis-2-pentene	627-20-3	C627-20-3	5	OLE2	OLE2	n/a	0.238	0.300	0.289	0.275	n/a
2-methyl-2-butene	513-35-9	C513-35-9	5	OLE2	OLE2	0.604	0.778	0.732	n/a	0.586	0.604
C5 Internal Alkenes	n/a	SM-C5-OLE2	5	OLE2	OLE2	3.716	n/a	n/a	n/a	n/a	3.716
2-methyl-1-butene	563-46-2	C563-46-2	5	OLE2	OLE2	1.075	0.411	0.577	n/a	0.462	1.075
trans-1,3-pentadiene	2004-70-8	C2004-70-8	5	OLEM	OLE2	n/a	0.022	n/a	n/a	n/a	n/a
1,4-pentadiene	591-93-5	C591-93-5	5	OLEM	OLE2	n/a	0.000	n/a	n/a	n/a	n/a
cyclopentene	142-29-0	C142-29-0	5	OLE2	OLE2	n/a	0.190	0.217	n/a	0.174	n/a
1,3-cyclopentadiene	542-92-7	C542-92-7	5	OLE2	OLE2	n/a	0.002	n/a	n/a	n/a	n/a
cis-2-hexene	7688-21-3	C7688-21-3	6	OLE2	OLE2	n/a	0.067	0.114	n/a	0.091	n/a
trans-2-hexene	4050-45-7	C4050-45-7	6	OLE2	OLE2	n/a	0.170	0.505	n/a	0.404	n/a
4-methyl-trans-2-hexene	3683-22-5	C3683-22-5	6	OLE2	OLE2	n/a	0.103	n/a	n/a	n/a	n/a
3-methyl-trans-2-hexene	20710-38-7	C20710-38-7	6	OLE2	OLE2	n/a	0.019	n/a	n/a	n/a	n/a
cis-3-hexene	7642-09-3	C7642-09-3	6	OLE2	OLE2	n/a	0.023	n/a	n/a	n/a	n/a
2-methyl-2-pentene	625-27-4	C625-27-4	6	OLE2	OLE2	n/a	0.152	0.387	n/a	0.310	n/a
trans-3-hexene	13269-52-8	C13269-52-8	6	OLE2	OLE2	n/a	0.054	n/a	n/a	n/a	n/a
3-methyl-cis-2-pentene	922-62-3	C922-62-3	6	OLE2	OLE2	n/a	0.021	n/a	n/a	n/a	n/a
C6 Internal Alkenes	n/a	SM-C6-OLE2	6	OLE2	OLE2	1.410	0.007	n/a	n/a	n/a	1.410
2,3-dimethyl-1-butene	563-78-0	C563-78-0	6	OLE2	OLE2	n/a	0.018	n/a	n/a	n/a	n/a
2-ethyl-1-butene	760-21-4	C760-21-4	6	OLE2	OLE2	n/a	0.007	n/a	n/a	n/a	n/a
2-methyl-1-pentene	763-29-1	C763-29-1	6	OLE2	OLE2	n/a	0.086	0.142	n/a	0.114	n/a
cyclohexene	110-83-8	C110-83-8	6	OLE2	OLE2	0.246	0.060	n/a	n/a	n/a	0.246
3-methylcyclopentene	1120-62-3	C1120-62-3	6	OLE2	OLE2	n/a	0.075	n/a	n/a	n/a	n/a
1-methylcyclopentene	693-89-0	C693-89-0	6	OLE2	OLE2	n/a	0.028	n/a	n/a	n/a	n/a
2-methyl-2-hexene	2738-19-4	C2738-19-4	7	OLE2	OLE2	n/a	0.014	n/a	n/a	n/a	n/a
3-methyl-cis-2-hexene	10574-36-4	C10574-36-4	7	OLE2	OLE2	n/a	0.045	n/a	n/a	n/a	n/a
3-methyl-trans-3-hexene	3899-36-3	C3899-36-3	7	OLE2	OLE2	n/a	0.014	n/a	n/a	n/a	n/a

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2,3-Dimethyl-2-Hexene	7145-20-2	C7145-20-2	7	OLE2	OLE2	n/a	0.008	n/a	n/a	n/a	n/a
2,4-dimethyl-2-pentene	625-65-0	C625-65-0	7	OLE2	OLE2	n/a	0.033	n/a	n/a	n/a	n/a
2-methyl-trans-3-hexene	692-24-0	C692-24-0	7	OLE2	OLE2	n/a	0.031	n/a	n/a	n/a	n/a
3-methyl-cis-3-hexene	4914-89-0	C4914-89-0	7	OLE2	OLE2	n/a	0.006	n/a	n/a	n/a	n/a
trans-2-heptene	14686-13-6	C14686-13-6	7	OLE2	OLE2	n/a	0.030	n/a	n/a	n/a	n/a
cis-2-heptene	6443-92-1	C6443-92-1	7	OLE2	OLE2	n/a	0.030	n/a	n/a	n/a	n/a
trans-3-heptene	14686-14-7	C14686-14-7	7	OLE2	OLE2	n/a	0.055	n/a	n/a	n/a	n/a
3-ethyl-2-pentene	816-79-5	C816-79-5	7	OLE2	OLE2	n/a	0.005	n/a	n/a	n/a	n/a
cis-3-heptene	7642-10-6	C7642-10-6	7	OLE2	OLE2	n/a	0.000	n/a	n/a	n/a	n/a
C7 Internal Alkenes	n/a	SM-C7-OLE2	7	OLE2	OLE2	0.716	0.016	n/a	n/a	n/a	0.716
2,4-dimethyl-1-pentene	2213-32-3	C2213-32-3	7	OLE2	OLE2	n/a	0.016	n/a	n/a	n/a	n/a
C7 Cyclic or di-olefins	n/a	SM-C7-OL2D	7	OLE2	OLE2	0.313	0.000	n/a	n/a	n/a	0.313
trans-4-octene	14850-23-8	C14850-23-8	8	OLE2	OLE2	n/a	0.002	n/a	n/a	n/a	n/a
trans-2-octene	13389-42-9	C13389-42-9	8	OLE2	OLE2	n/a	0.007	n/a	n/a	n/a	n/a
Trans 2,5-Dimethyl 3-Hexene	692-70-6	C692-70-6	8	OLE2	OLE2	n/a	0.000	n/a	n/a	n/a	n/a
2,4,4-trimethyl-1-pentene	107-39-1	C107-39-1	8	OLE2	OLE2	n/a	n/a	0.198	n/a	0.159	n/a
C8 Internal Alkenes	n/a	SM-C8-OLE2	8	OLE2	OLE2	0.403	0.008	n/a	n/a	n/a	0.403
C8 Cyclic or di-olefins	n/a	SM-C8-OL2D	8	OLE2	OLE2	n/a	0.330	n/a	n/a	n/a	n/a
Trans-4-Nonene	10405-85-3	C10405-85-3	9	OLE2	OLE2	n/a	0.001	n/a	n/a	n/a	n/a
c9 internal alkenes	n/a	S2-98042	9	OLE2	OLE2	0.515	0.009	n/a	n/a	n/a	0.515
C9 Cyclic or di-olefins	n/a	SM-C9-OL2D	9	OLE2	OLE2	n/a	0.019	n/a	n/a	n/a	n/a
3,4-Diethyl-2-Hexene (E)	59643-70-8	C59643-70-8	10	OLE2	OLE2	n/a	0.009	n/a	n/a	n/a	n/a
Trans-4-Decene	19398-89-1	C19398-89-1	10	OLE2	OLE2	n/a	0.009	n/a	n/a	n/a	n/a
c10 internal alkenes	n/a	S2-98039	10	OLE2	OLE2	0.224	0.041	n/a	n/a	n/a	0.224
C10 Cyclic or di-olefins	n/a	SM-C10-OL2D	10	OLE2	OLE2	n/a	0.000	n/a	n/a	n/a	n/a
c11 internal alkenes	n/a	S2-43146	11	OLE2	OLE2	0.492	0.028	n/a	n/a	n/a	0.492
Trans-5-Dodecene	7206-16-8	C7206-16-8	12	OLE2	OLE2	n/a	0.002	n/a	n/a	n/a	n/a
3,4,6-trimethyl-2-heptene	n/a	Sx-012	13	OLE2	OLE2	n/a	0.006	n/a	n/a	n/a	n/a
Trans-5-Tridecene	23051-84-5	C23051-84-5	13	OLE2	OLE2	n/a	0.005	n/a	n/a	n/a	n/a
Trans-5-Tetradecene	41446-66-6	C41446-66-6	14	OLE2	OLE2	n/a	0.000	n/a	n/a	n/a	n/a
styrene	100-42-5	C100-42-5	8	STYR	OLE2	n/a	0.251	1.477	2.096	1.992	n/a
b-methylstyrene	637-50-3	C637-50-3	9	STYR	OLE2	n/a	0.011	n/a	n/a	n/a	n/a

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indene	95-13-6	C95-13-6	9	STYR	OLE2	n/a	0.008	n/a	n/a	n/a	n/a
a-methylstyrene	98-83-9	C98-83-9	9	STYR	OLE2	n/a	0.000	n/a	n/a	n/a	n/a
C9 Styrenes	n/a	SM-C9-STYR	9	STYR	OLE2	1.007	n/a	n/a	n/a	n/a	1.007
C10 Styrenes	n/a	SM-C10-STYR	10	STYR	OLE2	0.851	0.000	n/a	n/a	n/a	0.851
1,3-butadiyne	460-12-8	C460-12-8	4	ALYN2	OLE2	n/a	0.008	n/a	n/a	n/a	n/a
2-butyne	503-17-3	C503-17-3	4	ALYN2	OLE2	n/a	0.004	n/a	n/a	n/a	n/a
2-methyl-3-buten-2-ol	115-18-4	C115-18-4	5	MUNST	OLE2	n/a	0.808	n/a	n/a	n/a	n/a
methyl methacrylate	80-62-6	C80-62-6	5	MUNST	OLE2	n/a	0.061	n/a	n/a	n/a	n/a
isoprene	78-79-5	C78-79-5	5	ISOP	ISOP	1.522	10.692	0.313	1.206	1.146	1.522
3-carene	13466-78-9	C13466-78-9	10	TERP	TERP	0.448	1.247	n/a	n/a	n/a	0.448
Sabinene	3387-41-5	C3387-41-5	10	TERP	TERP	n/a	0.790	n/a	n/a	n/a	n/a
d-limonene	5989-27-5	C5989-27-5	10	TERP2	TERP	n/a	0.966	n/a	n/a	n/a	n/a
a-pinene	80-56-8	C80-56-8	10	APIN	TERP	1.186	3.283	n/a	n/a	n/a	1.186
b-pinene	127-91-3	C127-91-3	10	BPIN	TERP	n/a	2.040	n/a	n/a	n/a	n/a
benzene	71-43-2	C71-43-2	6	BENZ	BENZ	4.634	3.531	5.056	2.842	2.700	4.634
chlorobenzene	108-90-7	C108-90-7	6	HBEN1	ARO1	n/a	0.078	n/a	n/a	n/a	n/a
p-dichlorobenzene	106-46-7	C106-46-7	6	HBEN1	ARO1	n/a	0.397	n/a	n/a	n/a	n/a
o-dichlorobenzene	95-50-1	C95-50-1	6	HBEN1	ARO1	n/a	0.049	n/a	n/a	n/a	n/a
ethylbenzene	100-41-4	C100-41-4	8	ARO1	ARO1	2.395	2.382	3.111	2.020	1.920	2.395
cumene (isopropyl benzene)	98-82-8	C98-82-8	9	ARO1	ARO1	0.403	0.109	0.228	0.498	0.473	0.403
n-propylbenzene	103-65-1	C103-65-1	9	ARO1	ARO1	0.761	0.384	0.852	0.747	0.710	0.761
C9 Monosubstituted Benzenes	n/a	SM-C9-BEN1	9	ARO1	ARO1	0.336	n/a	n/a	n/a	n/a	0.336
(1-methylpropyl)benzene (sec-butyl benzene)	135-98-8	C135-98-8	10	ARO1	ARO1	0.537	0.036	2.094	n/a	1.551	0.537
C10 Monosubstituted Benzenes	n/a	SM-C10-BEN1	10	ARO1	ARO1	0.425	0.046	n/a	n/a	n/a	0.425
n-butylbenzene	104-51-8	C104-51-8	10	ARO1	ARO1	n/a	0.111	n/a	n/a	n/a	n/a
t-butylbenzene	98-06-6	C98-06-6	10	ARO1	ARO1	n/a	0.028	n/a	n/a	n/a	n/a
C11 Monosubstituted Benzenes	n/a	SM-C11-BEN1	11	ARO1	ARO1	1.679	0.036	n/a	n/a	n/a	1.679
n-pentylbenzene	538-68-1	C538-68-1	11	ARO1	ARO1	n/a	0.021	n/a	n/a	n/a	n/a
C12 Monosubstituted Benzenes	n/a	SM-C12-BEN1	12	ARO1	ARO1	0.067	0.015	n/a	n/a	n/a	0.067
C13 Monosubstituted Benzenes	n/a	SM-C13-BEN1	13	ARO1	ARO1	n/a	0.005	n/a	n/a	n/a	n/a
toluene	108-88-3	C108-88-3	7	TOLU	ARO1	15.155	12.605	19.109	18.481	17.563	15.155

