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Preliminary Analyses of Houston Auto-GC 1998-2001 Data: Episode/Non-episode Differences

Interim Report
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1. INTRODUCTION AND OBJECTIVES

As a part of Task 2 of this work assignment to acquire, review, and analyze automatic gas chromatograph (auto-GC) data collected in Houston from 1998 through 2001, this interim report documents the preliminary exploration of the data with a focus on the episode/non-episode characteristics.

TNRCC collected hourly speciated hydrocarbon data at numerous sites for several years using auto-GCs as a part of monitoring efforts to better understand ozone precursor concentrations and composition in the Houston area. The auto-GCs record hourly concentrations of nearly 60 hydrocarbons. Other air quality parameters (such as ozone and NO_x) and meteorological data are also collocated at these sites.

One of the primary hypotheses being investigated in this memorandum is whether selected olefins (e.g., ethene, propene, 1,3-butadiene) or aromatics (e.g., toluene, 1,2,4-trimethylbenzene, styrene) are a greater fraction of the total nonmethane organic compounds (TNMOC) in the mornings of ozone episodes. One of the implications of higher reactive TNMOC fractions is that unique (or industrial upset) conditions may lead to these high concentrations and trigger ozone episodes. To pursue this hypothesis, we focused on the summer months of July-September, when there were a large number of days with high ozone concentrations. We defined an ozone episode day as a day in which the ozone concentration in the Houston area exceeded 125 ppb.

In this memorandum, we report on the preliminary results of analyses structured to explore overall characteristics of the data, episode versus non-episode differences, composition/concentration differences with respect to wind quadrant, and combinations of these investigations. Subsequent analyses will continue to focus on the details.

2. SUMMARY OF CONCLUSIONS

The conclusions summarized below resulted from our preliminary analyses:

- Concentrations of all species are generally higher during the mornings of ozone episode days. This finding is consistent with other investigations of episodes/non-episodes (e.g., Main and O'Brien, 2001).
- Overall, there is little difference in composition (weight percent) between episode and non-episode mornings when all data are included regardless of wind direction. This finding may be modified as we investigate the data further.
- Weight percents of reactive species (e.g., ethylene, propylene, xylenes, etc.) are actually higher on non-episode days at a number of sites and during some years; and most sites show no consistency as to whether the reactive species are higher during episodes or non-episodes from year to year. Again, we need to investigate this finding with respect to wind direction.

- The reactivity-weighted concentrations are very similar between episode and non-episode days at Clinton in 1999 during the morning. Exceptions include the aromatic hydrocarbons, C4 and C5 alkanes, and isoprene, which are slightly higher on episode mornings, and reactivity-weighted concentrations of ethene, which are significantly higher on episode mornings (while propene is not). We need to further investigate the relationship of these findings with wind direction.
- While the lack of significant compositional differences between mornings of ozone episodes and non-episodes suggests that emissions are similar on both ozone episode and non-episode days, concentrations and composition are highly dependent on wind direction at Clinton and Deer Park (at least), and further investigations are ongoing.

3. DATA AVAILABILITY AND COMPLETENESS

Hourly auto-GC data were collected from 1998-2001 year-round at Clinton and Deer Park, at Bayland from January 1998 to August 2000, at Aldine during September 2000, and at Channelview, HRM-3 and HRM-7 from August through October 2001. Data were previously validated by TNRCC staff and reviewed by STI. We summarized our data validation efforts for data in 1998-2000 Main et al., 2001, and for 2001 data in Main and Brown, 2002. **Table 3-1** summarizes the sites and missing data during the summers of 1998-2001. The percentage available is equal to the number of hourly samples divided by the number of expected hourly samples during periods in which the sites were operational. We assumed that there were 22 hourly samples in a given day and that the remaining two hours were devoted to calibrations (no data reported). There are many gaps in the data; the times and dates of missing auto-GC data are detailed in Appendix A.

Generally, more than 75% of the data (a commonly used threshold for completeness) are available during the time periods of interest. Only Bayland 1998, Clinton 2000, and Deer Park 2000 have less than 75% data availability during the July-September period. Missing data become a problem during ozone episodes when analyses are focused on hour-to-hour details.

Table 3-1. Table of expected and available auto-GC data during July-September 1998-2000 and August-October 2001. Counts are based on concentration data.

		TNRCC		Number of Hourly Data (1 day = 22 sample hours, 2 calibration hours)		
Site	Year	Site Code	Operational	Expected	Available	% Available
Bayland[a]/Aldine	2000	C8/C108/C150	7/1-8/6, 9/1-9/30	1452	935	64
Bayland	1999	C53/C146/C181	7/1-9/30	2024	1567	77
Bayland	1998	C53/C146/C181	7/1-9/30	2024	1084[b]	53
Channelview	2001	C15/C115	8/4-10/31	1958	1525[c]	78
Clinton	2001	C403/C113/C304	8/1-10/31	2024	1820	90
Clinton	2000	C403/C113/C304	7/1-9/30	2024	1260	62
Clinton	1999	C403/C113/C304	7/1-9/30	2024	1696	83
Clinton	1998	C403/C113/C304	7/1-9/30	2024	1758[d]	86
Deer Park	2001	C35/C139	8/1-10/31	2024	1697[e]	84
Deer Park	2000	C35/C139	7/1-9/30	2024	425	21
Deer Park	1999	C35/C139	7/1-9/30	2024	1768	86
Deer Park	1998	C35/C139	7/1-9/30	2024	1533[f]	75
HRM-3-Haden	2001	C603/C114	8/21-10/31	1584	1355[g]	86
HRM-7-Baytown	2001	C148	8/27-10/31	1452	1295[h]	89

[a] The site at Bayland was moved to Aldine 8/6; no data were collected 8/7-8/31, overall data recovery is 46%.
[b] 94 of these hours have no TNMOC data with which to calculate weight percent (48% availability).
[e] 97 of these hours have no TNMOC data with which to calculate weight percent (73 % availability).
[d] 809 of these hours have no TNMOC data with which to calculate weight percent (46% availability).
[c] 60 of these hours have no TNMOC data with which to calculate weight percent (72 % availability).
[f] 1299 of these hours have no TNMOC data with which to calculate weight percent (11% availability).
[g] 266 of these hours have no TNMOC data with which to calculate weight percent (69% availability).
[h] 82 of these hours have no TNMOC data with which to calculate weight percent (84% availability).

4. ABUNDANT SPECIES

In order to examine the species with the greatest potential to impact ozone formation in the Houston area, the most abundant species at the various sites from July through September were identified. Abundance was assessed on both a concentration and a reactivity-weighted compositional basis. This assessment was based on the fact that while some hydrocarbons are very copious (e.g., ethane and propane), they play a minor role in ozone formation. This phenomenon is in contrast to other, more reactive compounds which are found in smaller concentrations but, due to their high reactivity, are very important to ozone formation. There are a number of different scales on which to gauge this reactivity, such as reaction rates with OH, propylene equivalents, and maximum incremental reactivity (MIR) scale.

The MIR scale (Carter, 1994; Carter, 2000) is used in this analysis to characterize the reactivity of the individual compounds in the auto-GC samples. This scale provides an estimation of moles ozone formed per mole carbon of each hydrocarbon sampled, where the ozone formation estimates are intended to be used in a relative rather than absolute manner. To facilitate this, the reactivity of each species is found by multiplying the relative MIR scale factor and weight percent of each species (for each hourly sample). The result is the relative ranking of the species.

Tables 4-1 and 4-2 list the ten most abundant hydrocarbons on a concentration and reactivity-weight percent basis, respectively, at various sites and years in the Houston area. Important findings are that

- The same species are abundant on both a concentration (ethane, propane, isopentane, n-butane, isobutane) and reactivity-weight percent (ethylene, propylene, toluene, isopentane, xylenes) basis between years and sites.

- The importance of olefins and aromatics in ozone production is illustrated when presented on the reactivity-weight percent basis. Abundant species on this scale at most sites and during most years include ethylene, propylene, toluene, isopentane, xylenes and 1,2,4-trimethylbenzene.

- Isoprene is generally not an abundant species, indicating a lower amount of biogenic emissions than found in places such as the northeastern United States (Main et al., 1999). The one notable exception is that isoprene concentrations at Bayland in 2000 are very high, with a median concentration of 2 ppbC translating to 4.6% of the total non-methane hydrocarbons. The data appear to be valid, as there is a consistent diurnal pattern of high concentrations in the morning and afternoon, dropping off in the evening.

We also investigated abundance on a wind-direction basis using the 2000 data (Main et al., 2001). **Table 4-3** provides an example of results at the Clinton site for reactivity-weighted data. The six most abundant species are consistent across all wind quadrants while the other abundant species vary.

Table 4-1. Ten most abundant hydrocarbons by concentration during July-September at each site and year.

Species	ethan	propa	ispna	nbuta	isbta	ethyl	tolu	npnta	t2bte	nhexa	prpyl	xyl	2mpnta	acety	ispre	benz
Deer Park 1998	1	2	3	4	5	6	7	8	9	10						
Deer Park 1999	1	2	3	5	4	6	7	8			9	10				
Deer Park 2000	1	2	3	4	5	7	6	10			8	9				
Deer Park 2001	1	2	5	4	3	6	7	9		10	8					
Clinton 1998	3	2	1	4	6	8	9	7			10	5				
Clinton 1999	3	2	1	4	6	9	8	7			10	5				
Clinton 2000	3	2	1	4	5		6	8				9	10	7		
Clinton 2001	2	1	4	3	5	9	6	7			10	8				
Bayland 1998	1	2	3	4	7	8	5	6				9	10			
Bayland 1999	1	2	3	5	7	8	4	6				9	10			
Bayland 2000	1	2	3	4	8	7	6	9				10			5	
Aldine 2000	1	2	3	4	5	6	7			10		8	9			
Channelview 2001	2	1	5	3	4	6	7	9			8					10
HRM-3 2001	2	1	4	3	5	8	6	9			7	10				
HRM-7 2001	2	1	4	3	5	9	7	6		8	10					

Where

ethan = ethane
propa = propane
ispna = i-pentane
nbuta = n-butane
isbta = i-butane
ethyl = ethene
tolu = toluene
npnta = n-pentane
t2bte = t-2-butene
nhexa = n-hexane
prpyl = propene
xyl = xylenes
2mpnta = 2-methylpentane
acety = acetylene
ispre = isoprene
benz = benzene

Table 4-2. Ten most abundant hydrocarbons by reactivity weight during July-September at each site and year. Species abbreviations are provided in Appendix B.

	ethyl	prpyl	xyl	ispna	tolu	isbta	nbuta	propa	ispre	124tmb	123tmb	3m1bte	t2bte	c2be	ethan	13buta	npnta
Deer Park 1998	1	2	4	5	6	7	8	9	10					3			
Deer Park 1999	1	2	5	4	3	6	10	8	7	9							
Deer Park 2000	1	2	5	4	3	6	8	7	9						10		
Deer Park 2001	1	2	8	6	3	4	5	7							9		10
Clinton 1998	3	2	1	4	5	8	7		10	6		9					
Clinton 1999	3	2	1	5	6	9			8	4	7	10					
Clinton 2000	3	2	1	4	5	8	7		10	6		9					
Clinton 2001	1	2	3	4	5	7	6						8			10	9
Bayland 1998	1	2	7	6	4		10		3	5	8		9				
Bayland 1999	1	2	5	7	3		9			6	8		4	10			
Bayland 2000	1	2		4	3	10	7	8		6	5	9					
Aldine 2000	1	2	7	5	4		9	10	3	6	8						
Channelview 2001	2	1	6	7	3	5	4	8	9		10						
HRM-3 2001	2	1	3	5	4	7	6	8	9								10
HRM-7 2001	2	1	6	4	7	8	5	9								3	10

Where

- ethyl = ethene
- prpyl = propene
- xyl = xylenes
- ispna = i-pentane
- tolu = toluene
- isbta = i-butane
- nbuta = n-butane
- propa = propane
- ispre = isoprene
- 124tmb = 1,2,4-trimethylbenzene
- 123tmb = 1,2,3-trimethylbenzene
- 3m1bte = 3-methyl-1-butene
- t2bte = t-2-butene
- c2be = c-2-butene
- ethan = ethane
- 13buta = 1,3-butadiene
- npnta = n-pentane

Table 4-3. Ten most abundant hydrocarbons by wind quadrant on a reactivity-weighted basis (using Carter's MIR) at Clinton in 2000.

Species	Wind Quadrant							
	0-45°	45-90°	90-135°	135-180°	180-225°	225-270°	270-315°	315-360°
ethene	1	2	2	5	3	2	1	2
xylenes	2	5	3	1	2	3	2	1
propene	3	1	1	3	1	1	3	3
toluene	4	7	6	7	7	4	4	5
n-butane	5	4	5	4	8	7	8	4
isopentane	6	3	4	2	6	6	5	6
propane	7	9				10	10	8
1,2,4-trimethylbenzene	8				4	5	6	7
isobutane	9	8	7		10			9
ethane	10							
n-pentane			9					
isoprene							7	
1-butene		10	8	10				
1,2,3-trimethylbenzene						9		
3-methyl-1-butene			10	9	9	8	9	10
1,3-butadiene		6			5			
trans-2-butene				6				
cis-2-butene				8				

5. EPISODE ANALYSIS

Ozone episode days were defined as days in which an ozone monitor in the Houston area recorded a 1-hr ozone concentration of 125 ppb or above. The list was provided by TNRCC and confirmed by STI to be consistent with other investigations. To explore the role of individual compounds in ozone formation, the median values of PAMS species' concentration, weight percent and reactivity-weighted data were examined on days of ozone episodes and non-episode days for a variety of sites from July-September 1998-2000. Some of the investigations were focused on the 0500-to-0900 time period because this is the critical period when emissions are high, mixing heights are low, and the ozone formation chemistry is set.

5.1 FINGERPRINT ANALYSIS

Figure 5-1 shows an example fingerprint plot for Clinton 1999 in which the median concentration of each of the PAMS hydrocarbons during the morning (0500-0900) hours for episode and non-episode days are shown in elution order. **Figures 5-2 through 5-4** show the episode/non-episode fingerprints at Clinton 1999 using the median weight percent, reactivity-weighted composition, and reactivity-weighted concentrations, respectively.