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o-chlorotoluene	95-49-8	C95-49-8	7	TOLU	ARO1	n/a	0.001	n/a	n/a	n/a	n/a
benzyl alcohol	100-51-6	C100-51-6	7	BOAT	ARO1	n/a	0.005	n/a	n/a	n/a	n/a
phthalic anhydride	85-44-9	C85-44-9	8	BOAT	ARO1	n/a	0.003	n/a	n/a	n/a	n/a
2-phenoxyethanol	122-99-6	C122-99-6	8	BOAT	ARO1	n/a	0.006	n/a	n/a	n/a	n/a
dibutyl phthalate	84-74-2	C84-74-2	16	BOAT	ARO1	n/a	0.001	n/a	n/a	n/a	n/a
thiobencarb	28249-77-6	C28249-77-6	12	MARO	ARO1	n/a	0.002	n/a	n/a	n/a	n/a
o-xylene	95-47-6	C95-47-6	8	OXYL	ARO2	3.425	2.589	3.956	2.510	2.386	3.425
m-xylene	108-38-3	C108-38-3	8	MXYL	ARO2	4.097	5.290	5.261	3.254	3.092	4.097
p-xylene	106-42-3	C106-42-3	8	PXYL	ARO2	4.097	1.099	5.261	3.254	3.092	4.097
m-xylene and p-xylene	n/a	S1-90010	9	ARO2	ARO2	n/a	n/a	n/a	n/a	n/a	n/a
1,2,4-trimethylbenzene	95-63-6	C95-63-6	9	B124	ARO2	n/a	1.777	2.094	2.664	2.532	n/a
m-ethyltoluene	620-14-4	C620-14-4	9	ARO2	ARO2	n/a	1.228	1.457	1.872	1.779	n/a
p-ethyltoluene	622-96-8	C622-96-8	9	ARO2	ARO2	n/a	0.570	2.810	1.292	1.228	n/a
1,3,5-trimethylbenzene	108-67-8	C108-67-8	9	ARO2	ARO2	1.522	0.639	1.713	1.079	1.026	1.522
o-ethyltoluene	611-14-3	C611-14-3	9	ARO2	ARO2	n/a	0.487	1.250	1.145	1.088	n/a
1,2,3-trimethylbenzene	526-73-8	C526-73-8	9	ARO2	ARO2	1.589	0.424	n/a	1.224	1.163	1.589
ethyltoluenes {methylethylbenzenes}	25550-14-5	C25550-14-5	9	ARO2	ARO2	5.216	n/a	n/a	n/a	n/a	5.216
trimethylbenzenes	25551-13-7	C25551-13-7	9	ARO2	ARO2	4.970	n/a	n/a	n/a	n/a	4.970
1,3-diethylbenzene (meta)	141-93-5	C141-93-5	10	ARO2	ARO2	n/a	0.098	n/a	1.106	1.051	n/a
1,4-diethylbenzene (para)	105-05-5	C105-05-5	10	ARO2	ARO2	n/a	0.095	n/a	0.627	0.596	n/a
c10 dialkyl benzenes	n/a	S2-45248	10	ARO2	ARO2	3.604	n/a	n/a	n/a	n/a	3.604
ethyldimethylbenzenes	n/a	S1-45243	10	ARO2	ARO2	3.761	n/a	n/a	n/a	n/a	3.761
c10 tetrasubstituted benzenes	n/a	S1-45244	10	ARO2	ARO2	0.985	n/a	n/a	n/a	n/a	0.985
1,2-diethylbenzene (ortho)	135-01-3	C135-01-3	10	ARO2	ARO2	n/a	0.042	n/a	n/a	n/a	n/a
1,2,4,5-tetramethylbenzene	95-93-2	C95-93-2	10	ARO2	ARO2	n/a	0.098	n/a	n/a	n/a	n/a
1,2,3,5-tetramethylbenzene	527-53-7	C527-53-7	10	ARO2	ARO2	n/a	0.132	n/a	n/a	n/a	n/a
1,2,3,4-tetramethylbenzene	488-23-3	C488-23-3	10	ARO2	ARO2	n/a	0.032	n/a	n/a	n/a	n/a
1-methyl-4-isopropylbenzene	99-87-6	C99-87-6	10	ARO2	ARO2	n/a	0.019	n/a	n/a	n/a	n/a
1-methyl-3-isopropylbenzene	535-77-3	C535-77-3	10	ARO2	ARO2	n/a	0.098	n/a	n/a	n/a	n/a
1,4-dimethyl-2-ethylbenzene	1758-88-9	C1758-88-9	10	ARO2	ARO2	n/a	0.141	n/a	n/a	n/a	n/a
1,3-dimethyl-4-ethylbenzene	874-41-9	C874-41-9	10	ARO2	ARO2	n/a	0.133	n/a	n/a	n/a	n/a

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1,2-dimethyl-4-ethylbenzene	934-80-5	C934-80-5	10	ARO2	ARO2	n/a	0.234	n/a	n/a	n/a	n/a
1,3-dimethyl-2-ethylbenzene	2870-04-4	C2870-04-4	10	ARO2	ARO2	n/a	0.059	n/a	n/a	n/a	n/a
1,2-dimethyl-3-ethylbenzene	933-98-2	C933-98-2	10	ARO2	ARO2	n/a	0.036	n/a	n/a	n/a	n/a
1,3-dimethyl-5-ethylbenzene	934-74-7	C934-74-7	10	ARO2	ARO2	n/a	0.210	n/a	n/a	n/a	n/a
1-methyl-3n-propylbenzene	1074-43-7	C1074-43-7	10	ARO2	ARO2	n/a	0.229	n/a	n/a	n/a	n/a
1-methyl-4n-propylbenzene	1074-55-1	C1074-55-1	10	ARO2	ARO2	n/a	0.111	n/a	n/a	n/a	n/a
1-methyl-2n-propylbenzene	1074-17-5	C1074-17-5	10	ARO2	ARO2	n/a	0.032	n/a	n/a	n/a	n/a
1-methyl-2-isopropylbenzene	527-84-4	C527-84-4	10	ARO2	ARO2	n/a	0.068	n/a	n/a	n/a	n/a
c11 dialkyl benzenes	n/a	S2-45245	11	ARO2	ARO2	0.246	n/a	n/a	n/a	n/a	0.246
c11 trialkyl benzenes	n/a	S2-45246	11	ARO2	ARO2	0.246	n/a	n/a	n/a	n/a	0.246
1-ethyl-2-propyl benzene	n/a	DMS-OC11BEN2-1	11	ARO2	ARO2	n/a	0.042	n/a	n/a	n/a	n/a
1-methyl-2-tert-butylbenzene	1074-92-6	C1074-92-6	11	ARO2	ARO2	n/a	0.002	n/a	n/a	n/a	n/a
1-methyl-3-butylbenzene	1595-04-6	C1595-04-6	11	ARO2	ARO2	n/a	0.013	n/a	n/a	n/a	n/a
C11 Tetrasubstituted Benzenes	n/a	SM-C11-BEN4	11	ARO2	ARO2	n/a	0.003	n/a	n/a	n/a	n/a
1,2-diethyl-4-methylbenzene	n/a	DMS-4C11BEN3-1	11	ARO2	ARO2	n/a	0.008	n/a	n/a	n/a	n/a
1,3,5-c11 trisubstituted benzenes	n/a	DMS-5C11BEN3	11	ARO2	ARO2	n/a	0.000	n/a	n/a	n/a	n/a
1,3-diethyl-5-methyl benzene	2050-24-0	C2050-24-0	11	ARO2	ARO2	n/a	0.000	n/a	n/a	n/a	n/a
pentamethylbenzene	700-12-9	C700-12-9	11	ARO2	ARO2	n/a	0.004	n/a	n/a	n/a	n/a
1-ethyl-4-propyl benzene	n/a	DMS-PC11BEN2-1	11	ARO2	ARO2	n/a	0.038	n/a	n/a	n/a	n/a
c12 dialkyl benzenes	n/a	S0-45247	12	ARO2	ARO2	0.246	n/a	n/a	n/a	n/a	0.246
C12 Trisubstituted Benzenes	n/a	SM-C12-BEN3	12	ARO2	ARO2	0.246	n/a	n/a	n/a	n/a	0.246
1,3-dipropylbenzene	n/a	DMS-MC12BEN2-1	12	ARO2	ARO2	n/a	0.032	n/a	n/a	n/a	n/a
1,4-dipropylbenzene	n/a	DMS-PC12BEN2-1	12	ARO2	ARO2	n/a	0.018	n/a	n/a	n/a	n/a
1,3-isodipropylbenzene	99-62-7	C99-62-7	12	ARO2	ARO2	n/a	0.001	n/a	n/a	n/a	n/a
1,4 diisopropyl benzene	100-18-5	C100-18-5	12	ARO2	ARO2	n/a	0.018	n/a	n/a	n/a	n/a
1-(1,1-dimethylethyl)-3,5-dimethylbenzene	98-19-1	C98-19-1	12	ARO2	ARO2	n/a	0.015	n/a	n/a	n/a	n/a
1,2,4-c12 trisubstituted benzenes	n/a	DMS-4C12BEN3	12	ARO2	ARO2	n/a	0.026	n/a	n/a	n/a	n/a
1,3,5-c12 trisubstituted benzenes	n/a	DMS-5C12BEN3	12	ARO2	ARO2	n/a	0.010	n/a	n/a	n/a	n/a
1,2-dipropylbenzene	n/a	DMS-OC12BEN2-1	12	ARO2	ARO2	n/a	0.000	n/a	n/a	n/a	n/a