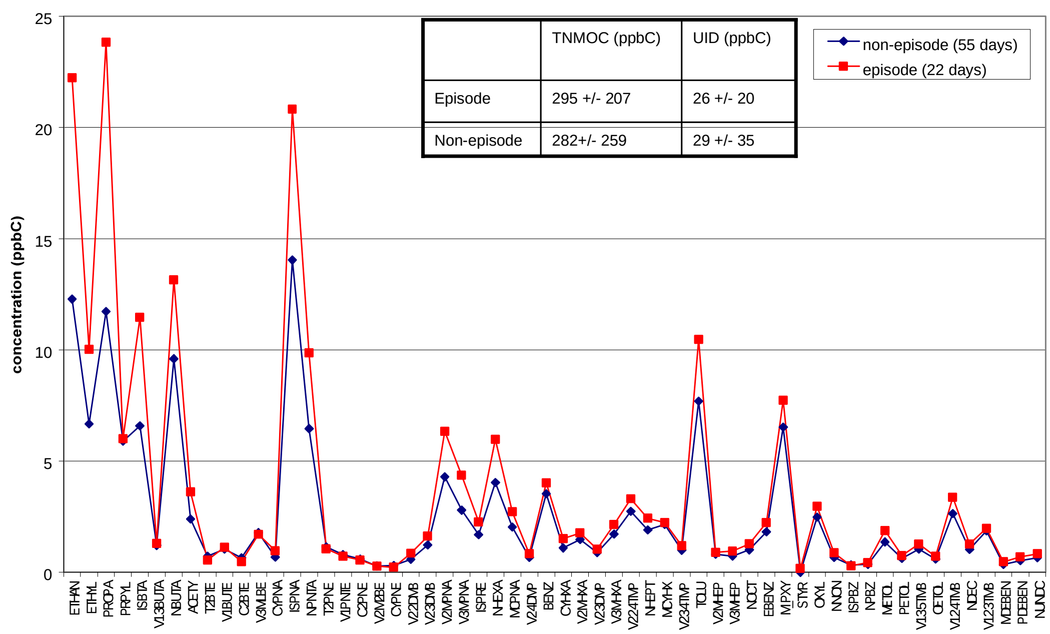

Figure 5-1. Fingerprint of PAMS hydrocarbon median concentrations (ppbC) by episode and non-episode days at Clinton, July-September 1999 (0500-0900). Species abbreviations are listed in Appendix B. UID = unidentified mass.

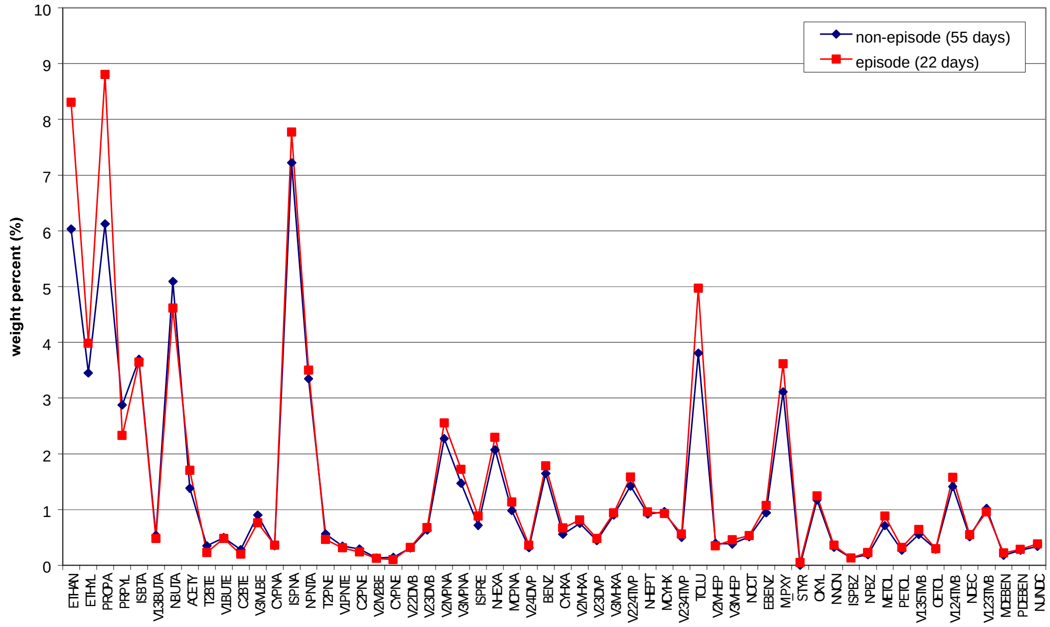

Figure 5-2. Fingerprint of PAMS hydrocarbon median weight percent by episode and non-episode days at Clinton, July-September 1999 (0500-0900). Species abbreviations are listed in Appendix B.

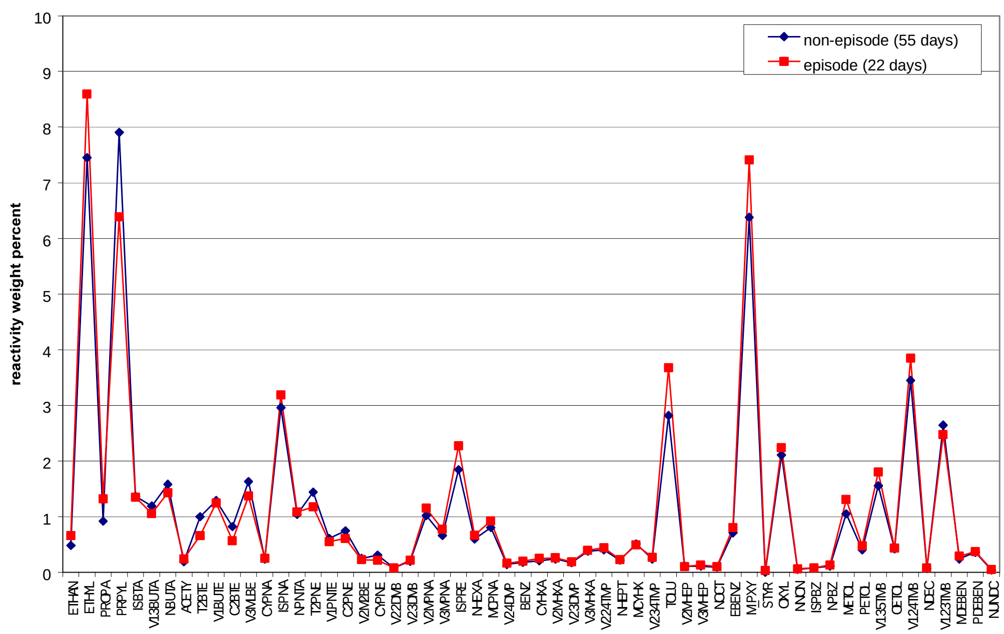

Figure 5-3. Fingerprint of PAMS hydrocarbon median reactivity-weight percent by episode and non-episode days at Clinton, July-September 1999 (0500-0900) hours. Species abbreviations are listed in Appendix B.

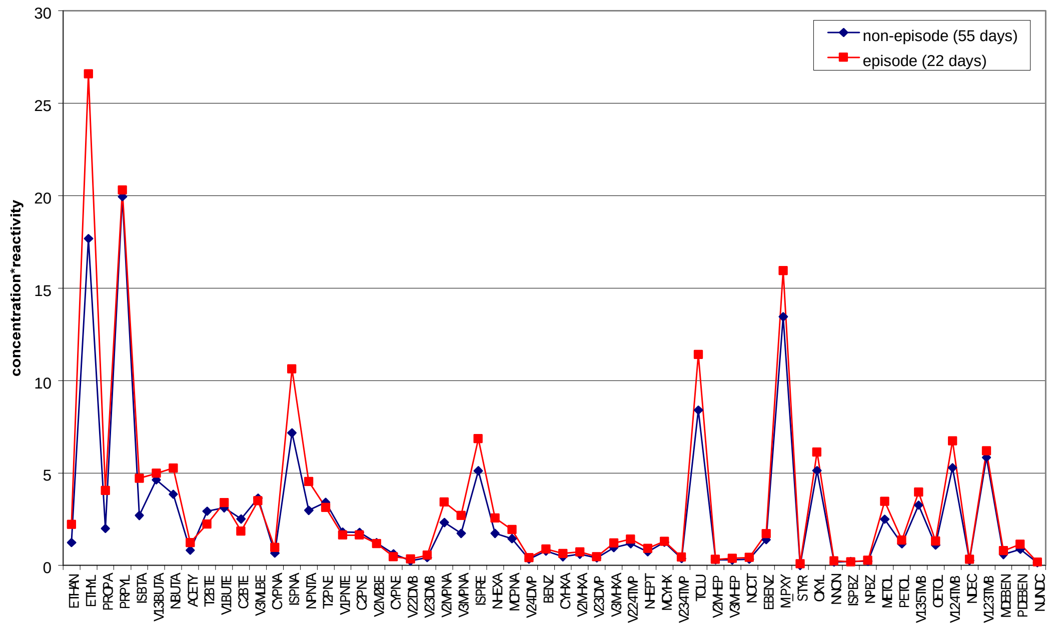

Figure 5-4. Fingerprint of PAMS hydrocarbon median concentration*reactivity by episode and non-episode days at Clinton, July-September 1999 (0500-0900). Species abbreviations are listed in Appendix B.

General findings resulting from an analysis of these fingerprints plots follow:

- Concentrations of all species are generally higher during the mornings of ozone episode days. This finding is consistent with other investigations of episodes/non-episodes (e.g., Main and O'Brien, 2001).
- There is little difference in composition (weight percent) between episode and non-episode mornings when all data are included regardless of wind direction. This finding may be modified as we investigate the data further.
- Weight percents of reactive species (e.g., ethylene, propylene, xylenes, etc.) are actually higher on non-episode days at a number of sites and during some years, and most sites show no consistency as to whether the reactive species are higher during episodes or non-episodes are higher from year to year. Again, we need to investigate this finding with respect to wind direction.
- The lack of compositional difference between mornings of ozone episodes and non-episodes suggests that emissions are similar on both ozone episode and non-episode days. If there is no difference in emissions on days of episodes and non-episodes, it would appear that, on any given day with the correct meteorology, an ozone episode would occur.
- The reactivity-weighted concentrations are very similar between episode and non-episode days at Clinton in 1999 during the morning. The aromatic hydrocarbons, C4 and C5 alkanes, and isoprene are slightly higher on episode mornings. Reactivity-weighted

concentrations of ethene are significantly higher on episode mornings while propene is not.

5.2 HYDROCARBONS OF INTEREST

Because of the general interest in the more reactive hydrocarbons, ethylene, propylene, isoprene, 1,3-butadiene, m- and p-xylenes, toluene and total reactivity were investigated further. **Table 5-1** lists, for each site and year (July-September, 0500-0900), whether episode or non-episode median weight percents are higher and whether the values are different at a 95% confidence level in accordance with a t-test. Few consistent patterns were observed. Key findings of this analysis are that

- Ethene weight fractions were higher on episode mornings in 1999 at Clinton and Deer Park.
- Propene weight fractions were higher on non-episode mornings in 1998 at Bayland and in 1998, 1999, and 2000 at Clinton.
- 1,3-butadiene fractions were higher on non-episode mornings in 2000 at Aldine and in 1999 and 2000 at Clinton. 1,3-butadiene fractions were higher on episode mornings at Deer Park in 2000.
- Toluene fractions were higher on episode mornings in 1998 at Bayland and in 1998 and 1999 at Clinton.
- 1,2,4-trimethylbenzene fractions were higher on non-episode mornings in 1999 at Bayland and Deer Park and in 2000 at Clinton.

Ethylene and propylene are reactive olefins that are among the most abundant on a reactivity-weight percent basis and, as such, can play an important role in ozone formation. Previous investigations have suggested that these two compounds may be elevated on ozone episode days (Fehling, 2002). Both compounds generally had higher concentrations on episode days, but not always on a relative basis (as shown in Table 5-1). T-tests also confirm that ethylene and propylene weight percents are generally not statistically different between episode and non-episode days. The only exceptions were that ethylene was higher on a weight-percent basis on episode days at Deer Park and Clinton during summer 1999, and propylene was statistically higher on non-episode days at Clinton in 1998-2000 and Bayland in 1998. At most sites, there is no consistency among years as to whether non-episode or episode median weight percents are higher. At Deer Park, ethylene was higher on episode days in 1999 and 2000, and propylene was higher on non-episode days at Clinton in 1998-2000; all other sites showed little consistency from year to year. Ethylene and propylene do not follow the same pattern as to whether episode or non-episode median weight percents are higher; it may be that these two compounds are more independent of each other in Houston than at other sites.

Isoprene is a reactive olefin that is emitted from biogenic sources (Stoeckenius et al., 1994; Main and Roberts, 2000); it can be an important contributor to ozone formation. Anthropogenic sources are possibly important in the Houston Ship Channel as isoprene is also used in the polymer and rubber industry. Fingerprint analysis shows that isoprene is sometimes higher in concentration in Houston on days of ozone episodes, consistent with findings from other parts of the country (Dye et al., 1998). Again, there is no compositional (weight-percent) difference between episode and non-episode mornings. Isoprene was consistently higher on episode days (though statistically different only in 1998) at Clinton in 1998-2000 and was higher on non-episode days at Deer Park in 1999-2000. Other sites had no consistent results as to whether episode or non-episode days were higher from year to year.

1,3-butadiene is another highly reactive and toxic compound and is used as a tracer for motor vehicle exhaust. This compound was generally higher on non-episode days, consistently so at Clinton in 1998-2000 (and significantly different in 1999-2000). It was statistically higher on non-episode days at Aldine in 2000, but statistically higher on episode days at Deer Park in 2000. Sites other than Clinton were not consistent from year to year.

Toluene is a fairly reactive compound that is emitted mainly from solvent use, refining, and mobile source emissions. Due to its high reactivity and potential for ozone formation, as well as its abundance in the urban Houston area, toluene is of interest. Toluene was generally higher on a weight-percent basis on episode days, but only significantly so at Bayland in 1998, and at Clinton in 1998 and 1999; weight percents were higher on non-episode days (though not significantly) at Bayland in 2000 and Deer Park in 1999. Note that toluene was consistently higher on episode days at Clinton in 1998-2000, and significantly so in 1998 and 1999. The other sites showed little consistency on an annual basis.

Other reactive aromatics include the three xylene isomers and 1,2,4-trimethylbenzene, which can be emitted from sources such as refining, mobile sources, and solvent use. These compounds showed no consistent difference in weight percent between episode and non-episode days. Xylenes were significantly higher on episode days at Bayland in 1998, but significantly higher on non-episode days at Deer Park in 1999. 1,2,4-trimethylbenzene was significantly higher on non-episode days at Bayland in 1999, Clinton in 2000 and Deer Park in 1999. The only site that was consistent year to year was Deer Park, where 1,2,4-trimethylbenzene was higher on non-episode days in 1999-2000.

For the final report, we will also investigate the total reactivity on episode and non-episode mornings.

Table 5-1. Results of two-sample t-tests for ethylene, propylene, and isoprene by location and year, July-September, 0500-0900: number of days in each episode and non-episode median, whether episode or non-episode median weight percents are higher and whether episode and non-episode weight percents are different at a 95% confidence level. Significant differences are highlighted in bold.

Species	Site	Year	Number of days/ episode	Number of days/ non-episode	Which median weight percent is higher?	Different at a 95% confidence level?
Ethylene	Aldine	2000	5	16	ep>non	No
Ethylene	Bayland	2000	8	19	non>ep	No
Ethylene	Bayland	1999	22	48	ep>non	No
Ethylene	Bayland	1998	7	36	non>ep	No
Ethylene	Clinton	2000	*23*	*35*	non>ep	No
Ethylene	Clinton	1999	22	54	ep>non	**Yes**
Ethylene	Clinton	1998	16	26	non>ep	No
Ethylene	Deer Park	2000	8	9	ep>non	No
Ethylene	Deer Park	1999	24	54	ep>non	**Yes**
Propylene	Aldine	2000	5	16	ep>non	No
Propylene	Bayland	2000	*6*	*15*	ep>non	No
Propylene	Bayland	1999	22	48	ep>non	No
Propylene	Bayland	1998	7	*26*	non>ep	**Yes**
Propylene	Clinton	2000	*48*	*23*	non>ep	**Yes**
Propylene	Clinton	1999	22	54	non>ep	**Yes**
Propylene	Clinton	1998	16	26	non>ep	**Yes**
Propylene	Deer Park	2000	8	9	non>ep	No
Propylene	Deer Park	1999	24	54	ep>non	No
Isoprene	Aldine	2000	5	16	ep>non	No
Isoprene	Bayland	2000	8	19	non>ep	**Yes**
Isoprene	Bayland	1999	22	48	non>ep	No
Isoprene	Bayland	1998	7	36	ep>non	No
Isoprene	Clinton	2000	*48*	*23*	ep>non	No
Isoprene	Clinton	1999	22	54	ep>non	No
Isoprene	Clinton	1998	16	26	ep>non	**Yes**
Isoprene	Deer Park	2000	8	9	non>ep	No
Isoprene	Deer Park	1999	24	54	non>ep	No
1,3butadiene	Aldine	2000	5	16	non>ep	**Yes**
1,3butadiene	Bayland	2000	7	26	non>ep	No
1,3butadiene	Bayland	1999	22	48	ep>non	No
1,3butadiene	Bayland	1998	7	36	non>ep	No
1,3butadiene	Clinton	2000	*24*	*31*	non>ep	**Yes**
1,3butadiene	Clinton	1999	22	54	non>ep	**Yes**
1,3butadiene	Clinton	1998	16	26	non>ep	No
1,3butadiene	Deer Park	2000	8	9	ep>non	**Yes**
1,3butadiene	Deer Park	1999	24	54	non>ep	No

Table 5-1. Results of two-sample t-tests for ethylene, propylene, and isoprene by location and year, July-September, 0500-0900: number of days in each episode and non-episode median, whether episode or non-episode median weight percents are higher and whether episode and non-episode weight percents are different at a 95% confidence level. Significant differences are highlighted in bold.

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Species	Site	Year	Number of days/ episode	Number of days/ non-episode	Which median weight percent is higher?	Different at a 95% confidence level?
Toluene	Aldine	2000	5	16	ep>non	No
Toluene	Bayland	2000	*6*	*15*	non>ep	No
Toluene	Bayland	1999	22	48	ep>non	No
Toluene	Bayland	1998	7	*26*	ep>non	**Yes**
Toluene	Clinton	2000	32	48	ep>non	No
Toluene	Clinton	1999	22	54	ep>non	**Yes**
Toluene	Clinton	1998	16	26	ep>non	**Yes**
Toluene	Deer Park	2000	8	9	ep>non	No
Toluene	Deer Park	1999	24	54	non>ep	No
m-&p-xylene	Aldine	2000	5	16	non>ep	No
m-&p-xylene	Bayland	2000	*6*	*15*	non>ep	No
m-&p-xylene	Bayland	1999	22	48	ep>non	No
m-&p-xylene	Bayland	1998	7	*26*	ep>non	**Yes**
m-&p-xylene	Clinton	2000	32	48	ep>non	No
m-&p-xylene	Clinton	1999	22	54	non>ep	No
m-&p-xylene	Clinton	1998	16	26	non>ep	No
m-&p-xylene	Deer Park	2000	8	9	ep>non	No
m-&p-xylene	Deer Park	1999	24	54	non>ep	**Yes**
1,2,4trimethylbenzene	Aldine	2000	5	16	ep>non	No
1,2,4trimethylbenzene	Bayland	2000	*6*	*15*	non>ep	No
1,2,4trimethylbenzene	Bayland	1999	22	48	non>ep	**Yes**
1,2,4trimethylbenzene	Bayland	1998	7	*26*	ep>non	No
1,2,4trimethylbenzene	Clinton	2000	32	48	non>ep	**Yes**
1,2,4trimethylbenzene	Clinton	1999	22	54	ep>non	No
1,2,4trimethylbenzene	Clinton	1998	16	26	non>ep	No
1,2,4trimethylbenzene	Deer Park	2000	8	9	non>ep	No
1,2,4trimethylbenzene	Deer Park	1999	24	54	non>ep	**Yes**

5.3 DIURNAL CHARACTERISTICS

Box whisker plots are commonly used to display a large amount of data and are particularly useful in assessing differences among data. Box whisker plots are drawn in different ways by different software programs. However, most box whisker plots show an interquartile range (i.e., 25^{th} to 75^{th} percentile) and some way to illustrate data outside this range. **Figure 5-5** shows an illustrated box whisker and notched box whisker plot. The box shows the 25^{th}, 50^{th} (median), and 75^{th} percentiles. The whiskers always end on a data point, so when the plots show no data beyond the end of a whisker, the whisker shows the value of the highest or lowest data point. The whiskers have a maximum length equal to 1.5 times the length of the box (the interquartile range). If there are data outside this range, the points are shown on the plot and the whisker ends on the highest or lowest data point within the range of the whisker. The "outliers" are also further identified with asterisks representing the points that fall within three times the interquartile range from the end of the box and circles representing points beyond this.

Since sample size is also an important consideration when one begins to stratify data, notched box whisker plots have been used to analyze data in this study (see Figure 5-5). These plots include notches that mark confidence intervals. The boxes are notched (narrowed) at the median and return to full width at the lower and upper confidence interval values[1]. We selected 95% confidence intervals. If the 95% confidence interval is beyond the 25th or 75th percentile, then the notches extend beyond the box (hence the "folded" appearance).

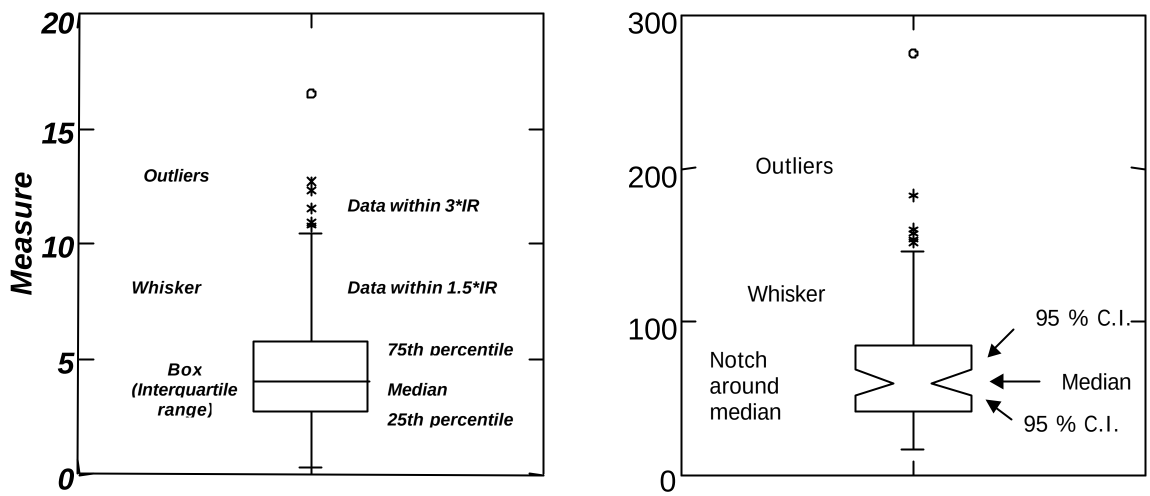

Figure 5-5. Illustration of a box-whisker plot and a notched box whisker plot as defined by SYSTAT statistical software.

Sixteen species for each site, based on their abundance in concentration and reactivity-weight percent, were examined on an hourly basis for days of ozone episodes and non-episodes. Hourly notched box plots of these species were generated by episode and non-episode in order to examine any diurnal variations between ozone episode and non-episode days. Example notched box plots of isobutane, ethylene, propylene and toluene by weight percent at Clinton in 1999 for episode and non-episode days are shown in **Figures 5-6 and 5-7**.

While concentration differences were observed for most species between episode and non-episode days, there was generally little difference in weight percent or reactivity-weighted data between ozone episodes and non-episodes.

[1] SYSTAT literature uses methodology documented by McGill, Tukey, and Larsen (1978) to show simultaneous confidence intervals on the median of several groups in a box plot. If the intervals around two medians do not overlap, one can be confident at about the 95% level that the two population medians are different.

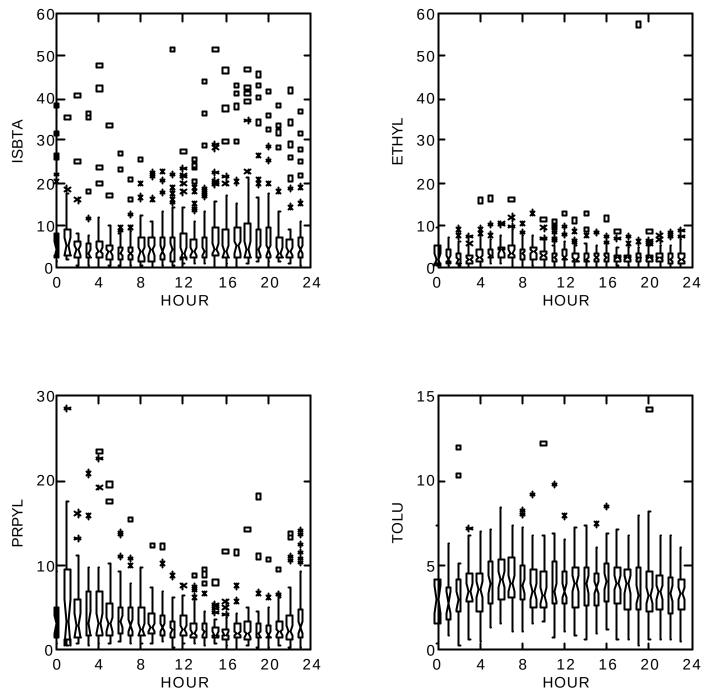

Figure 5-6. Notched box plots of isobutane (ISBTA), ethylene (ETHYL), propylene (PRPYL), and toluene (TOLU) by weight percent for non-episode days at Clinton, July-September 1999.

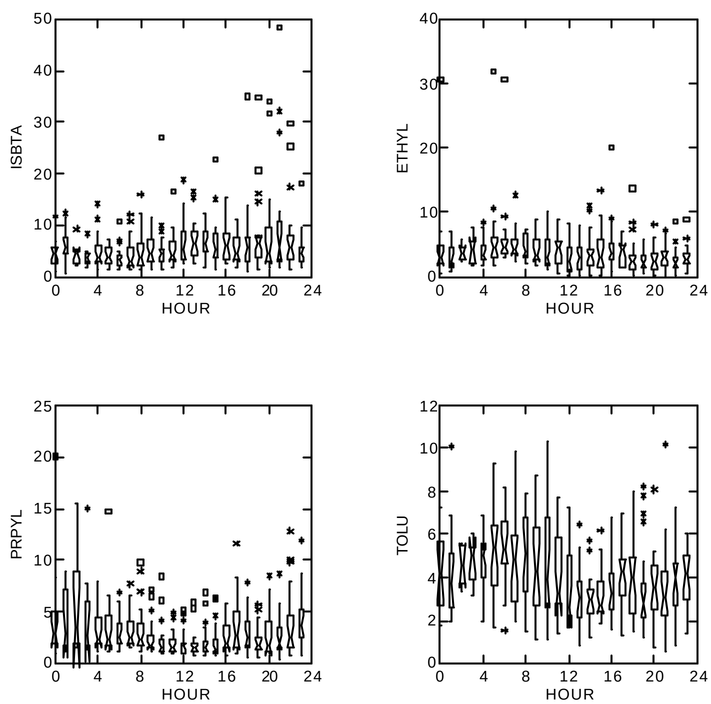

Figure 5-7. Notched box plots of isobutane (ISBTA), ethylene (ETHYL), propylene (PRPYL), and toluene (TOLU) by weight percent for episode days at Clinton, July-September 1999.

5.4 EPISODE ANALYSIS BY WIND DIRECTION

We prepared several maps of the monitoring sites to assist us in understanding the layout of the Houston Ship Channel including the location of potential sources (e.g., freeways, industrial complexes) near the sites. **Figures 5-8 through 5-14** show aerial photographs of the areas surrounding the auto-GC data collection sites. The figures also include some landmarks such as freeways and major arterial roads. **Figure 5-15** shows the VOC sources reporting more than 99 tons per year in the 1999 TNRCC emission inventory. These maps coupled with site visits indicate the likelihood of a directional dependence on composition and concentration.