Species	CAS Number	Carter SDB ID [a]	#C	Carter Emis-sion Group [a]	S07 Spec. Group [a]	ARBROG profile [b]	Emission LA [c]	SCOS97 LA Average [c]	PAMS LA Average [c]	PAMS / SCOS patch [c]	PAMS / SCOS / Emis patch [d]
1-propyl-3-n-butylbenzene	n/a	DMS-MC13BEN2-1	13	ARO2	ARO2	n/a	0.005	n/a	n/a	n/a	n/a
1,2-diethyl-4-propylbenzene	n/a	DMS-4C13BEN3-1	13	ARO2	ARO2	n/a	0.006	n/a	n/a	n/a	n/a
indan	496-11-7	C496-11-7	9	NAPT	ARO2	n/a	0.205	n/a	n/a	n/a	n/a
methylindans	27133-93-3	C27133-93-3	10	NAPT	ARO2	n/a	0.338	n/a	n/a	n/a	n/a
tetralin	119-64-2	C119-64-2	10	NAPT	ARO2	n/a	0.000	n/a	n/a	n/a	n/a
napthalene	91-20-3	C91-20-3	10	NAPT	ARO2	n/a	0.281	n/a	n/a	n/a	n/a
C11 Tetralin or Indane	n/a	SM-C11-TET	11	NAPT	ARO2	n/a	0.028	n/a	n/a	n/a	n/a
2-methylnaphthalene	91-57-6	C91-57-6	11	NAPT	ARO2	n/a	0.061	n/a	n/a	n/a	n/a
1-methyl naphthalene	90-12-0	C90-12-0	11	NAPT	ARO2	n/a	0.036	n/a	n/a	n/a	n/a
C12 Monosubstituted Naphthalene	n/a	SM-C12-NAP1	12	NAPT	ARO2	n/a	0.008	n/a	n/a	n/a	n/a
dimethyl napthalenes	28804-88-8	C28804-88-8	12	NAPT	ARO2	n/a	0.015	n/a	n/a	n/a	n/a
2,3-dimethylnaphthalene	581-40-8	C581-40-8	12	NAPT	ARO2	n/a	0.000	n/a	n/a	n/a	n/a
C12 Tetralin or Indane	n/a	SM-C12-TET	12	NAPT	ARO2	n/a	0.000	n/a	n/a	n/a	n/a
trimethylnaphthalene	28652-77-9	C28652-77-9	13	NAPT	ARO2	n/a	0.000	n/a	n/a	n/a	n/a
C13 monosubstituted naphthalene	n/a	DMS-C13-NAP1	13	NAPT	ARO2	n/a	0.000	n/a	n/a	n/a	n/a
phenol (carbolic acid)	108-95-2	C108-95-2	6	PHEN	CRES	n/a	0.112	n/a	n/a	n/a	n/a
o-cresol (2-methyl-benzenol)	95-48-7	C95-48-7	7	CRES	CRES	n/a	0.008	n/a	n/a	n/a	n/a
m-cresol (3-methyl-benzenol)	108-39-4	C108-39-4	7	CRES	CRES	n/a	0.007	n/a	n/a	n/a	n/a
p-cresol (4-methyl-benzenol)	106-44-5	C106-44-5	7	CRES	CRES	n/a	0.007	n/a	n/a	n/a	n/a
2,3-dimethyl phenol	526-75-0	C526-75-0	8	CRES	CRES	n/a	0.000	n/a	n/a	n/a	n/a
c9 phenols	n/a	S1-45311	9	CRES	CRES	n/a	0.000	n/a	n/a	n/a	n/a
c10 alkylphenols	n/a	S0-45303	10	CRES	CRES	n/a	0.027	n/a	n/a	n/a	n/a
c11 alkylphenols	n/a	S0-45304	11	CRES	CRES	n/a	0.003	n/a	n/a	n/a	n/a
formaldehyde	50-00-0	C50-00-0	1	HCHO	HCHO	1.858	2.790	n/a	5.430	5.160	1.858
acetaldehyde	75-07-0	C75-07-0	2	CCHO	CCHO	2.238	1.758	n/a	6.760	6.424	2.238
propionaldehyde	123-38-6	C123-38-6	3	RCHO	RCHO	0.492	0.295	n/a	n/a	n/a	0.492
C4 aldehydes	n/a	SM-C4-RCHO	4	RCHO	RCHO	0.291	n/a	n/a	n/a	n/a	0.291
butyraldehyde	123-72-8	C123-72-8	4	RCHO	RCHO	n/a	0.370	n/a	n/a	n/a	n/a

Species	CAS Number	Carter SDB ID [a]	#C	Carter Emis-sion Group [a]	S07 Spec. Group [a]	ARBROG profile [b]	Emission LA [c]	SCOS97 LA Average [c]	PAMS LA Average [c]	PAMS / SCOS patch [c]	PAMS / SCOS / Emis patch [d]
isobutyraldehyde	78-84-2	C78-84-2	4	RCHO	RCHO	n/a	0.000	n/a	n/a	n/a	n/a
c5 aldehyde	n/a	S2-43512	5	RCHO	RCHO	1.253	n/a	n/a	n/a	n/a	1.253
isovaleraldehyde (3-methylbutanal)	590-86-3	C590-86-3	5	RCHO	RCHO	n/a	0.043	n/a	n/a	n/a	n/a
n-pentanal (n-valeraldehyde)	110-62-3	C110-62-3	5	RCHO	RCHO	n/a	0.009	n/a	n/a	n/a	n/a
glutaraldehyde (a dialdehyde)	111-30-8	C111-30-8	5	RCHO	RCHO	n/a	0.008	n/a	n/a	n/a	n/a
c6 aldehydes	n/a	S2-98095	6	RCHO	RCHO	1.030	n/a	n/a	n/a	n/a	1.030
hexanal (hexanaladehyde)	66-25-1	C66-25-1	6	RCHO	RCHO	n/a	0.733	n/a	n/a	n/a	n/a
benzaldehyde	100-52-7	C100-52-7	7	AALD	BALD	0.269	0.425	n/a	n/a	n/a	0.269
methylbenzaldehyde isomers	1334-78-7	C1334-78-7	8	AALD	BALD	n/a	0.274	n/a	n/a	n/a	n/a
acetone	67-64-1	C67-64-1	3	ACET	ACET	2.171	6.239	n/a	23.601	22.429	2.171
methyl ethyl ketone (mek) (2-butanone)	78-93-3	C78-93-3	4	MEK	MEK	1.029	1.247	n/a	n/a	n/a	1.029
methyl propyl ketone (2-pentanone)	107-87-9	C107-87-9	5	KET1	MEK	n/a	0.000	n/a	n/a	n/a	n/a
diacetone alcohol (4-hydroxy-4-methyl-2-pentanone)	123-42-2	C123-42-2	6	HKET	MEK	n/a	0.047	n/a	n/a	n/a	n/a
cyclohexanone	108-94-1	C108-94-1	6	KET2	PRD2	n/a	0.053	n/a	n/a	n/a	n/a
methyl n-butyl ketone	591-78-6	C591-78-6	6	KET2	PRD2	n/a	0.159	n/a	n/a	n/a	n/a
methyl isobutyl ketone	108-10-1	C108-10-1	6	KET2	PRD2	n/a	0.139	n/a	n/a	n/a	n/a
methyl amyl ketone	110-43-0	C110-43-0	7	KET2	PRD2	n/a	0.144	n/a	n/a	n/a	n/a
2-methyl-3-hexanone	7379-12-6	C7379-12-6	7	KET2	PRD2	n/a	0.127	n/a	n/a	n/a	n/a
C8 Cyclic Ketones	n/a	SM-KET8C	8	KET2	PRD2	n/a	0.003	n/a	n/a	n/a	n/a
C9 Ketones	n/a	SM-KET9	9	KET2	PRD2	n/a	0.012	n/a	n/a	n/a	n/a
2-propyl cyclohexanone	94-65-5	C94-65-5	9	KET2	PRD2	n/a	0.000	n/a	n/a	n/a	n/a
4-propyl cyclohexanone	40649-36-3	C40649-36-3	9	KET2	PRD2	n/a	0.000	n/a	n/a	n/a	n/a
camphor	76-22-2	C76-22-2	10	KET2	PRD2	n/a	0.000	n/a	n/a	n/a	n/a
formic acid	64-18-6	C64-18-6	1	HCOOH	FACD	n/a	0.000	n/a	n/a	n/a	n/a
acetic acid	64-19-7	C64-19-7	2	CCOOH	AACD	n/a	0.024	n/a	n/a	n/a	n/a
glycolic acid {hydroxyacetic acid}	79-14-1	C79-14-1	2	RCOOH	PACD	n/a	0.000	n/a	n/a	n/a	n/a
propionic acid	79-09-4	C79-09-4	3	RCOOH	PACD	n/a	0.000	n/a	n/a	n/a	n/a
acetylene	74-86-2	C74-86-2	2	ACTYL	ACYE	4.567	4.736	11.802	4.610	4.381	4.567

Species	CAS Number	Carter SDB ID [a]	#C	Carter Emis-sion Group [a]	S07 Spec. Group [a]	ARBROG profile [b]	Emission LA [c]	SCOS97 LA Average [c]	PAMS LA Average [c]	PAMS / SCOS patch [c]	PAMS / SCOS / Emis patch [d]
methyl alcohol	67-56-1	C67-56-1	1	MEOH	MEOH	n/a	1.845	n/a	n/a	n/a	n/a
2-amino-2-methyl-1-propanol	124-68-5	C124-68-5	4	INHIB	NROG	n/a	0.001	n/a	n/a	n/a	n/a
octamethylcyclotetrasiloxane	556-67-2	C556-67-2	8	INHIB	NROG	n/a	0.628	n/a	n/a	n/a	n/a
2,4-toluene diisocyanate {tdi}	584-84-9	C584-84-9	9	INHIB	NROG	n/a	0.000	n/a	n/a	n/a	n/a
methene(b)4-phenylisocyanate {methylenediphenyldiisocyanate}	101-68-8	C101-68-8	15	INHIB	NROG	n/a	0.000	n/a	n/a	n/a	n/a
Unreactive compounds	n/a	INERT	1	INERT	NROG	n/a	0.015	n/a	n/a	n/a	n/a
methyl chloride	74-87-3	C74-87-3	1	INERT	NROG	n/a	0.000	n/a	n/a	n/a	n/a
Chloroform	67-66-3	C67-66-3	1	INERT	NROG	n/a	0.001	n/a	n/a	n/a	n/a
carbon tetrachloride	56-23-5	C56-23-5	1	INERT	NROG	n/a	0.000	n/a	n/a	n/a	n/a
methylene bromide	74-95-3	C74-95-3	1	INERT	NROG	n/a	0.000	n/a	n/a	n/a	n/a
methyl bromide	74-83-9	C74-83-9	1	INERT	NROG	n/a	0.025	n/a	n/a	n/a	n/a
nitromethane	75-52-5	C75-52-5	1	INERT	NROG	n/a	0.001	n/a	n/a	n/a	n/a
ethylene oxide	75-21-8	C75-21-8	2	INERT	NROG	n/a	0.007	n/a	n/a	n/a	n/a
1,1,1-trichloroethane	71-55-6	C71-55-6	2	INERT	NROG	n/a	2.593	n/a	n/a	n/a	n/a
1,1-difluoroethane (hfc-152a)	75-37-6	C75-37-6	2	INERT	NROG	n/a	0.105	n/a	n/a	n/a	n/a
3,3-dichloro-1,1,1,2,2-pentafluoropropane {hcfc-225ca}	422-56-0	C422-56-0	3	INERT	NROG	n/a	0.000	n/a	n/a	n/a	n/a
1,3-dichloro-1,1,2,2,3-pentafluoropropane {hcfc-225cb}	507-55-1	C507-55-1	3	INERT	NROG	n/a	0.000	n/a	n/a	n/a	n/a
1,1,1,2,3,4,4,5,5,5-decafluoropentane {hfc-43-10mee}	138495-42-8	C138495-42-8	5	INERT	NROG	n/a	0.000	n/a	n/a	n/a	n/a
1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-butane {c4f9och3}	163702-07-6	C163702-07-6	5	INERT	NROG	n/a	0.000	n/a	n/a	n/a	n/a
2-(fl2methoxymethyl)-1,1,1,2,3,3,3-fl7propane {(cf3)2cfcf2och3}	163702-08-7	C163702-08-7	5	INERT	NROG	n/a	0.001	n/a	n/a	n/a	n/a
Nitrobenzene	98-95-3	C98-95-3	6	INERT	NROG	n/a	0.000	n/a	n/a	n/a	n/a
Glyoxal	107-22-2	C107-22-2	2	GLY	GLY	n/a	0.045	n/a	n/a	n/a	n/a
methyl glyoxal	78-98-8	C78-98-8	3	MGLY	MGLY	n/a	0.044	n/a	n/a	n/a	n/a
acrolein (2-propenal)	107-02-8	C107-02-8	3	ACRO	MACR	n/a	0.158	n/a	n/a	n/a	n/a