Figures 5-16 and 5-17 show scatter plots of the concentrations of selected hydrocarbons with respect to wind direction at the Clinton and Deer Park sites. Ambient concentrations at other sites did not show as much directional dependence. Observations from the figures follow:

- Toluene, 1,3-butadiene, and n-butane concentrations are higher when winds are from the south at the Clinton site. Other hydrocarbons showing similar patterns include C4 and C5 alkanes and propane. Ethene, propene and xylenes do not show clear patterns.
- Ethene, toluene, propene, and 1,3-butadiene concentrations are higher when winds are from the northeast at the Deer Park site. The butanes show a similar pattern.

Ethylene and propylene weight percents were also investigated by wind direction in order to determine whether there were any dominant sources of these hydrocarbons in a particular direction for each site. Wind octants (north, northeast, etc. shown in **Figure 5-18**) were assigned based on the wind direction for each hour's data, and the median values for each wind direction during the morning (0500-0900) for episode and non-episode days in 1998 through 2000 were found. The following observations resulted:

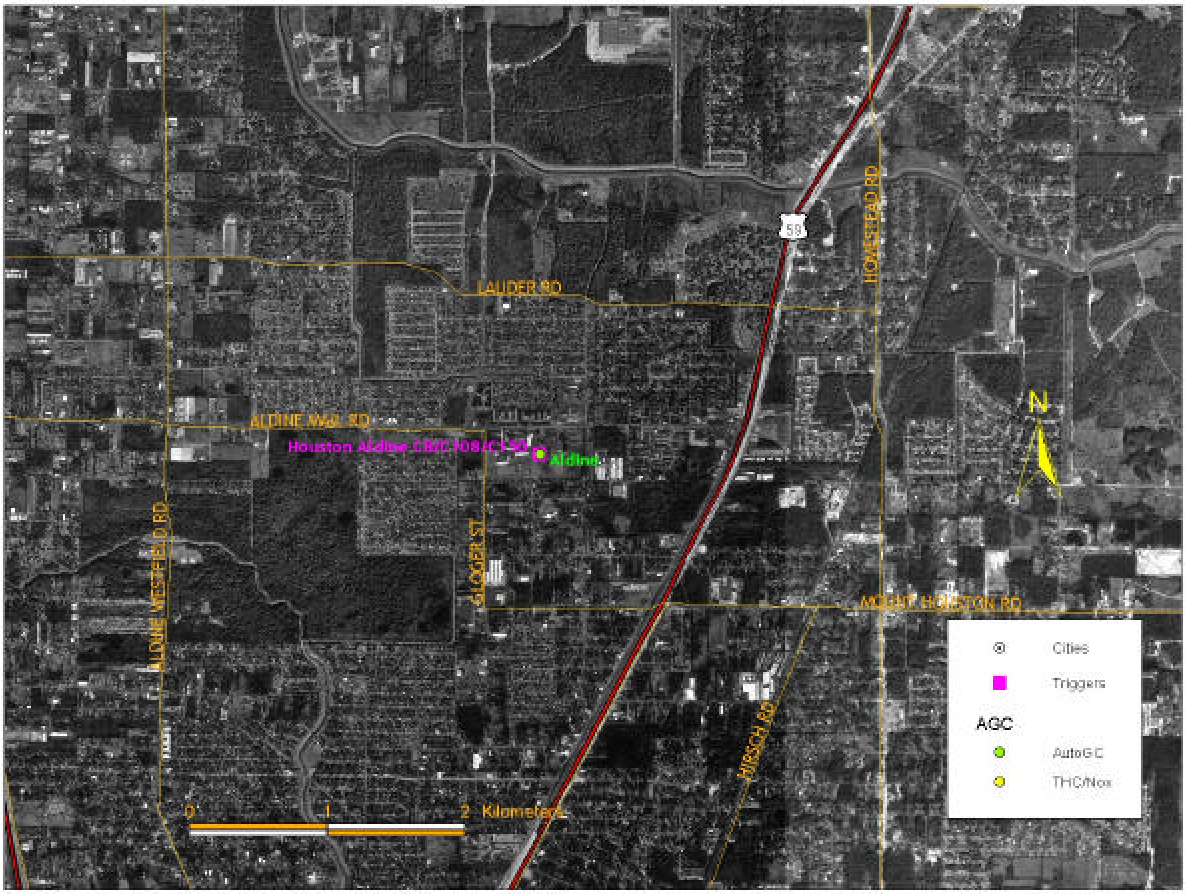

Figure 5-8. 3.5 minute digital orthophotoquads of the area surrounding the Aldine monitoring site. Photos are circa 1995 from the U.S. Geological Survey.

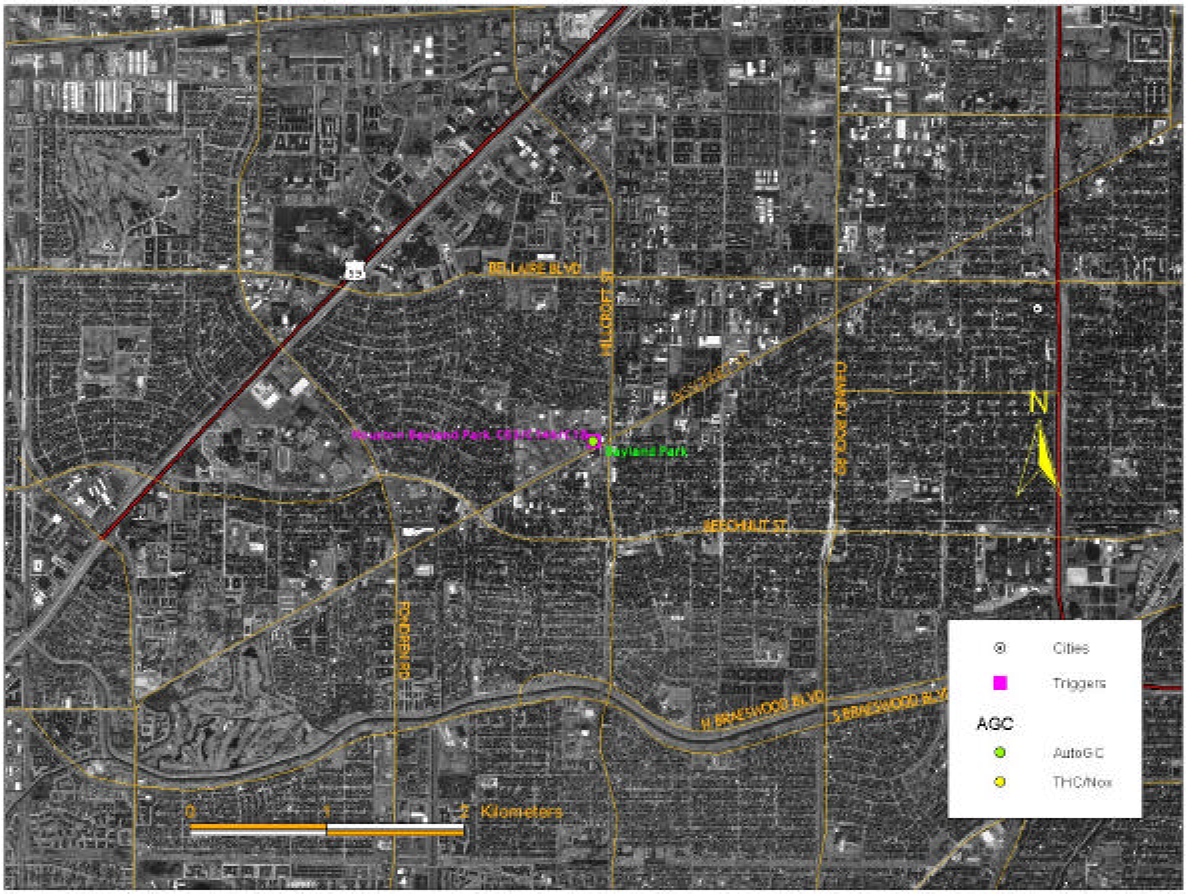

Figure 5-9. 3.5 minute digital orthophotoquads of the area surrounding the Bayland Park monitoring site. Photos are circa 1995 from the U.S. Geological Survey.

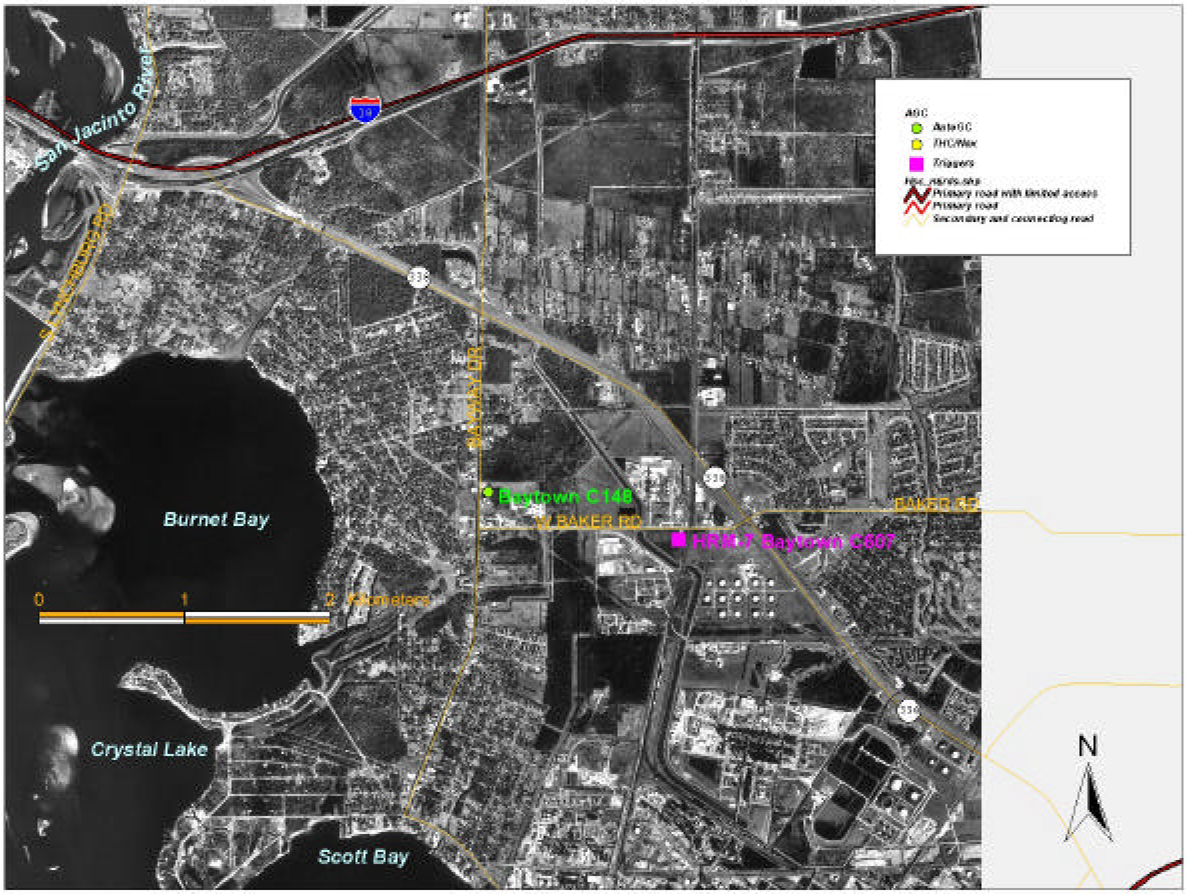

Figure 5-10. 3.5 minute digital orthophotoquads of the area surrounding the Baytown monitoring site. Photos are circa 1995 from the U.S. Geological Survey.

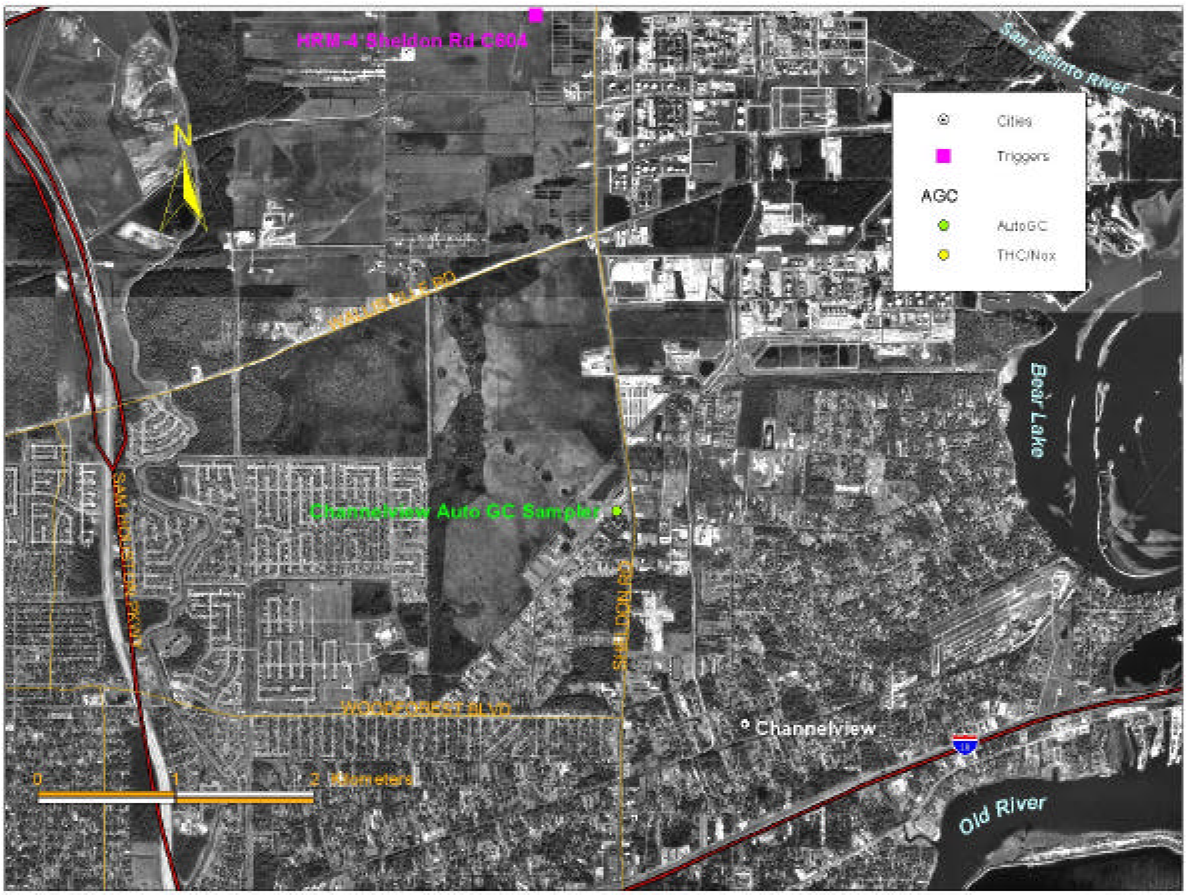

Figure 5-11. 3.5 minute digital orthophotoquads of the area surrounding the Channelview monitoring site. Photos are circa 1995 from the U.S. Geological Survey.