Species	CAS Number	Carter SDB ID [a]	#C	Carter Emis-sion Group [a]	S07 Spec. Group [a]	ARBROG profile [b]	Emission LA [c]	SCOS97 LA Average [c]	PAMS LA Average [c]	PAMS / SCOS patch [c]	PAMS / SCOS / Emis patch [d]
2-methyl-2-propenal (methacrolein)	78-85-3	C78-85-3	4	MACR	MACR	n/a	0.085	n/a	n/a	n/a	n/a
Crotonaldehyde	4170-30-3	C4170-30-3	4	UALD	IPRD	n/a	0.130	n/a	n/a	n/a	n/a
Chloropicrin	76-06-2	C76-06-2	1	PHOT	BACL	n/a	0.006	n/a	n/a	n/a	n/a
Nonvolatile compounds	n/a	NONVOL	0	NVOL	NVOL	n/a	0.000	n/a	n/a	n/a	n/a
Total						234.446	234.446	234.446	234.446	234.446	234.446

[a] Carter (2010b). [b] Carter (1993) and Carter (2008), standard mixture of hydrocarbon and oxygenated organics being in use for incremental reactivity scales. The all of the profiles in this table were factored to have total of 234.446 ppbC. [c] Developed in this study, not used for box modeling in this report [d] Used for box modeling in this report.

Table 10 Species concentration profiles in Table 9 corresponding to rotate principal components in Table 1, factors 2 and 3

Species	CAS Number	Num C's	Carter's Emis-sion Group	SAPRC 07 group	ARBROG profile	Emission LA	SCOS97 LA Average	PAMS LA Average	PAMS / SCOS patch	PAMS / SCOS / Emis patch
acrolein (2-propenal)	107-02-8	3	ACRO	MACR	n/a	0.158	n/a	n/a	n/a	n/a
formaldehyde	50-00-0	1	HCHO	HCHO	1.858	2.790	n/a	5.430	5.160	4.543
acetaldehyde	75-07-0	2	CCHO	CCHO	2.238	1.758	n/a	6.760	6.424	5.656
propionaldehyde	123-38-6	3	RCHO	RCHO	0.492	0.295	n/a	n/a	n/a	0.662
o-xylene	95-47-6	8	OXYL	ARO2	3.425	2.589	3.956	2.510	2.386	2.100
m-xylene	108-38-3	8	MXYL	ARO2	4.097	5.290	5.261	3.254	3.092	2.722
p-xylene	106-42-3	8	PXYL	ARO2	4.097	1.099	5.261	3.254	3.092	2.722
m-xylene and p-xylene	n/a	8	ARO2	ARO2	0.336	n/a	n/a	n/a	n/a	n/a
1,3-butadiene	106-99-0	4	13BDE	OLE2	0.582	0.752	0.683	n/a	0.547	0.481
methyl bromide	74-83-9	1	INERT	NROG	n/a	0.025	n/a	n/a	n/a	n/a
cis-1,3-dichloropropene	10061-01-5	3	OTH5	ALK5	n/a	0.014	n/a	n/a	n/a	n/a
trans-1,3-dichloropropene	10061-02-6	3	OTH6	ALK5	n/a	0.014	n/a	n/a	n/a	n/a

Table 11 Sum of MIR for six profiles. All profiles assumes total ROG of 234.4 ppbC

Profiles	ARBROG profile	Emission LA	SCOS97 LA Average	PAMS LA Average	PAMS / SCOS patch	PAMS / SCOS / Emis patch
Sum of MIR (ppb O_3)	253.58	256.86	199.95	202.65	209.10	208.16

As shown in Table 11, the reactivity of the PAMS average profile is 50.9 ppb O_3 less than that of the ARBROG profile expressed as sum of MIR. Figure 23 shows that the contribution of relatively reactive species has a different degree of contribution to overall reactivity. For example, the OLE2 group accounts for 6.9 and 37.3 ppb O_3 in MIR for the PAMS and ARBROG profile, respectively.

Part of the reason for the smaller contribution of this group of species arises from the smaller set of species that were measured in the PAMS program. Under the PAMS sampling, some 40 – 60 species are measured, and in the Los Angeles data only 54 hydrocarbon species and 3 carbonyl species are available. In comparison, the 1997 SCOS study identified 69 hydrocarbon species. Figure 24 compares C4 and C5 species of alkenes with kOH>7x10^4 $ppm^{-1}min^{-1}$ (corresponding to "OLE2" species in lumped SAPRC07 mechanism). The PAMS profile does not include 2-methylpropene, 1,3-butadiene, 2-methyl-2-butene, 2-methyl-1-butene and cyclopentene. The ARBROG profile also lacks some of these species, but it instead has species mixtures such as "C5 internal olefins".

In order to augment the set of species in the PAMS species list, the observations from the SCOS study were used in following manner. First, species in each profile were grouped into a SAPRC07 species group. Using the SCOS profile, the contribution of each species within a species group was determined by ppbC. Then if a species *i* that belonged to a species group *G* was not included in the PAMS profile but was included in SCOS profile, its missing concentration was estimated as follows:

First, every species found in both the PAMS and SCOS profiles was identified. Then for each species group the ratio between the sums of concentration of these common species was determined.

$$f_G = \frac{\sum_{j \in G \wedge j \in (PAMS \cap SCOS)} C_{PAMS,j}}{\sum_{j \in G \wedge j \in (PAMS \cap SCOS)} C_{SCOS,j}}$$

$$C_{PAMS,i} = f_G \times C_{SCOS,i}$$

In the above expressions, f_G is ratio of the contribution of group *G* in each profile, determined by species common to both PAMS and SCOS. Using this f_G, the concentration of species *i* in the PAMS profile was determined by product of f_G and concentration in the SCOS profile. After the concentration PAMS species profile was augmented by using the above method, the entire profile was renormalized to have the original concentration of 233.7 ppbC, and the resulting

augmented and modified profile is referred to as the "PAMS/SCOS patch" profile. The profile is shown in Table 9 with column title "PAMS/SCOS patch".

The "PAMS/SCOS patch" profile has slightly higher reactivity than the original PAMS profile (7.2 ppb O_3 in terms of MIR, see Table 11) but still has lower overall MIR value than the ARBROG profile (43.7 ppb O_3 in MIR).

The ARBROG profile is composed not only with single compounds but also with groups of related compounds (e.g., C5 Internal Alkenes). Such grouped species account for 22 percent of the overall mass (ppbC) and 25 percent of the reactivity (ppb O_3 of MIR). This appears to cause large differences between the ARBROG profile and the new profiles generated in this work based on PAMS and SCOS observation.

In order to evaluate the augmentation of profiles, the profiles based on observations (PAMS or PAMS/SCOS patch) were compared against the ARBROG profile and also against the profiles derived from the emission inventory. First, it was identified that the following nine groups of species are affected by the mixture of species found in ARBROG profile, in terms of ppbC and/or the MIR weighted ppb O_3:

- branched alkanes,
- cyclic and bi-cyclic alkanes,
- external alkenes,
- internal alkenes,
- cyclic and di-alkenes,
- mono-substituted aromatics,
- multi-substituted aromatics,
- aldehydes
- ketones.

Figure 25 shows the distribution of branched alkanes in different profiles. It shows that C5 through C7 branched alkanes contribute similarly to the overall VOC regardless of the profile. For C8 branched alkanes, the PAMS profile (without patch) has a significantly smaller presence when compared to the ARBROG or Emis profile. Because of patching with the SCOS profile, which covers a wider range of species, the PAMS/SCOS profile behaves similarly to the ARBROG/Emis profile for C8 species. For C9 and greater compounds, even the PAMS/SCOS profile (patched profile) shows less contribution of these larger molecules in comparison to the ARBROG or Emis profile.

Similarly, Figure 26 shows the distribution of internal alkenes. For this class of species, the contribution in the ARBROG profile is grossly exaggerated in comparison to the Emis or PAMS profiles for molecules of any number of carbons. In contrast, the Emis profile and PAMS/SCOS profile behave similarly for C4 thorough C6 compounds. For the larger species, the observations (PAMS/SCOS) do not meet the larger concentrations found in the Emis profiles. This analysis was repeated for the remaining seven classes of species. It was found that (1) ARBROG

overestimates multi-substituted aromatics when compared to ambient observations or emissions as was the case for internal olefins and (2) profiles behave similarly for smaller molecules regardless of the origin of the ROG profile, but observations (PAMS or PAMS/SCOS patch) underestimate the contribution of larger molecules due to lack of measurements.

In order to remedy the discrepancy between ambient observations and emissions, an approach similar to the earlier described PAMS/SCOS patching was performed. Instead of SAPRC07 species group, the above nine species classes were used to group species, and the Emis profile was used to patch the PAMS/SCOS profile. The entire profile was renormalized to have total of 233.7 ppbC. This profile is referred to as "PAMS/SCOS/Emis patched" profile. The profile is shown in Table 9 with column header "PAMS/SCOS/Emis patch". In Figures 25 and 26, this new patched profile has a distribution closer to that of Emis, particularly for larger molecules. The larger contribution of reactive species in ARBROG was supported neither by ambient observation (PAMS profile) nor the emission inventory (Emis profile), and this new profile has less total MIR value than ARBROG.

Thus the "PAMS/SCOS/Emis patched" profile is selected for further analysis as a candidate to replace "ARBROG" profile. Total number of species in this new profile was 294, including 5 species whose concentration was zero. Of 294 species, 244 species represents single compounds whereas remaining 50 species represents group of similar species (simple mixture). Table 12 summarizes count of species of all six profiles.

Table 12 Count of species in six profiles

Profiles	ARBROG profile	Emission LA	SCOS97 LA Average	PAMS LA Average	PAMS / SCOS patch	PAMS / SCOS / Emis patch
Single Compound	62	457	71	58	79	244
Mixture of Similar Compounds	42	64	0	0	0	50
Total [a]	104 (0)	521 (10)	71 (0)	58 (0)	79 (2)	294 (5)

[a] Species with zero concentration are shown in parenthesis.

Figure 22 Composition of profiles by SAPRC07 species group in ppbC

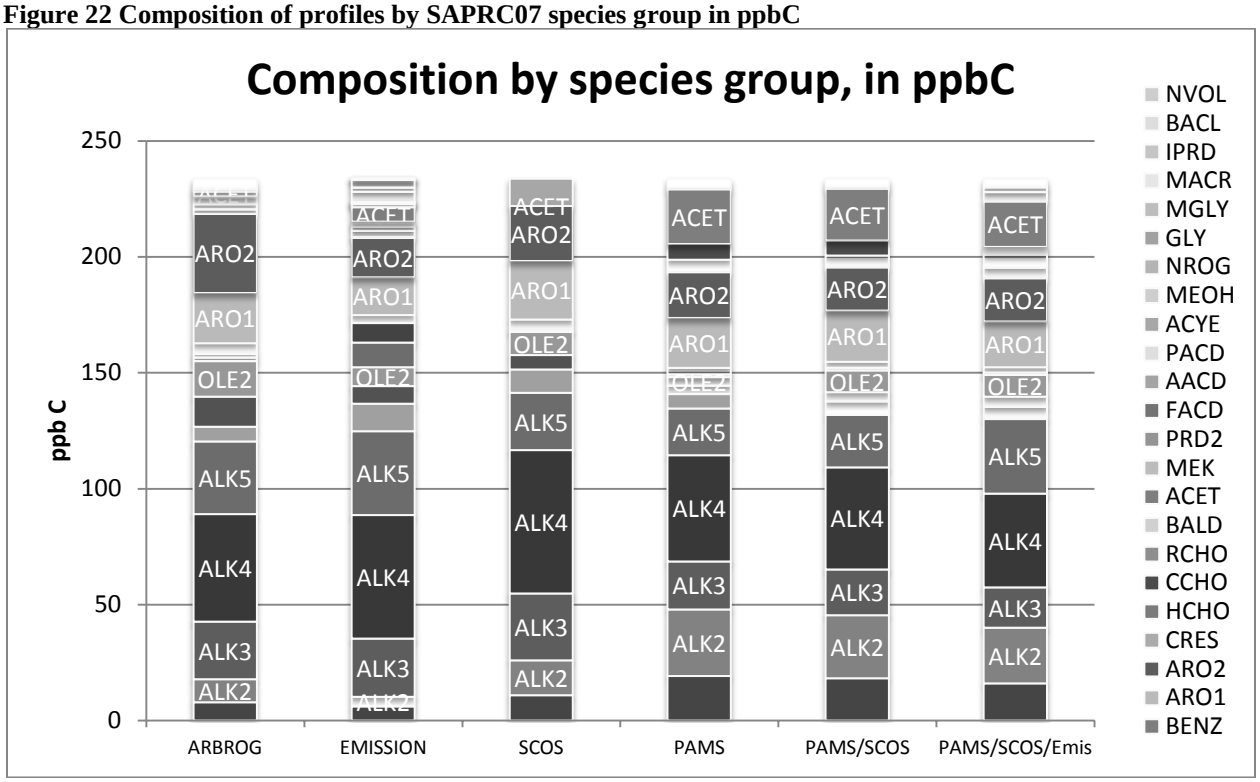


Figure 23 Composition of profiles by SAPRC07 species group in ppbO_3 estimated with MIR

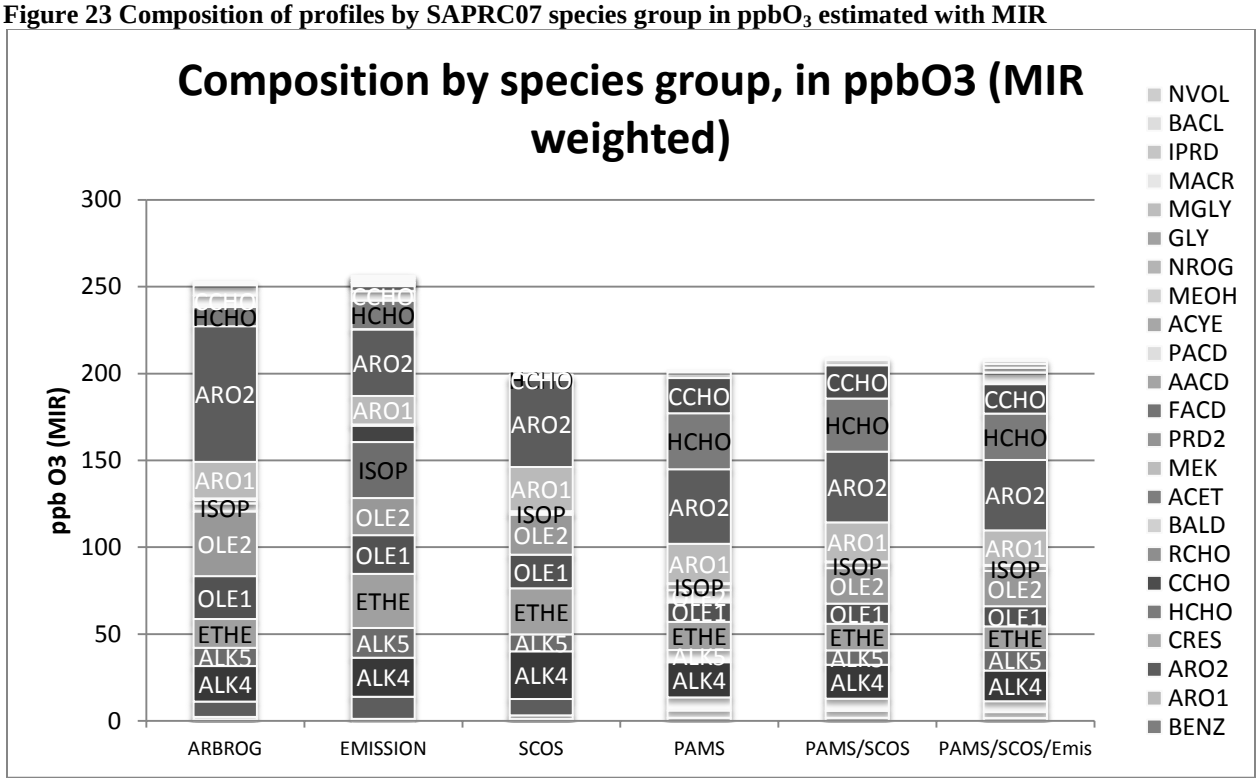


Figure 24 Comparison of C4 and C5 OLE2 species (mostly internal olefins)

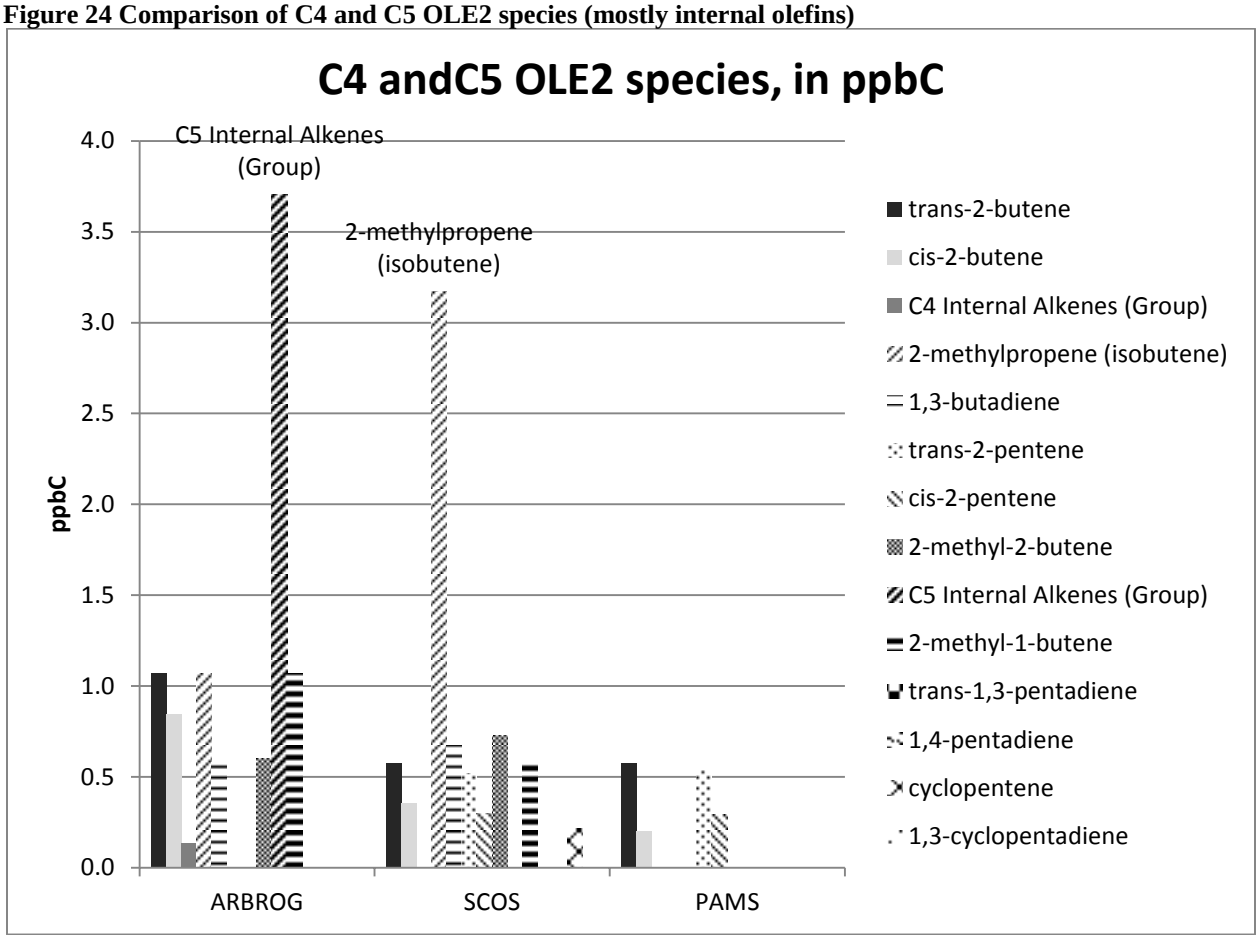


Figure 25 Concentration of branched alkanes in different profiles grouped by number of carbons (ppbC)