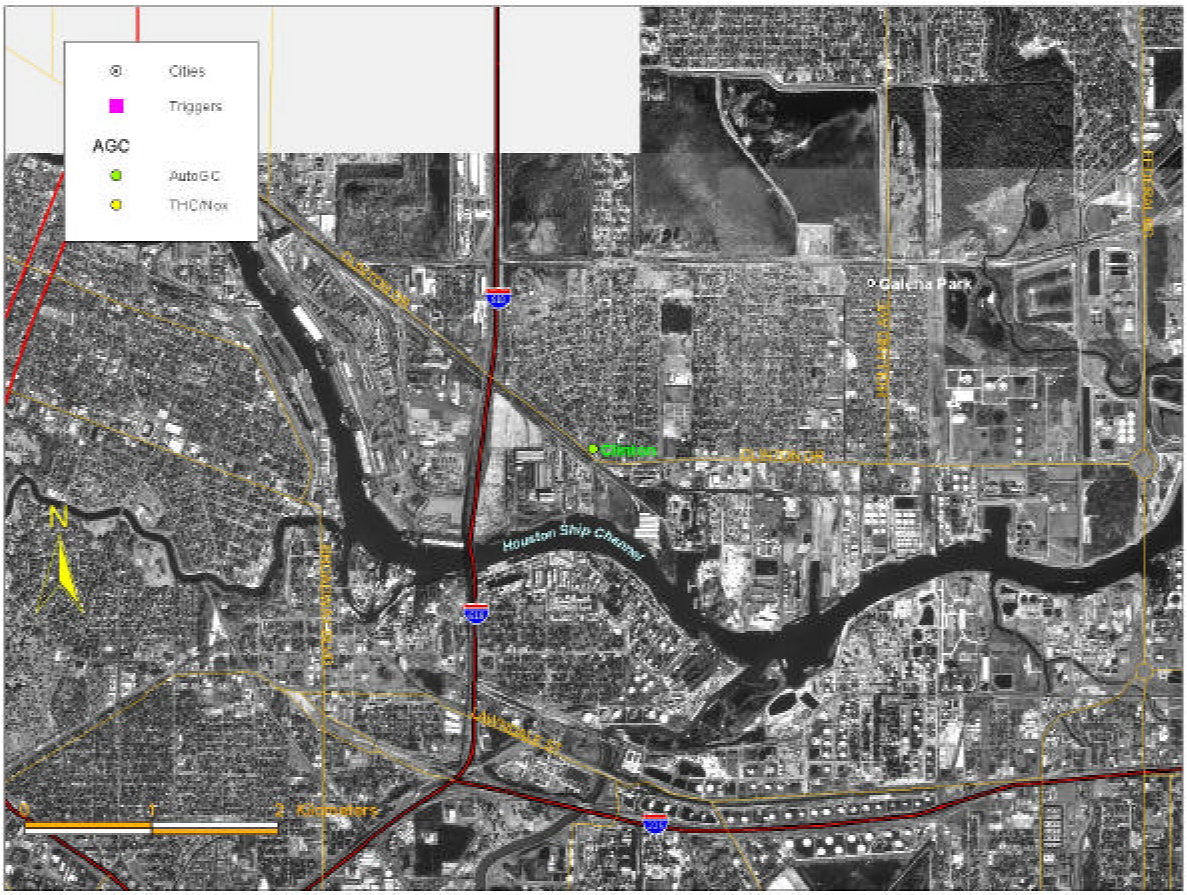

Figure 5-12. 3.5 minute digital orthophotoquads of the area surrounding the Clinton monitoring site. Photos are circa 1995 from the U.S. Geological Survey.

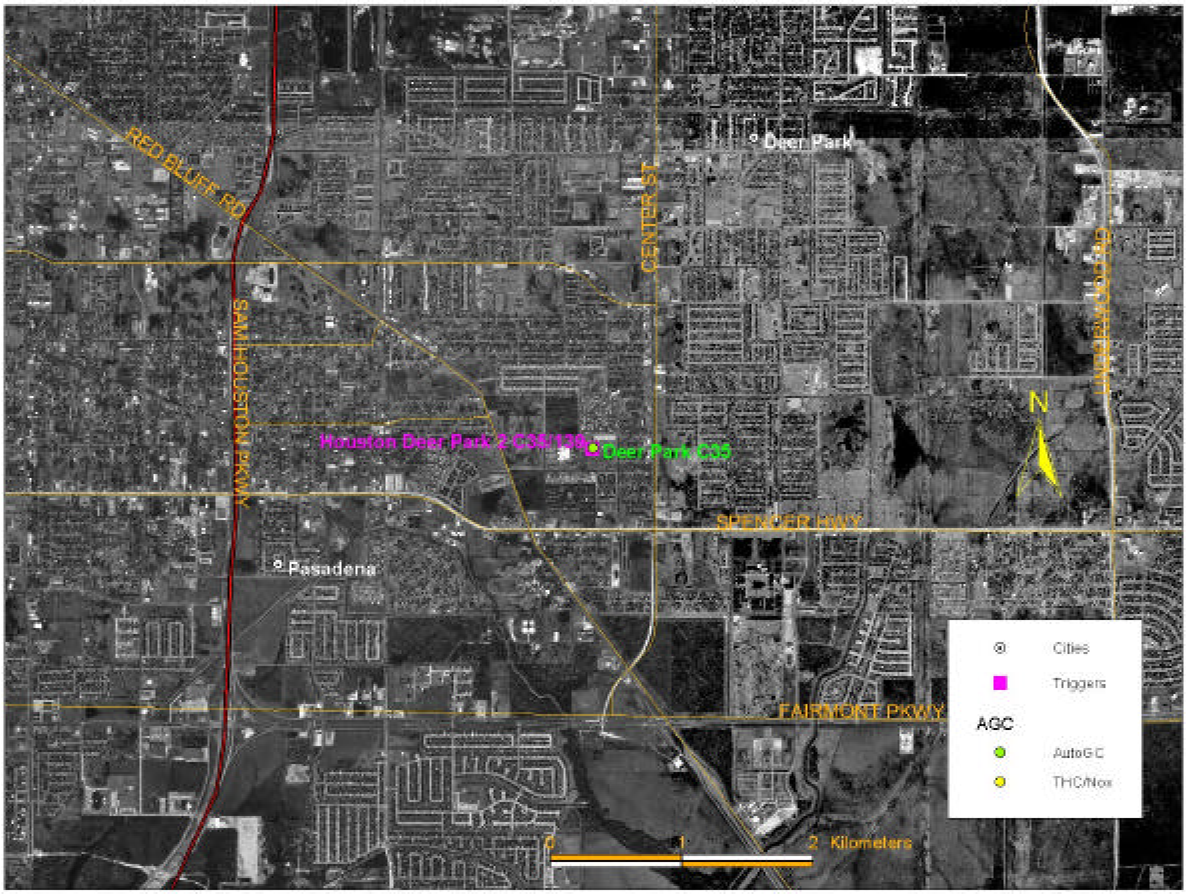

Figure 5-13. 3.5 minute digital orthophotoquads of the area surrounding the Deer Park monitoring site. Photos are circa 1995 from the U.S. Geological Survey.

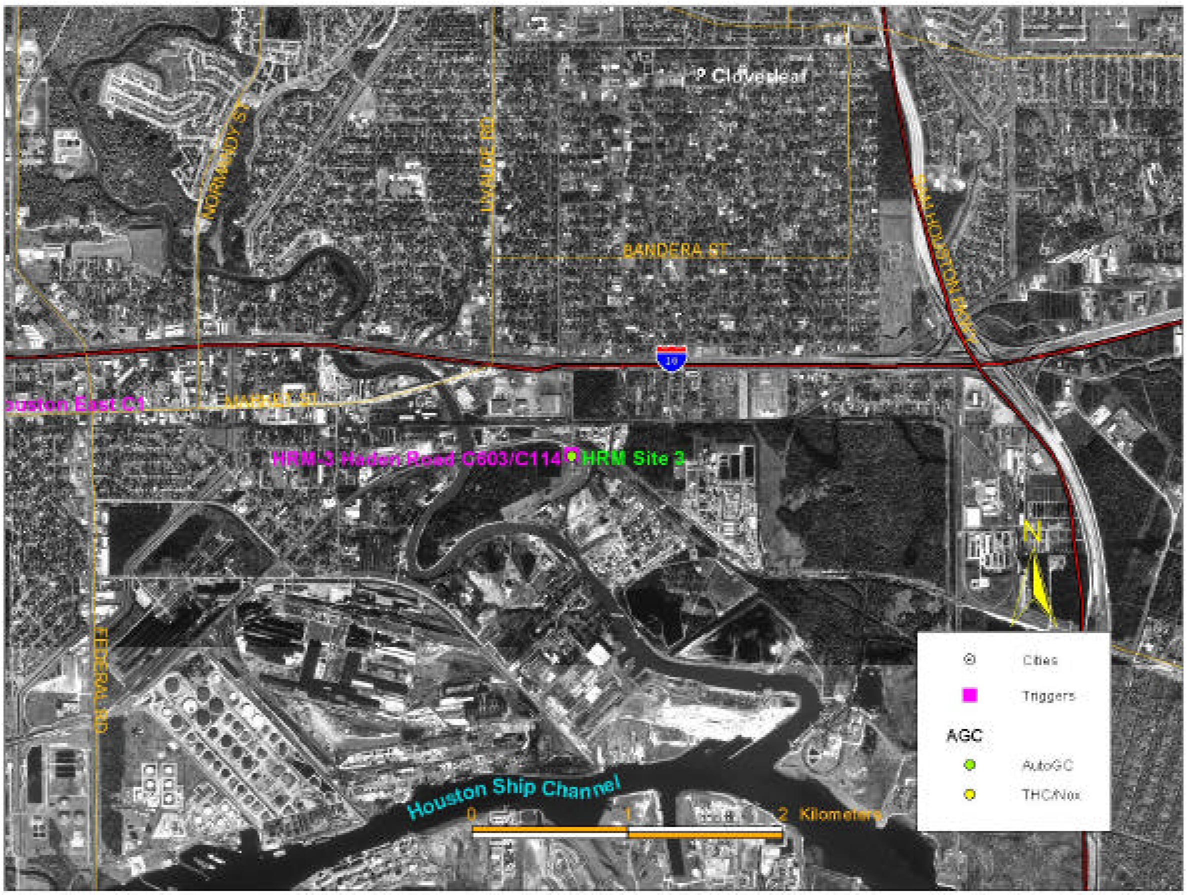

Figure 5-14. 3.5 minute digital orthophotoquads of the area surrounding the HRM-3 monitoring site. Photos are circa 1995 from the U.S. Geological Survey.

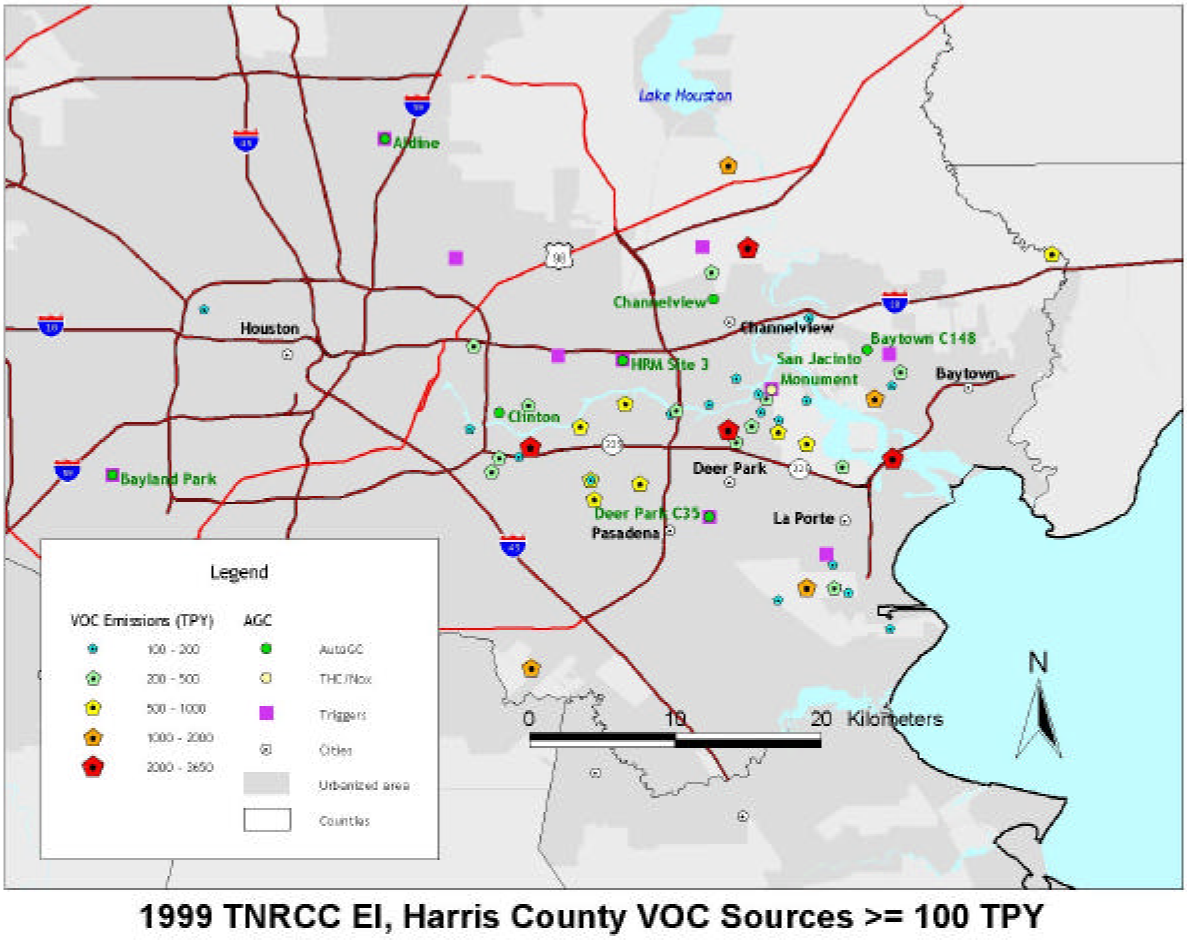

Figure 5-15. Harris County VOC sources greater than or equal to 100 tons per year (TNRCC emission inventory, 1999).