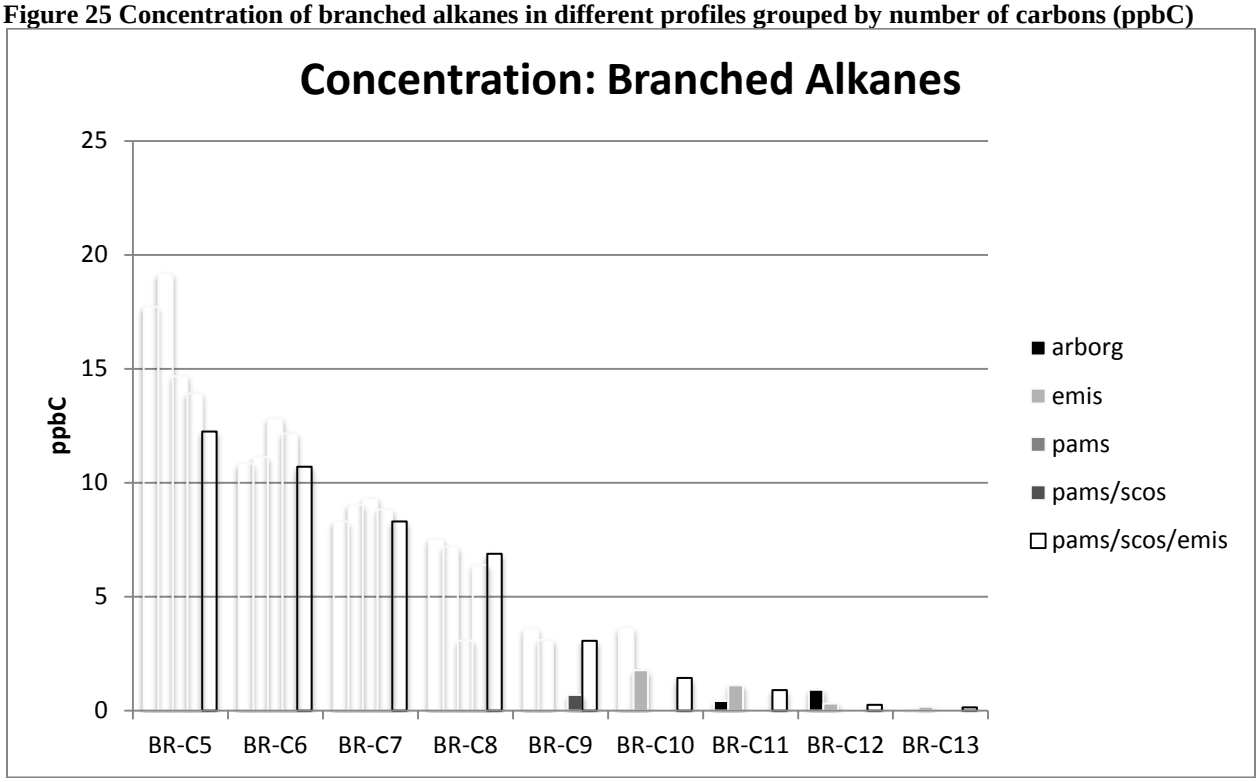
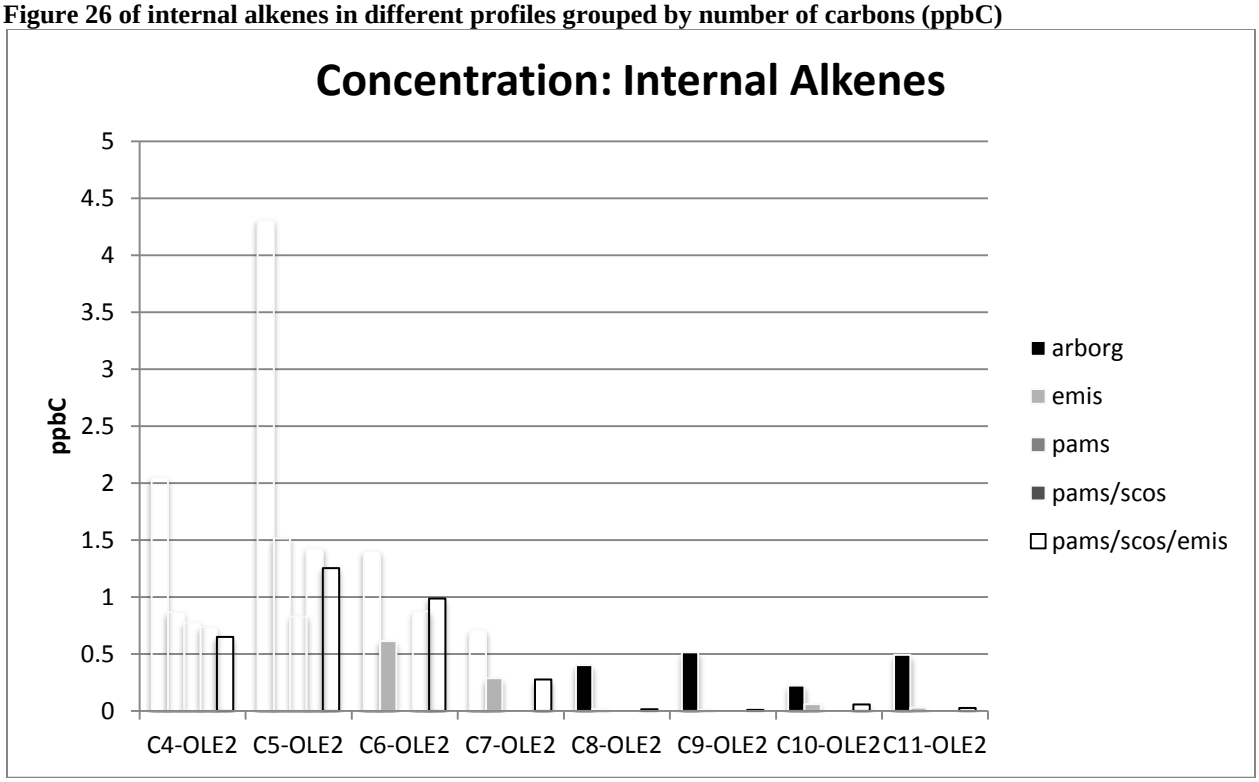


Figure 26 of internal alkenes in different profiles grouped by number of carbons (ppbC)



4 Results

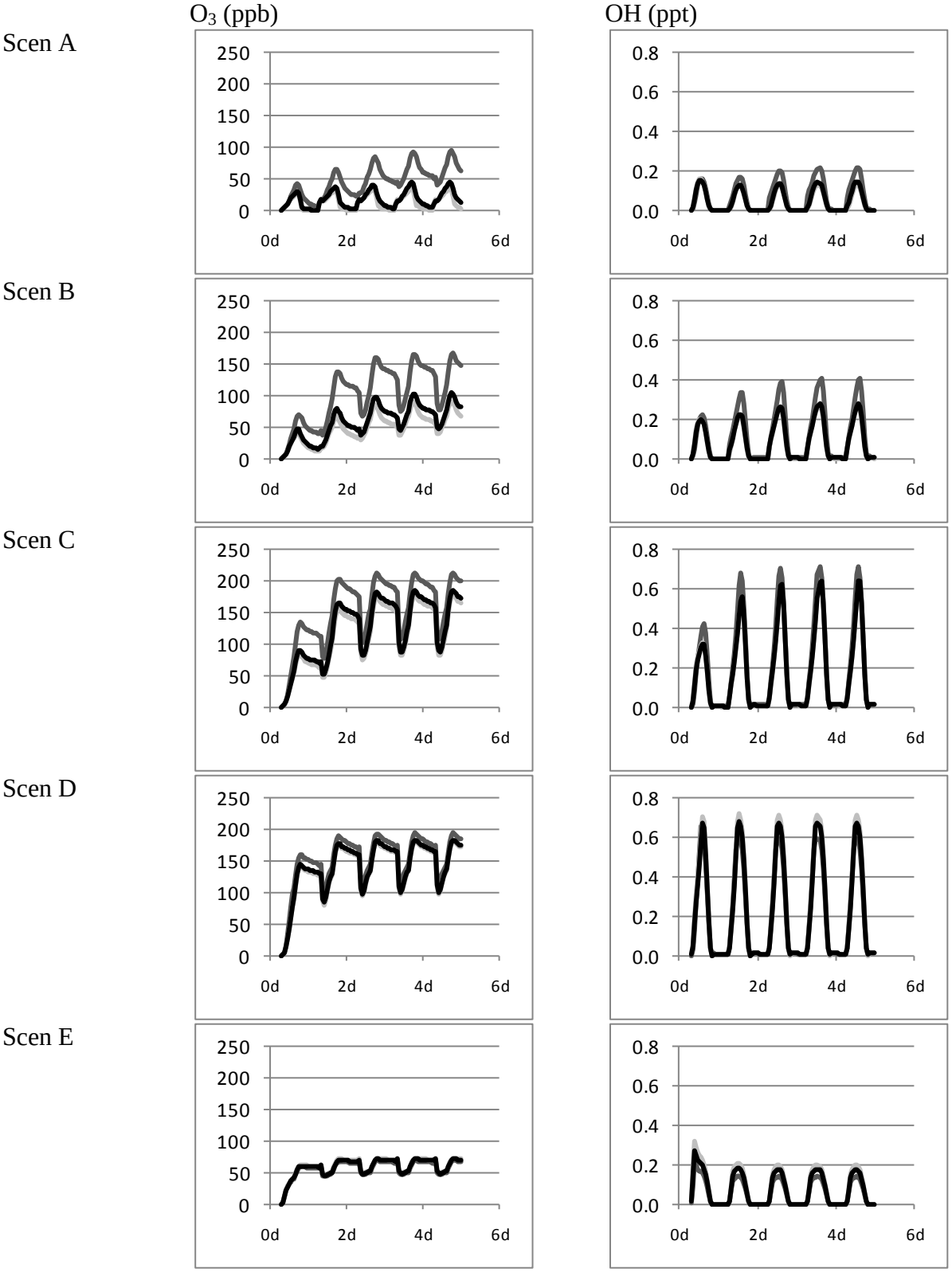
4.1 Time Series of Selected Species

In order to evaluate overall reactivity of the profiles as a whole, multi-day box model scenario simulations (Carter, 2010c) were performed with each of the six profiles. Time series of O_3 and OH for "ARBROG", "PAMS" (original observations without patching) and "PAMS/SCOS/Emis patch" profiles are shown in Figure 27. The daily maximum concentrations of those species for all profiles are summarized in Table 13. It is shown that the PAMS profile, even when patched with data from the SCOS study and the emission inventory, shows lower total reactivity at low NOx conditions (Scenario A and B) resulting in 48.8 and 63.0 ppb less daily maximum ozone in comparison to the ARBROG profile. The OH concentrations are also less by approximately 25 percent. The margin narrows when the system is not limited by VOC (Scenario C, D and E). As discussed in the previous section, the contribution of highly reactive species such as internal alkenes and aromatics becomes less significant for the PAMS profile and its derived profiles in comparison to the ARBROG profile. So the smaller predicted concentration of ozone and radicals are expected.

Table 13 Daily maximum O_3 and OH concentration with five-day scenario

Sce-nario	Input ROG/NOx ratio (ppbC/ppb)	O_3 (ppb)						OH (ppt)					
		ARBR OG	Emis	SCOS	PAMS	PAMS / SCOS	PAMS / SCOS / Emis	ARBR OG	Emis	SCOS	PAMS	PAMS / SCOS	PAMS / SCOS / Emis
A	3.85	95.2	100.7	32.3	35.6	46.1	46.0	0.220	0.213	0.122	0.159	0.158	0.152
B	4.94	167.3	179.9	115.5	91.0	105.0	104.3	0.411	0.407	0.282	0.267	0.291	0.279
C	7.04	213.6	223.5	202.8	178.5	187.0	186.2	0.711	0.664	0.666	0.646	0.673	0.643
D	11.0	194.5	201.7	191.4	181.2	183.9	183.9	0.664	0.623	0.626	0.725	0.713	0.684
E	70.4	69.6	70.6	71.0	73.5	73.2	72.0	0.227	0.196	0.295	0.320	0.288	0.271

Figure 27 Time Series of O_3 and OH concentration for multi-day scenario with ARBORG (dark grey), PAMS without patch (light grey) and PAMS/SCOS/Emis patch (black) profiles



4.2 Incremental Reactivity of the ROG mixture and Selected Species

The incremental reactivity of ROG mixtures was determined using the reactivity calculation package of Carter (2010a), using the AVGARB environmental scenario. "ARBROG" profile and "PAMS/SCOS/Emis patch" profile were used as base mixtures. The ratio of oxygenated species to hydrocarbons in each profile was 0.0475 and 0.2009, respectively, and these values are used to adjust level of base hydrocarbon in the model to the prescribed value. The chemical mechanistic for the lumped species was not updated with new profile, but the values determined using ARBROG profile was reused for new mechanisms.

Table 14 shows an example of the incremental reactivity using the two profiles with relative change. The first four rows show species from different classes (alkanes, alkenes, aromatics and oxygenates). The last row shows the incremental reactivity of the ROG mixture itself. The results indicate that the new profile ("PAMS/SCOS/Emis") has significantly smaller incremental reactivity than the older profile regardless of NOx level when tested ROG as a whole. This may be related to the fact that the overall reactivity of the new profile is smaller than that of the older profile. For the incremental reactivity of individual test species, the new profile predicts larger reactivity than the old profile for hydrocarbons, with exception of n-hexane at high NOx conditions. Formaldehydes incremental reactivity is smaller with new profile.

Figures 28 through 31 shows similar analysis applied to 251 alkanes, 170 alkenes, 197 aromatics, and 401 oxygenated species. The relative change in incremental reactivity is plotted against the magnitude incremental reactivity. Table 15 shows mean and standard deviation of relative changes in incremental reactivities, calculated for each species class. It shows that maximum incremental reactivity (MIR) increases with new profiles for alkanes, aromatics and oxygenated species, whereas alkenes may increase or decrease depending on species. The magnitude of change is within 10 percent for most species.

Table 14 Incremental reactivities using "ARBROG" and "PAMS/SCOS/Emis patch" profile as base mixture. AVGARB environmental scenario was used. Base uses base case HC to NOx ratio of the AVGARB scenario. Other three incremental reactivities using adjusted NOx levels to maximum incremental reactivity condition (MIR), maximum ozone condition (MIOR) and equal benefit condition (EBIR). Units are in $gO_3/gROG$.

	ARBROG				PAMS/SCOS/Emis patched				Relative Change			
	Base	MIR	MOIR	EBIR	Base	MIR	MOIR	EBIR	Base	MIR	MOIR	EBIR
HC/NOx ratio	6.58	3.70	5.63	8.85	6.58	3.81	5.82	9.28				
n-Henane	0.704	1.265	0.839	0.468	0.729	1.310	0.838	0.456	3.6%	3.6%	-0.1%	-2.6%
Propene	3.641	12.020	4.515	2.717	3.867	12.220	4.589	2.762	6.2%	1.7%	1.6%	1.7%
m-Xylene	2.335	10.020	3.127	1.452	2.522	10.120	3.180	1.469	8.0%	1.0%	1.7%	1.2%
Formaldehyde	1.968	9.782	2.738	1.272	2.046	9.288	2.647	1.227	4.0%	-5.1%	-3.3%	-3.5%
ROG	1.173	3.730	1.478	0.803	0.975	2.948	1.174	0.633	-16.9%	-21.0%	-20.6%	-21.2%

Table 15 Change in incremental reactivity calculated with ARBROG and PAMS/SCOS/Emis patch profiles, average across species of same class. Values in parenthesis shows one-standard deviation

	Base	MIR	MOIR	EBIR
Alkanes	6.4% (+/-1.5%)	6.3% (+/-2.3%)	1.2% (+/-0.8%)	-1.8% (+/-1.3%)
Alkenes	5.8% (+/-1.7%)	1.2% (+/-2.8%)	1.2% (+/-1.9%)	1.1% (+/-1.7%)
Aromatics	7.7% (+/-1.1%)	1.5% (+/-1.3%)	1.9% (+/-1.4%)	1.1% (+/-0.6%)
Oxygenates	5.5% (+/-1.5%)	3.1% (+/-2.3%)	2.3% (+/-4.3%)	0.0% (+/-1.8%)

Figure 28 Relative change in incremental reactivities between PAMS/SCOS/Emis profile and ARBROG profile: Alkanes.

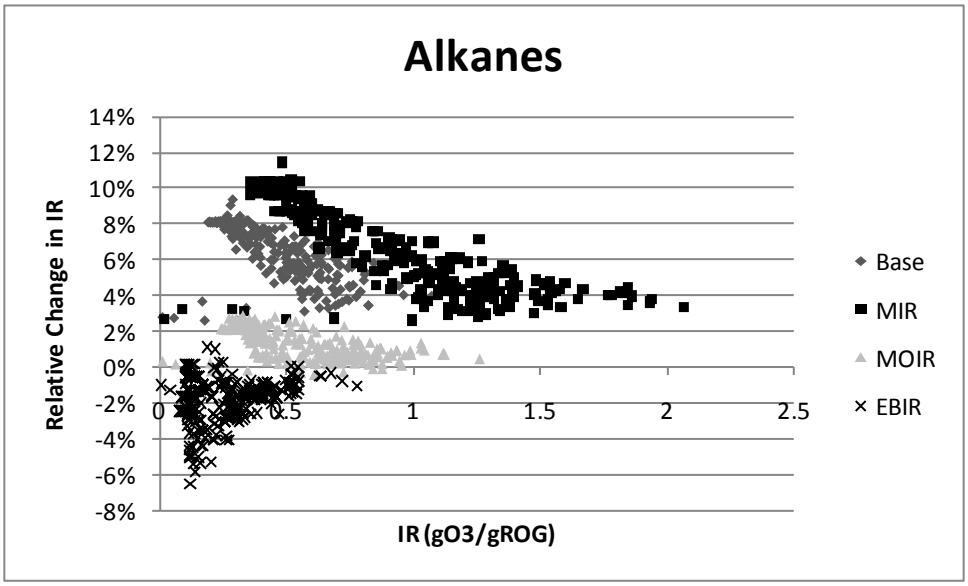


Figure 29 Relative change in incremental reactivities between PAMS/SCOS/Emis profile and ARBROG profile: Alkenes.

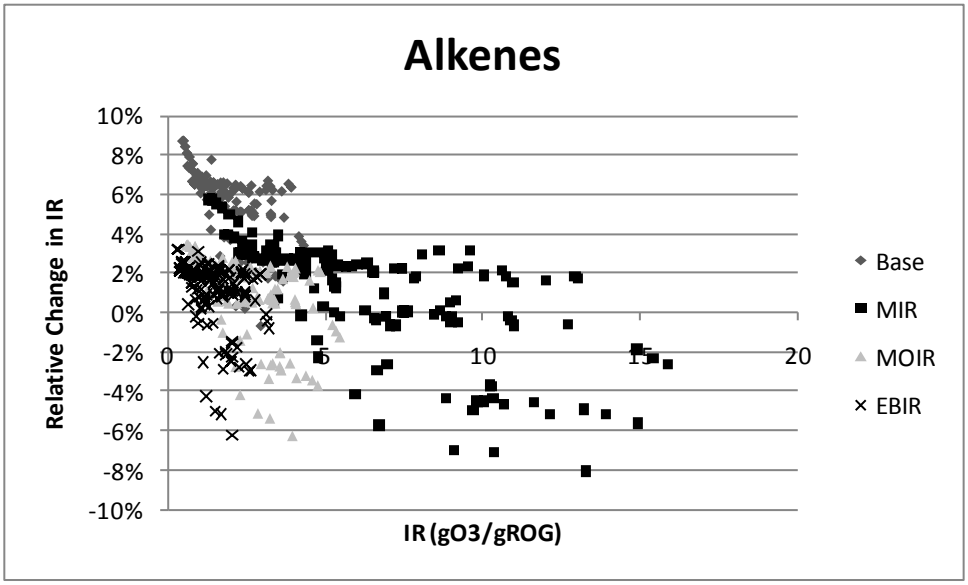


Figure 30 Relative change in incremental reactivities between PAMS/SCOS/Emis profile and ARBROG profile: Aromatics.

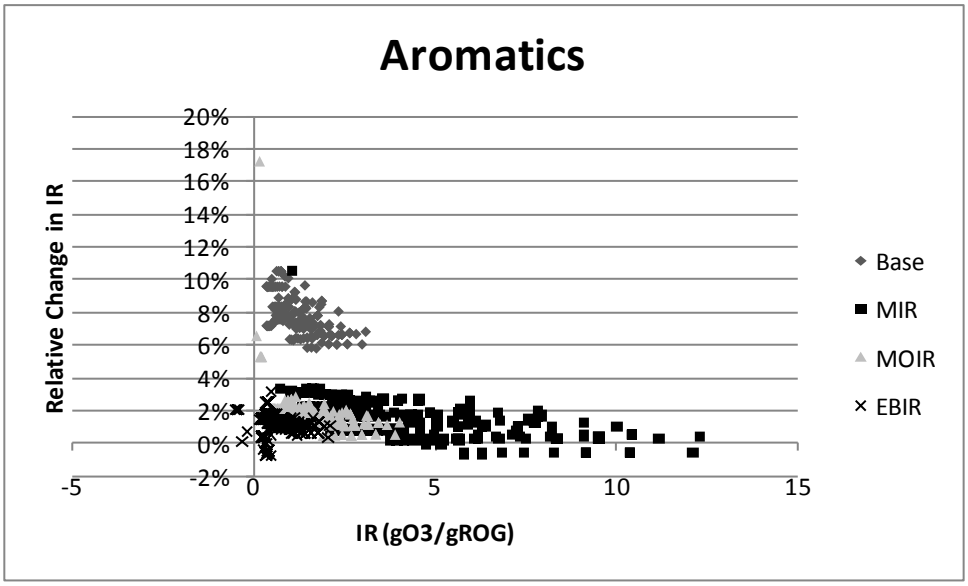
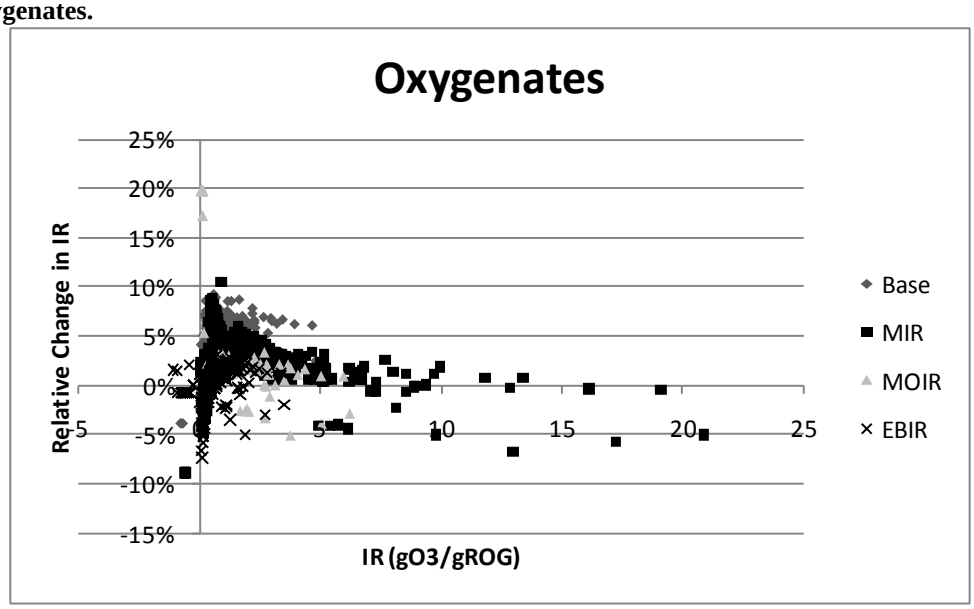


Figure 31 Relative change in incremental reactivities between PAMS/SCOS/Emis profile and ARBROG profile: Oxygenates.



5 Conclusions

The PAMS observations were augmented with SCOS97 observation and emission inventory in Los Angeles counties to develop new profile. In comparison to the older profile (ARBROG), several groups of species (e.g. alkenes and aromatics with relatively large molecules) were reduced.

The PAMS/SCOS/Emis patched profile generated less ozone than the ARBROG profile, particularly when VOC is scarce. OH was also lower in those scenarios.

The new profile seems to lead to larger maximum incremental reactivity for testing identical species, particularly for alkanes and aromatics. The margin of change is within 10 percent.