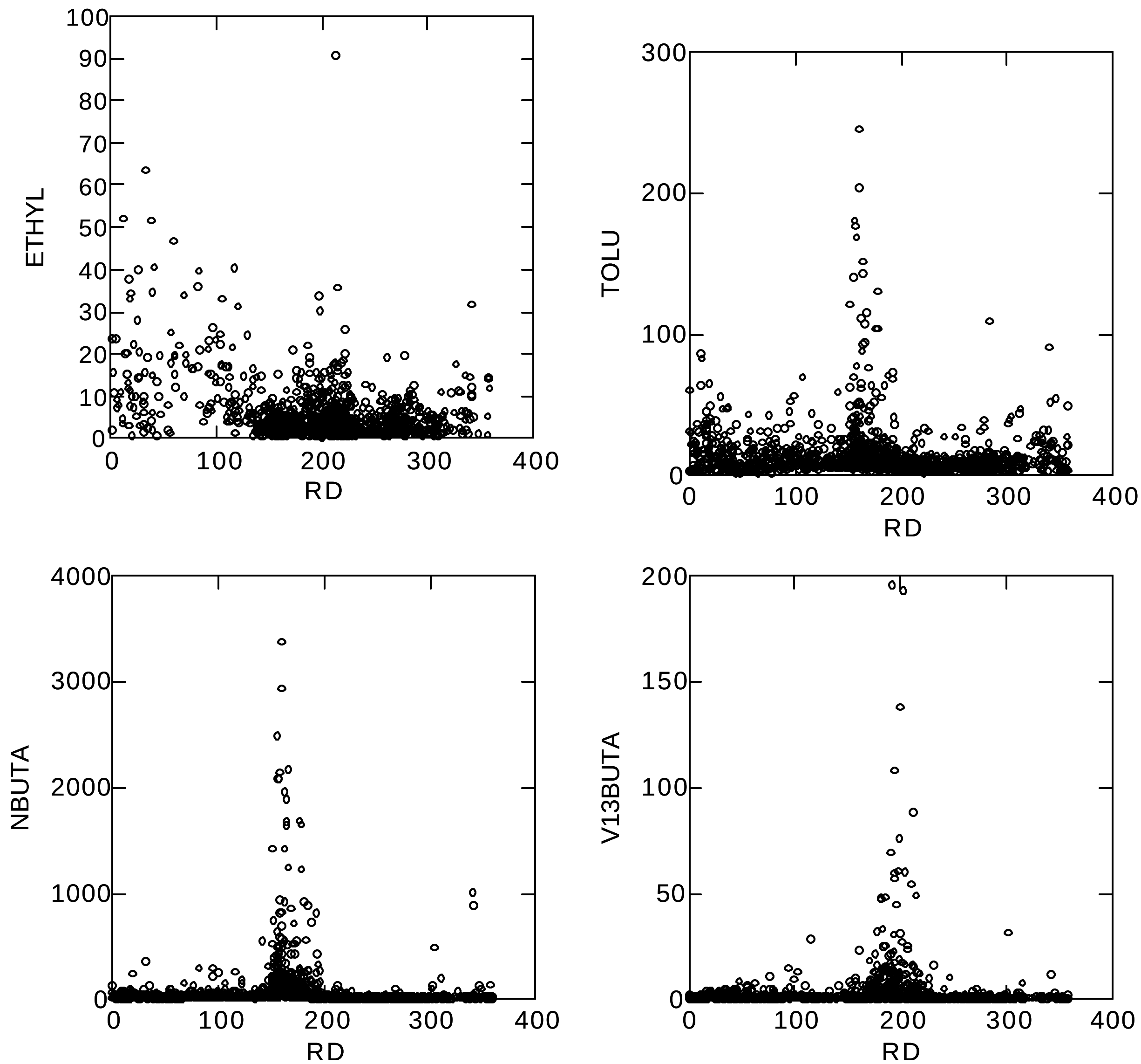

Figure 5-16. Concentrations of ethene (ETHYL), toluene (TOLU), n-butane (NBUTA), and 1,3-butadiene (V13BUTA) at Clinton during July, August, and September 2000 (all hours included).

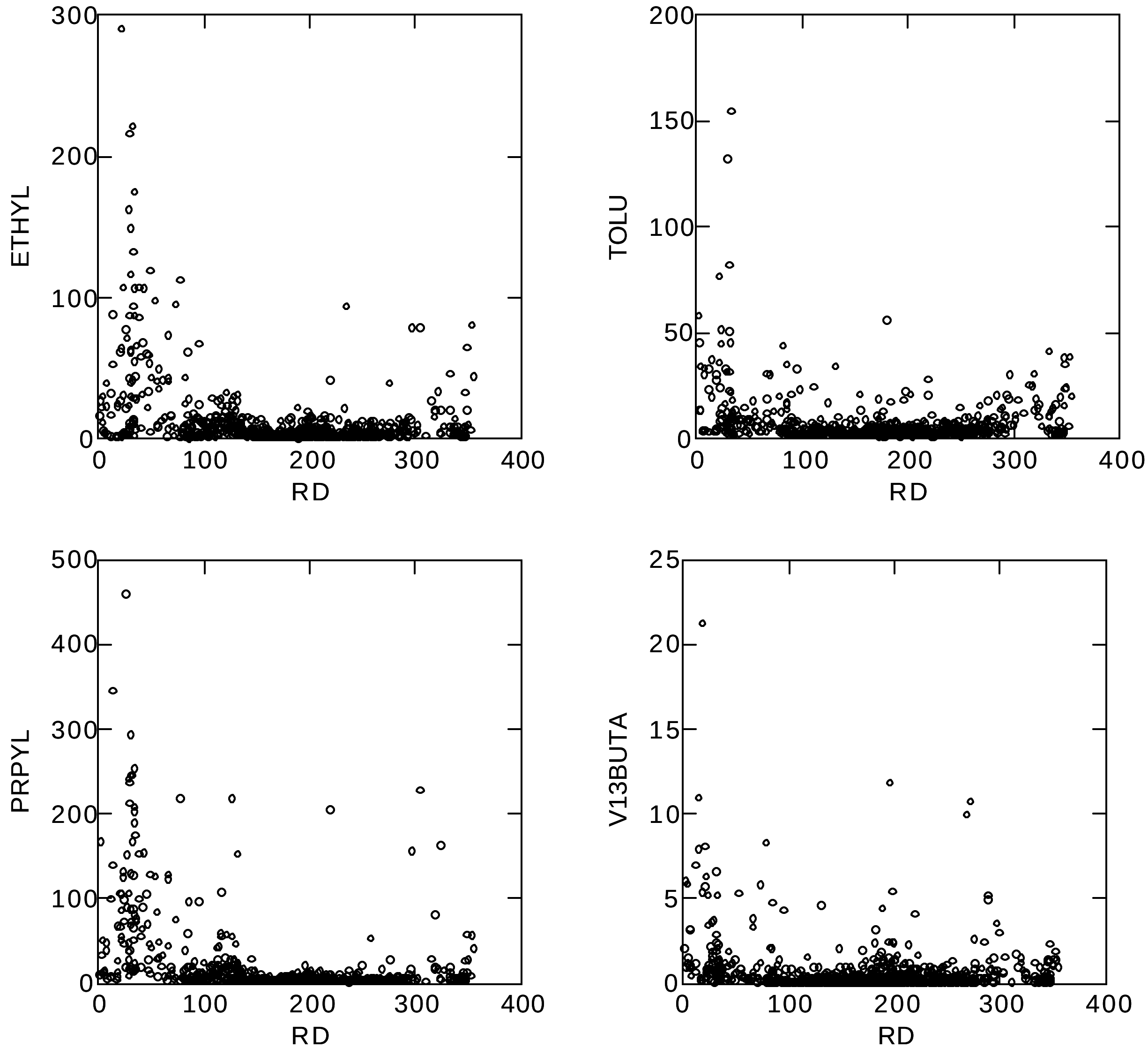

Figure 5-17. Concentrations of ethene (ETHYL), toluene (TOLU), propene (PRPYL), and 1,3-butadiene (V13BUTA) at Deer Park during July, August, and September 2000 (all hours included).

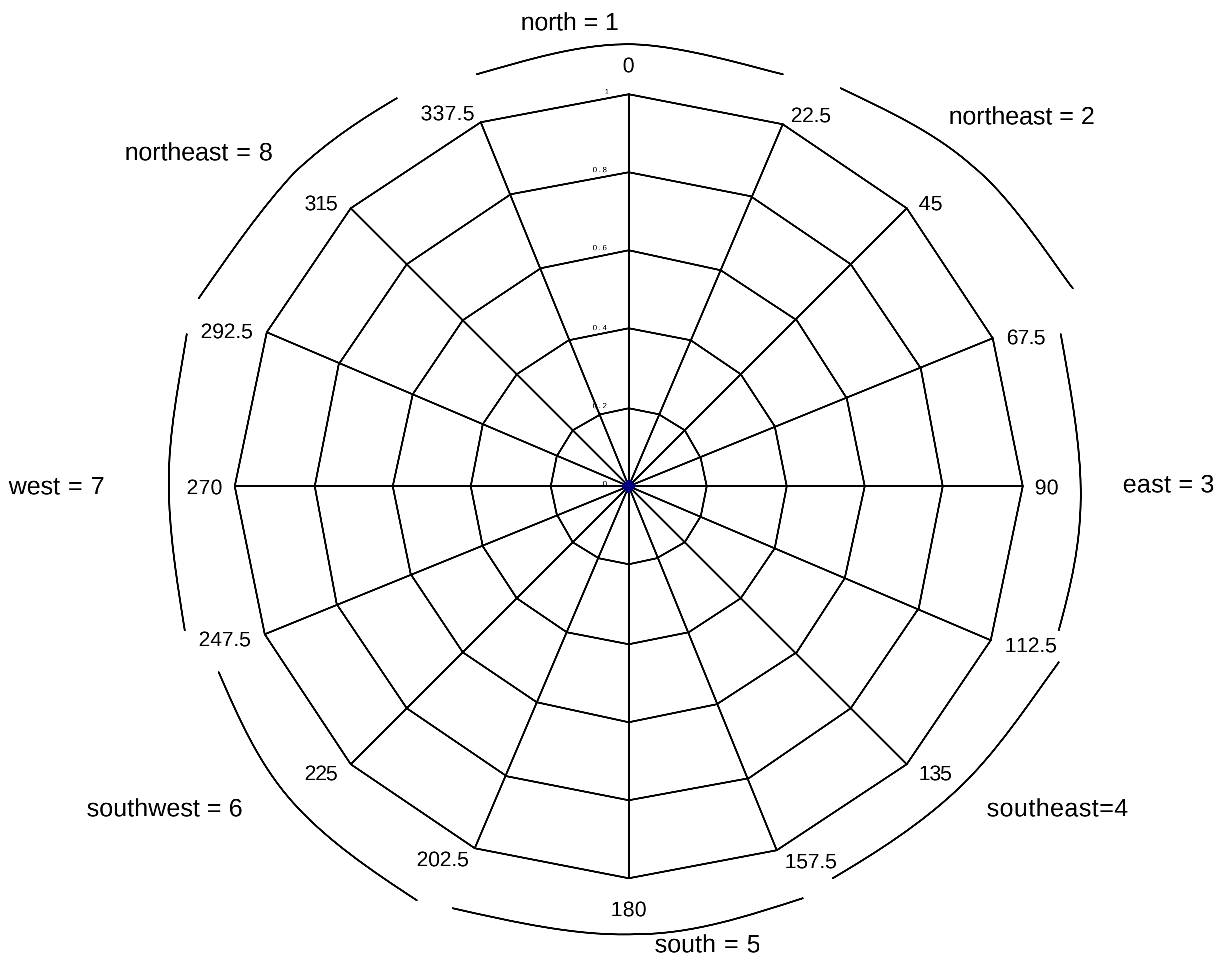

Figure 5-18. Sample radar plot showing assigned wind octants by degree (0-360).

- Aldine (September 2000). The weight percent of both ethylene and propylene were generally consistent from every direction though there is a spike in weight percent during episode days when the wind was from the north. However, there were a limited data from this site, which was operational for less than 20 days during September 2000.
- Bayland (July-September 1998-1999; July 1-August 6, 2000). Wind direction patterns for ethylene and propylene concentrations varied by year:
  - Concentrations were higher in 1998 on episode days when winds were from the east.
  - Concentrations were highest in 1999 on episode days when winds were from the northeast.
  - Little difference was observed in concentrations between episode and non-episode days in 2000. Note that data were only available for July.
  - On a weight-percent scale, ethylene and propylene fractions were consistently highest when winds were from the north and northeast. In 1999, ethylene and propylene had higher weight percents from these directions on episode days while in 1998 the weight percents were higher on non-episode days.
- Clinton (July-September 1998-2000). Ethylene and propylene were generally higher in concentration when winds were from the east in 1998 and from the northeast in 1999. On a weight-percent basis, these hydrocarbons were more abundant when winds were from the northeast on both episode and non-episode days (see **Figures 5-19 and 5-20**). 1,3-butadiene fractions show more of a westerly component on episode mornings and an easterly component on non-episode mornings (**Figure 5-21**). Toluene fractions are greater for winds from the northwest on both episode and non-episode mornings in 1999 (**Figure 5-22**) possibly influenced by presence of the freeway.
- Deer Park (July-September 1998-2000). Concentrations of both ethylene and propylene were significantly higher on episode and non-episode days when winds were from the north and northeast. Ethylene is higher in weight percent on episode days with winds from the northeast and east in 1999 and 2000. The high concentrations arriving from the north and northeast are consistent with the industrial activities along the Houston Ship Channel to the north.

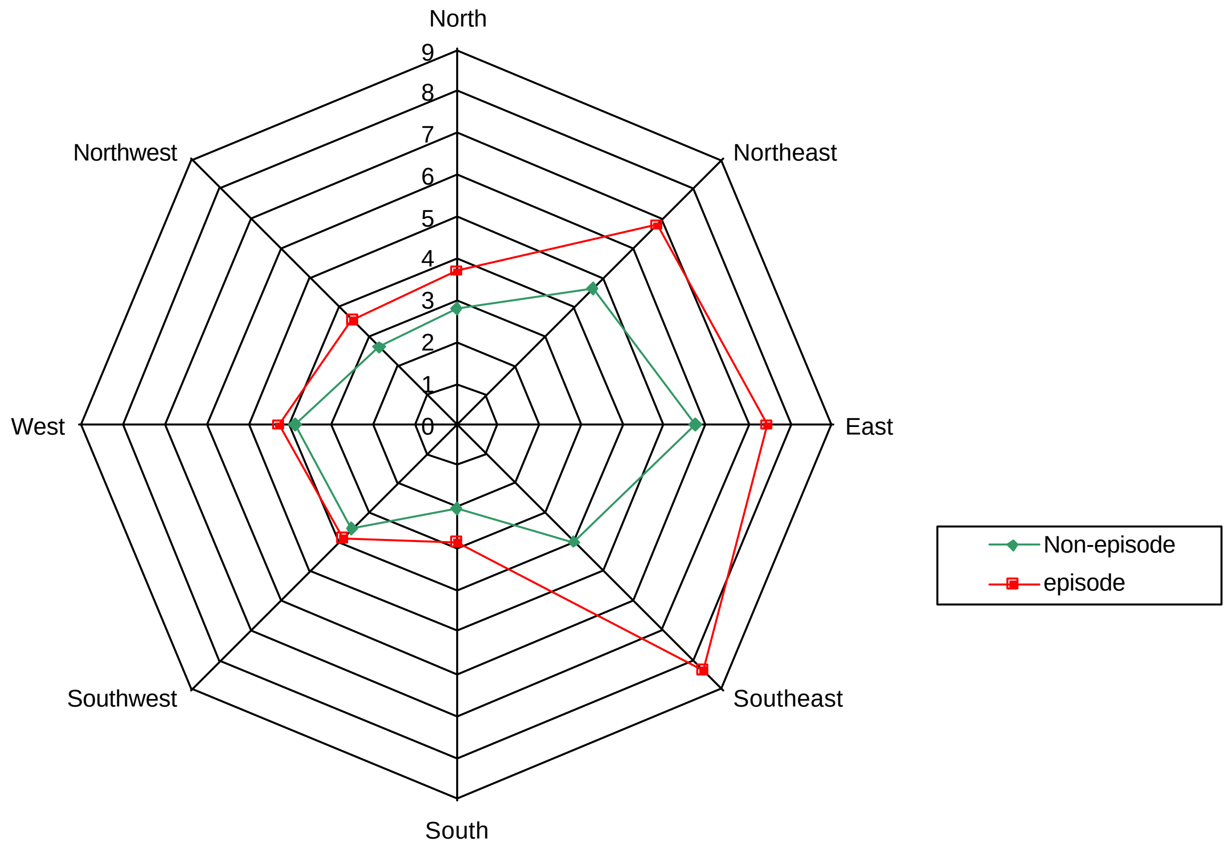

Figure 5-19. Radar plot of the median weight percent of ethylene by wind direction for episode and non-episode days at Clinton, July-September (0500-0900) 1999.

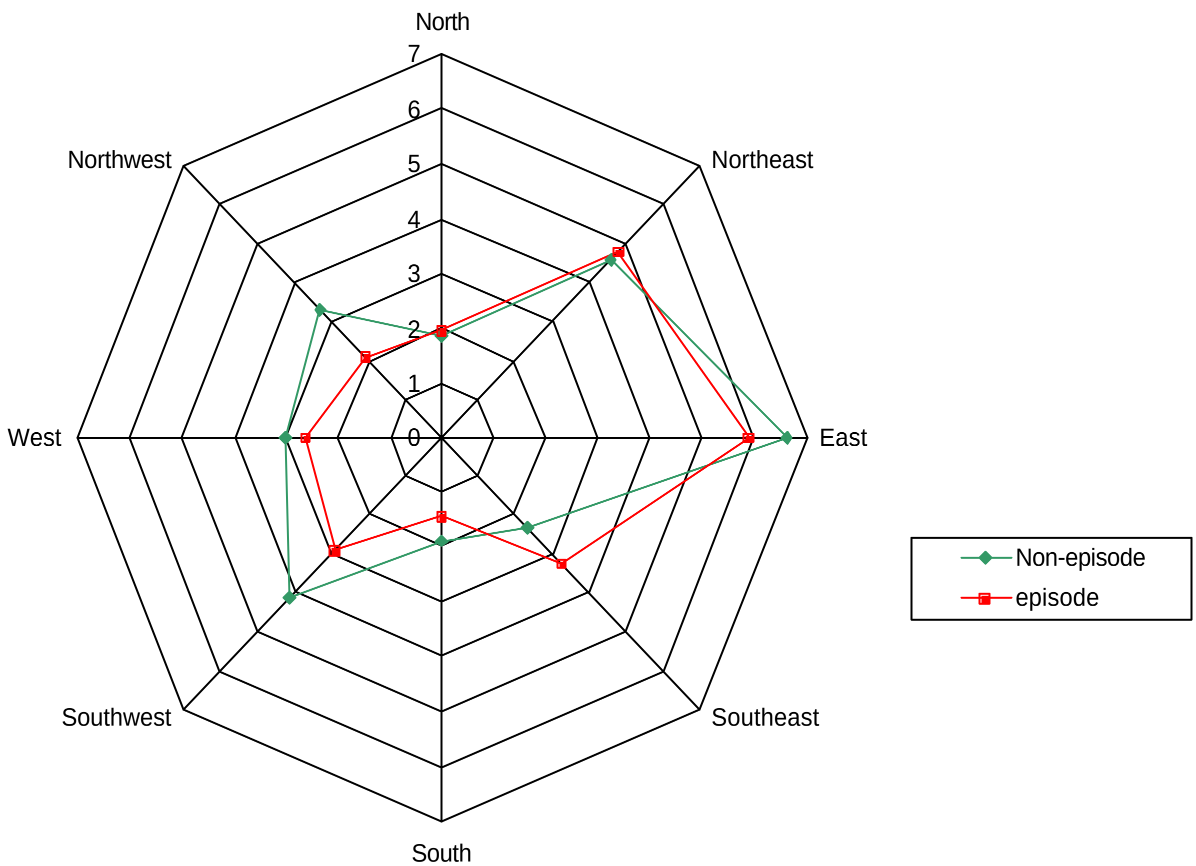

Figure 5-20. Radar plot of the median weight percent of propylene by wind direction for episode and non-episode days at Clinton, July-September (0500-0900) 1999.

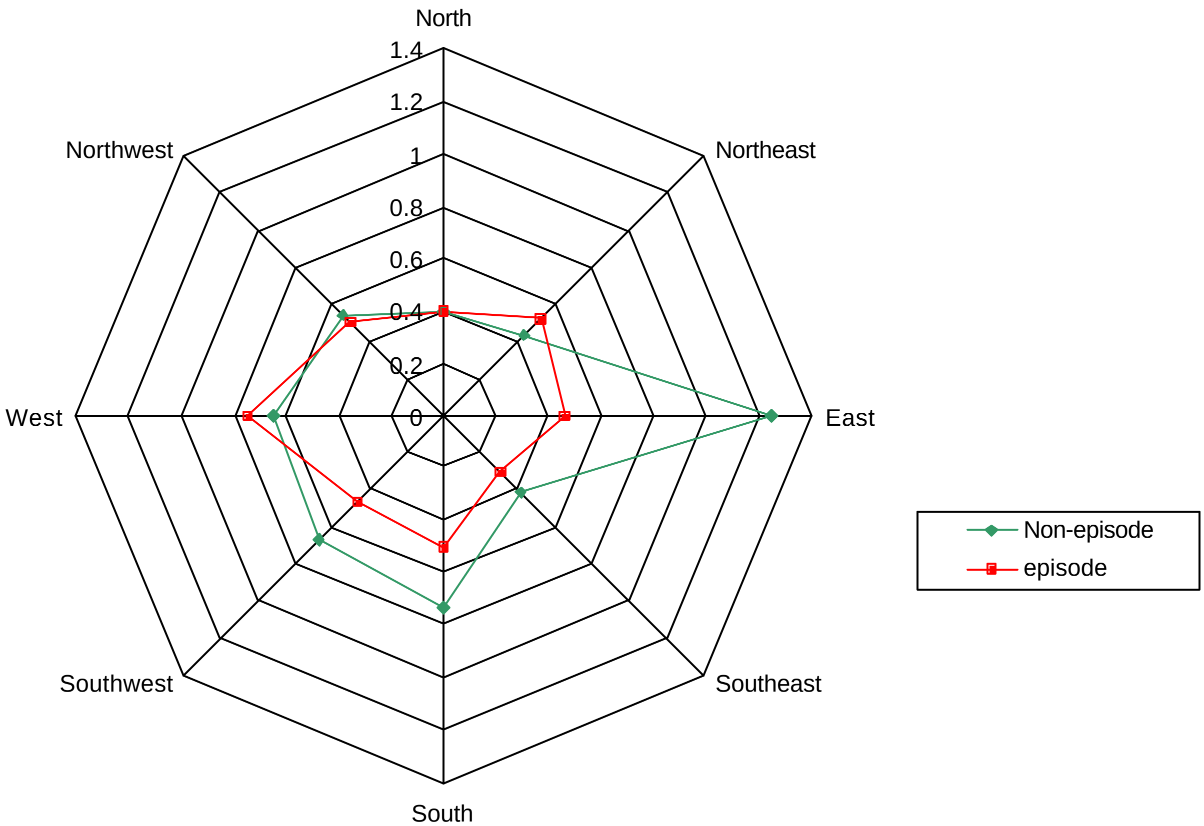

Figure 5-21. Radar plot of the median weight percent of 1,3-butadiene by wind direction for episode and non-episode days at Clinton, July-September (0500-0900) 1999.

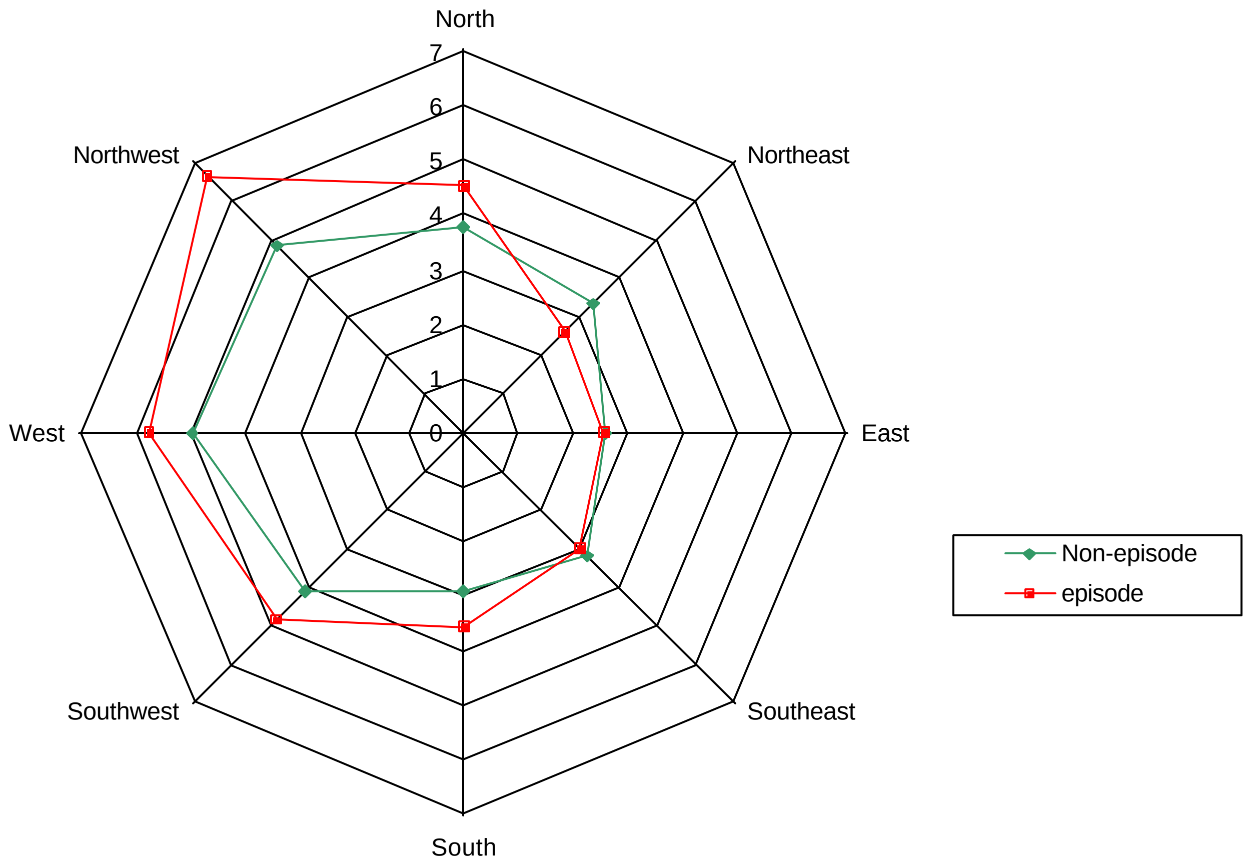

Figure 5-22. Radar plot of the median weight percent of toluene by wind direction for episode and non-episode days at Clinton, July-September (0500-0900) 1999.

Figures 5-23 and 5-24 show median concentration fingerprints for episode and non-episode days at Clinton during summer 2000. The fingerprints are provided by wind quadrant (where Northeast = 22.5 to 67.5 degrees, etc.). The fingerprints are on the same scale for comparison purposes. We made the following observations:

- On non-episode days concentrations tended to be highest when winds were from the east and south.
- On episode days, some hydrocarbons are highest when winds are from the north (e.g., toluene, xylenes, propane, several alkanes) while others were highest when winds were from the south (including butanes, C4 and C5 olefins, and 2,2,4-trimethylpentane). Ethene concentrations appear to be highest when winds are from the north, northeast, and east. There is little wind direction difference for propene.

It is clear from our analyses by wind direction that concentrations and composition are highly dependent on wind direction, particularly at Clinton and Deer Park. Future analyses include investigating additional scatter plots and fingerprints for episode and non-episode mornings and individual days, and fingerprints showing weight fractions and reactivity weighting.