The average of six monitors in Los Angeles County from PAMS observations were taken as bases for new ROG profile. The profile is augmented with SCOS97 observation and emission inventory in Los Angeles for species that is not reported in PAMS study yet may contribute to overall reactivity of the profile. These compounds typically are species with larger molecular weight. Total number of species included is 294, including five species whose concentration was zero. Of 294 species, 244 species represents single compounds whereas remaining 50 species represents group of similar species (simple mixture).

In comparison to the profile used in earlier works (ARBROG), overall reactivity of the profile was reduced. This was shown by (1) reduced total of MIR weighted sum of concentration and (2) decreased formation of O_3 and OH with new profile with box modeling, particularly when the ROG to NOx ratio in the system is low (VOC limited condition). The reduced reactivity can be attributed, but not limited to, reduced amount of "simple mixture" species of larger alkenes and aromatics. Reduction of the amount of these species is justified by incorporating SCOS97 study (more species are measured than PAMS study) and emission inventory of Los Angeles County.

Incremental reactivity of was calculated using the new profiles for selected 1181 organic species. The new profile leads to slightly higher maximum incremental reactivity (MIR) for alkanes, aromatics and oxygenated compounds. Average relative increase in MIR values were 6.3, 1.5 and 3.1 percent for each class of species with standard deviation of 2.3 percent, 1.3 percent and 2.3 percent, respectively. MIR of alkenes may increase or decrease depending on species. Maximum ozone incremental reactivity (MOIR) and equal benefit incremental reactivity (EBIR) are affected less by the change in profile. Incremental reactivity of ROG as a whole was decreased by approximately 20 percent for all of three incremental reactivity values.

6 Recommendations

This work was conducted with information on Los Angeles County. Upon adapting the results to other parts of the State of California or other parts of country, it is recommended to evaluate the overall MIR of the ROG profiles for those specific locations. The new profile derived in this work leads to fairly large differences in predicted ozone concentration but the incremental

reactivity was not affected as much. It would be useful if the sensitivity of the incremental reactivity with regard to the changes in the profile of the base ROG mixture were evaluated with a thorough examination of ambient observations and/or the emission inventory to determine the necessity of further development of profiles specific to places other than Los Angeles County.

The incremental reactivity was evaluated with the new base ROG profile, but the mechanistic parameters of the base mixture were not updated, and the values developed based on ARBROG (the previous profile) were reused. It is recommended to update the mechanistic parameters using the new profile and to re-evaluate the incremental reactivities.

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8 List of inventions reported and copyrighted materials produced

Not applicable

9 Glossary of Terms, Abbreviations

VOC – volatile organic compound

ROG – reactive organic gas

AQS – Air Quality System, an EPA database

PAMS – Photocehmical Assessment Monitoring Station

SCOS – Southern California Ozone Study

MIR – maximum incremental reactivity

MOIR – maximum ozone incremental reactivity

SAPRC – Chemical mechanism developed at University of California at Riverside.

ARBROG – The name of ROG profile that has been used for incremental reactivity calculations

AVGARB – Single day box model simulation conditions (scenario) developed based on conditions for 38 cities in the United States

NEI – National Emissions Inventory Database, an EPA database

PCA – principal component analysis, a common multivariate statistical technique

SAROAD – Storage and Retrieval of Aerometric Data an EPA database

10 Appendix - Data quality issues

Data concerns that led to this revised report are described in this appendix. The time series for the reactive hydrocarbon species 1-pentene for five Los Angeles sites appears in Figure 32. Table 16 lists the information about each site. The data come from 3-hour canister samples from July through September each year. Four of the sites have their concentrations in ppbC graphed on a scale from 0.0 to 14.5 ppbC, whereas the Burbank 060371002 site is graphed on a unique scale, which is nearly two orders of magnitude greater than the others.

Table 16 Los Angeles PAMS sites used in this analysis

name	AQS	Site Address	latitude	longitude	elevation (m)
Azusa	060370002	803 N. Loren Av, Azusa	34.136	-117.924	187
Burbank	060371002	228 W Palm Ave, Burbank	34.176	-118.317	171
Pico Rivera #2	060371602	4144 San Gabriel River Pkwy, Pico Rivera	34.010	-118.069	58
LAX - Hastings	060375005	7201 W Westchester Pkwy, Los Angeles	33.955	-118.430	37
Santa Clarita-Placerita	060376012	22224 Placerita Canyon Rd, Santa Clarita	34.383	-118.528	386

Figure 33 shows the time series for only the summer of 2007 for the Burbank 060371002 site. Two anomalous features appear in this figure: a sudden spike in the data from the beginning of July followed by a steady decline to July 5, and a larger spike in the data beginning September 3, peaking September 5, and then declining though mid-September. Looking back at Figure 32, a similar spike and decline appears at Pico Rivera #2 060371602 in the summer of 2008. This possible anomaly is not treated in this revision, as the "spike" feature is not as extreme as at the Burbank site.

Figure 34 shows the relationship of 1-pentene concentrations and the hourly wind directions. For simplicity, only the first hourly wind direction resultant in a three hour VOC sample was used in merging the meteorological and VOC data. As the elevated 1-pentene values are distributed across the range of observed wind directions, it appears the concentrations are likely not associated with any particular upwind source.

These investigations lead to the decision to exclude the data from the summer of 2007 for Burbank.

Figure 32 Summer VOC measurements at five Los Angeles PAMS sites for 1-pentene, ppbC units

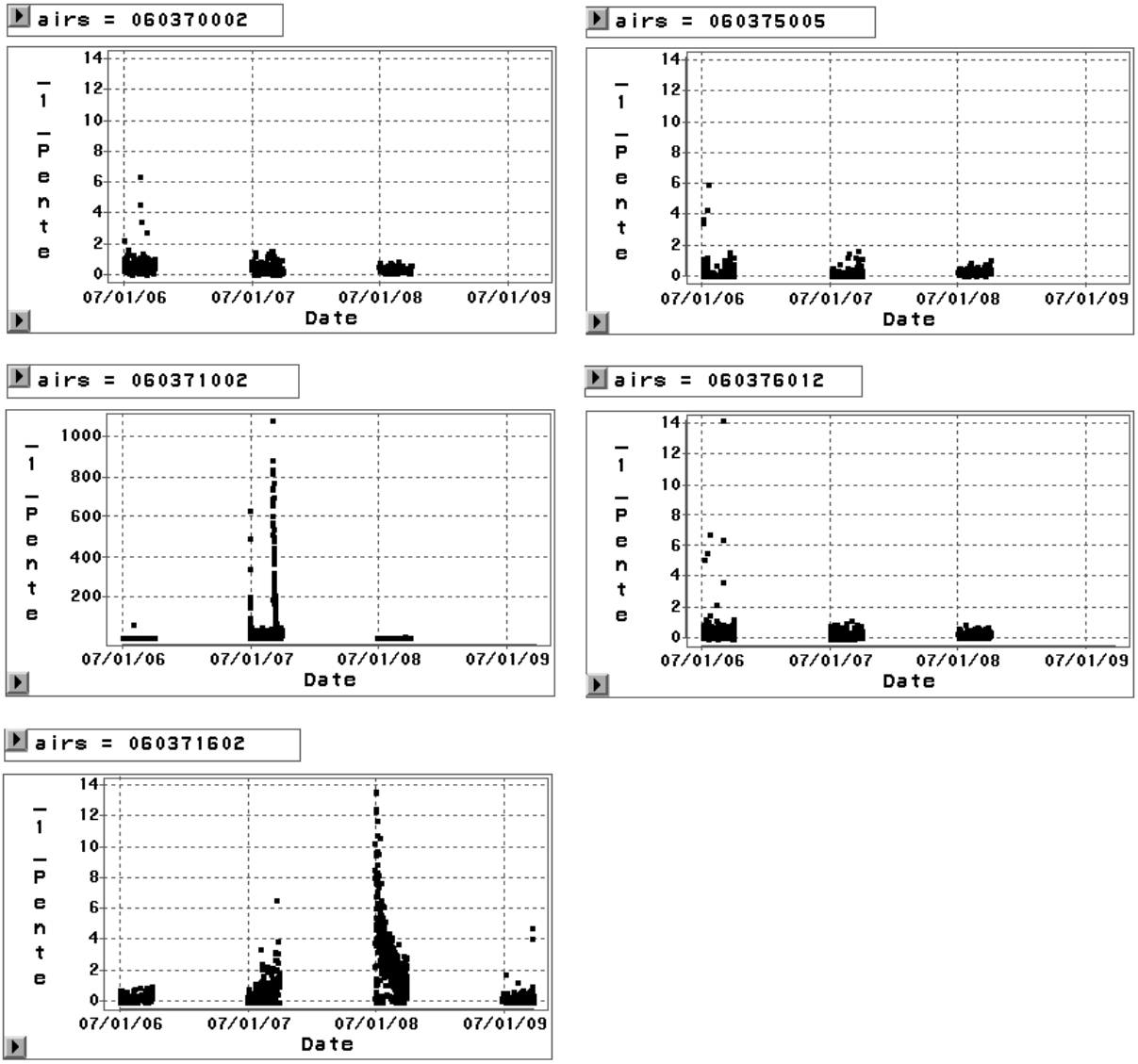

Figure 33 Time series Burbank 1-pentene 3-hour samples ppbC units, July 1 – September 30, 2007

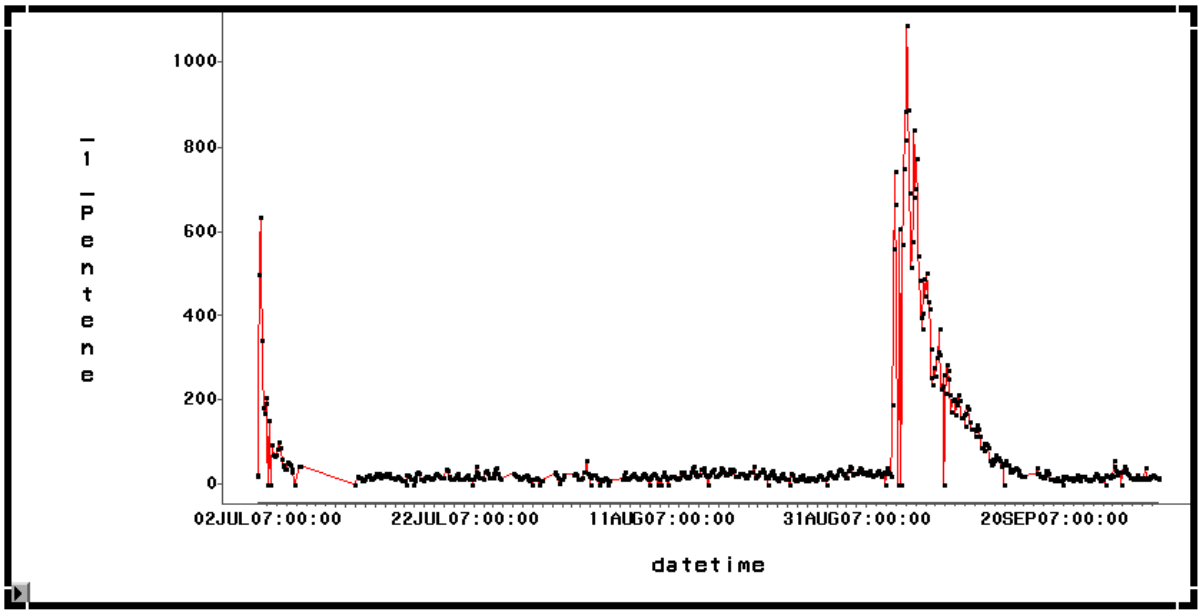

Figure 34 Burbank 1-pentene 3-hour samples vs. wind direction resultant July 1 – September 30, 2007