5.5 ANALYSIS OF THE AUGUST 23-SEPTEMBER 1, 2000 MODELING PERIOD

The period of August 23-September 1, 2000 was selected for detailed photochemical modeling; these dates were subject to more in-depth analysis of hydrocarbon composition and concentrations. Fingerprints were prepared for the mornings (0500-0700) of these dates using concentration, weight percent, and reactivity-weighted data. Specifically, days of ozone episodes (August 25-16 and August 29-September 1) were compared to non-episode days (August 23-24 and August 27-28) during the period.

Fingerprints of the median concentration, weight percent, and reactivity-weighted data for each morning (0500-0700) at Clinton are shown in **Figures 5-25 through 5-32**. Observations from these figures include the following:

- TNMOC concentrations are highest on the episode days of August 25-26, but the next highest days are the non-episode days of August 23-24. The episode days of August 30-September 1 all have much lower concentrations than the non-episode days of August 23-24. These findings suggest that high hydrocarbon concentrations may not necessarily facilitate an ozone episode.
- There is also no clear pattern in the weight-percent data between the episode and non-episode days. For example, ethane and propane fractions (good indicators of accumulation and carryover) vary from day to day with no clear pattern between the episode and non-episode days. Toluene and isopentane fractions are 6%-7% for all days, and m-&p-xylenes remain around 2%-3% for all days.
- There is no clear pattern in the reactivity-weighted data between episodes and non-episodes. The two most abundant species on this scale, ethylene and propylene, generally vary between 4% and 8% on both episode and non-episode days. Toluene and xylenes, also significant species on this scale, show no discernable difference between the episode and non-episode days.

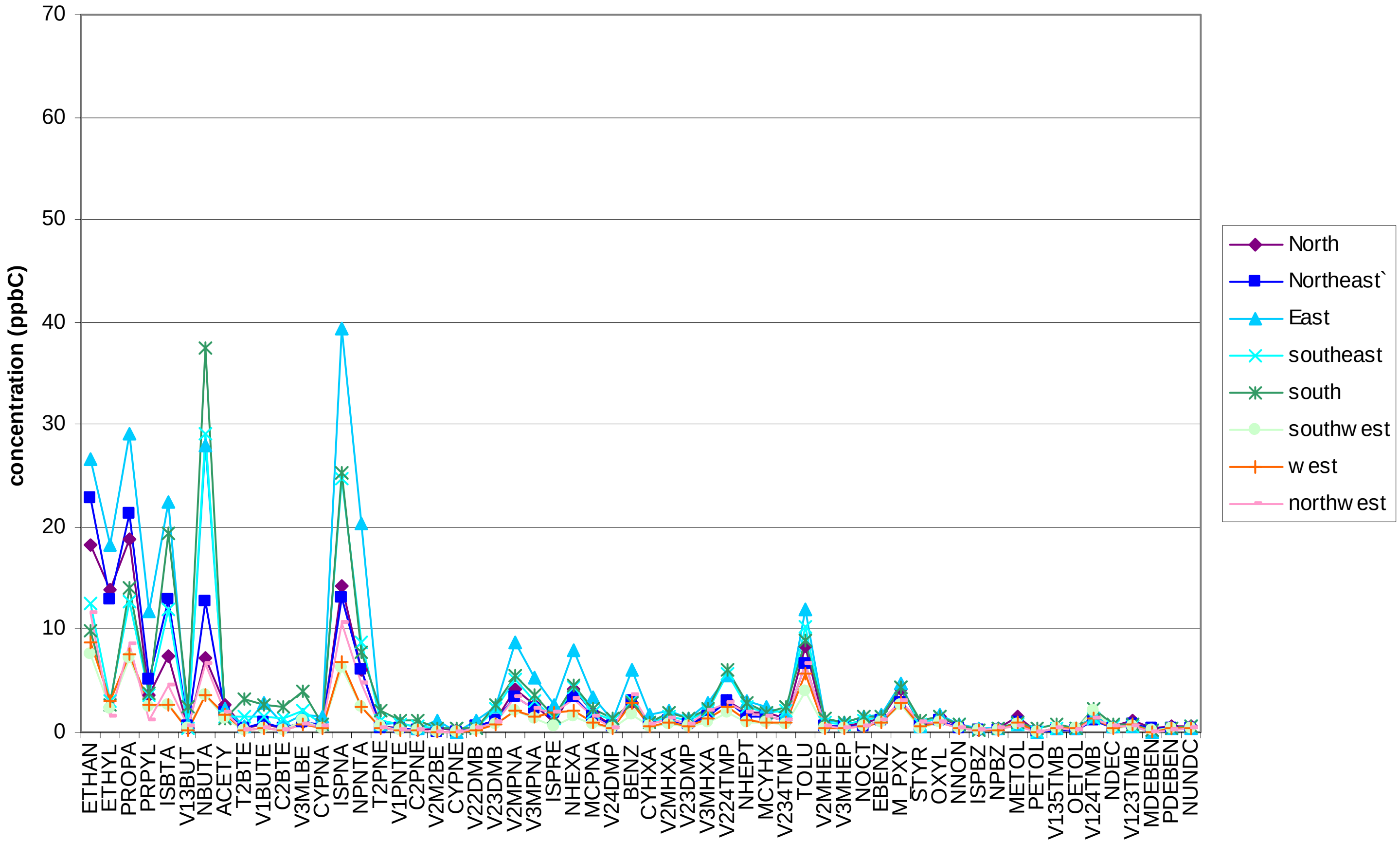

Figure 5-23. Fingerprint at Clinton, July-September 2000 (0500-0900): median concentrations (ppbC) during non-episode days by wind octant. Species abbreviations are found in Appendix B.

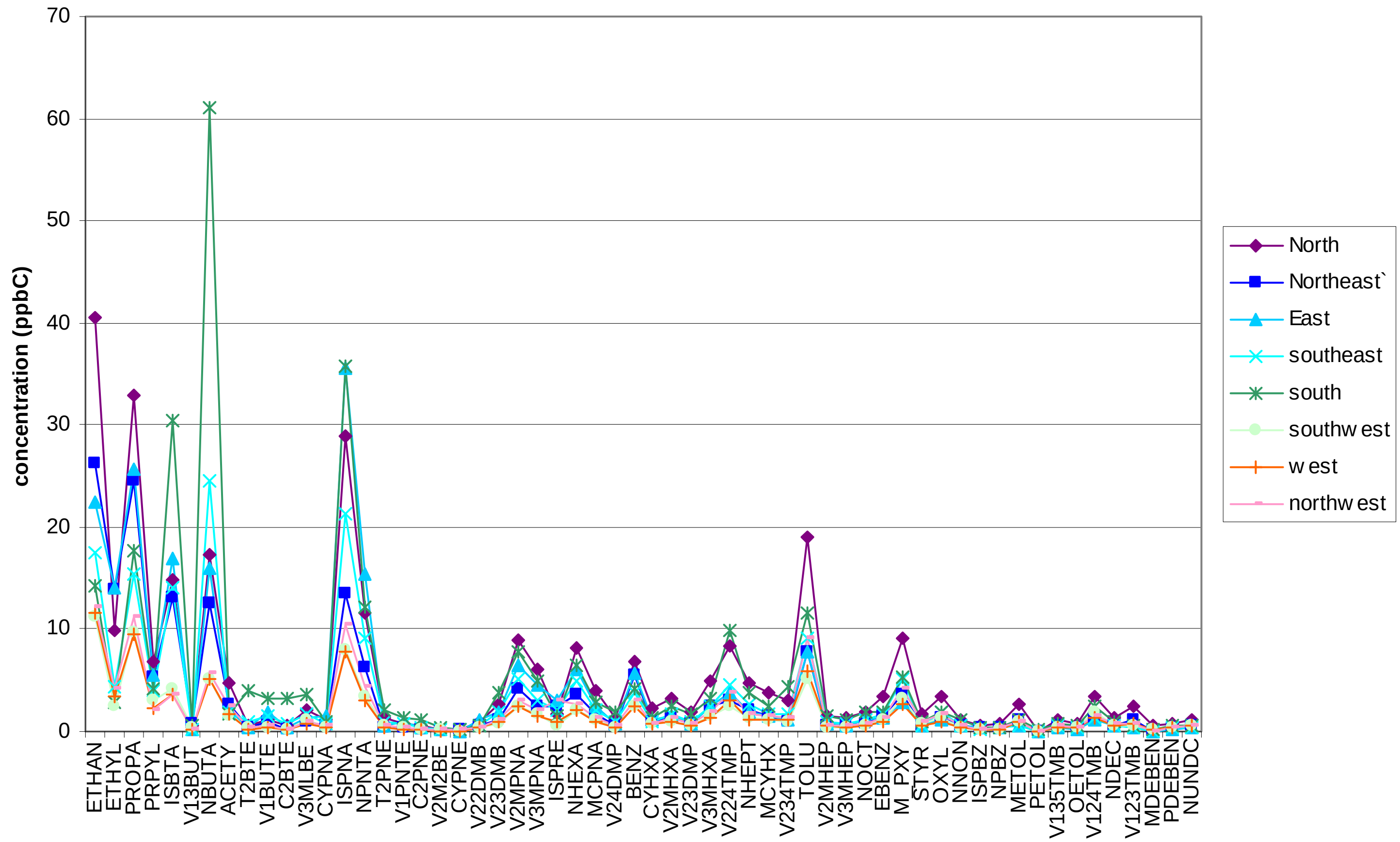

Figure 5-24. Fingerprint at Clinton, July-September 2000 (0500-0900): median concentrations (ppbC) during episode days by wind octant. Species abbreviations are found in Appendix B.

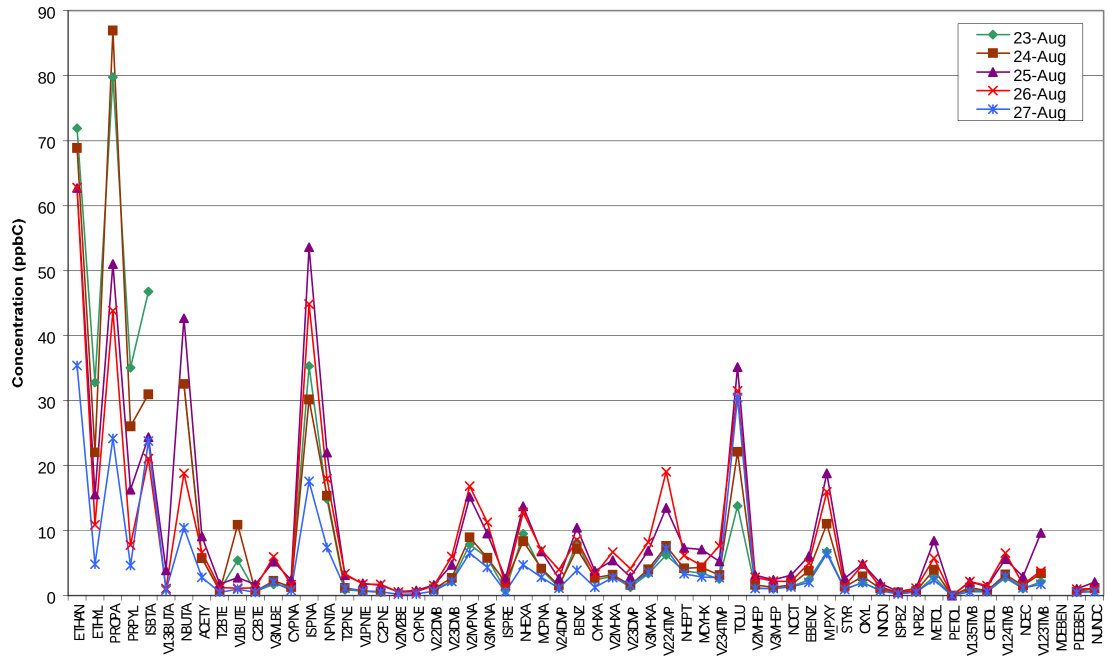

Figure 5-25. Median concentrations at Clinton, August 23-27, 2000 (0500-0700).

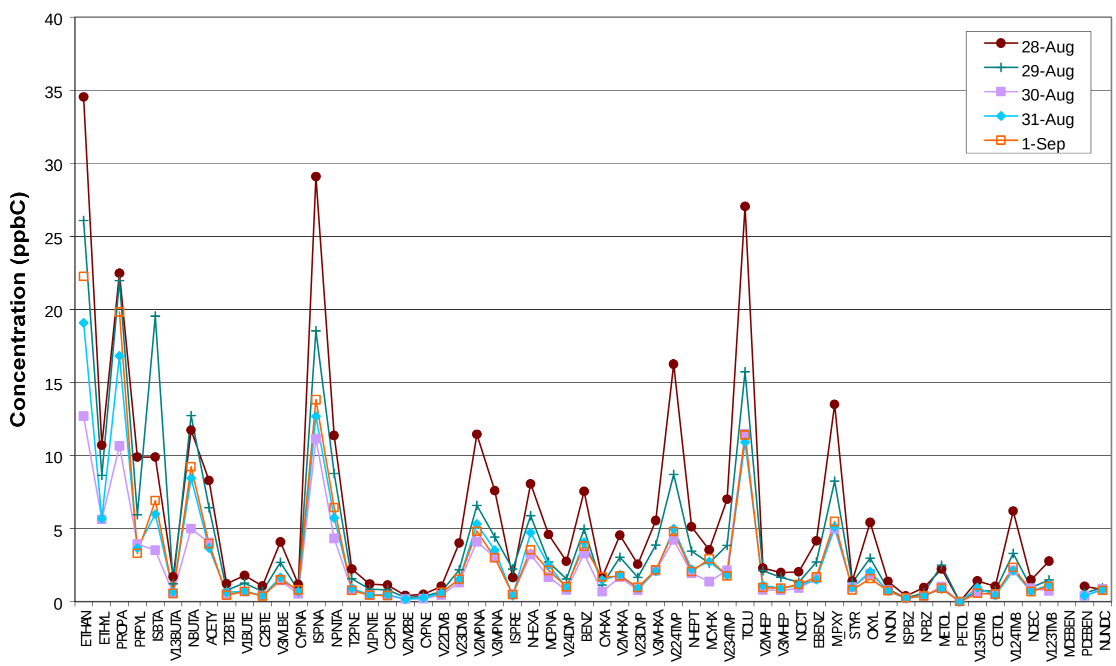

Figure 5-26. Median concentrations at Clinton August 28-September 1, 2000 (0500-0700).

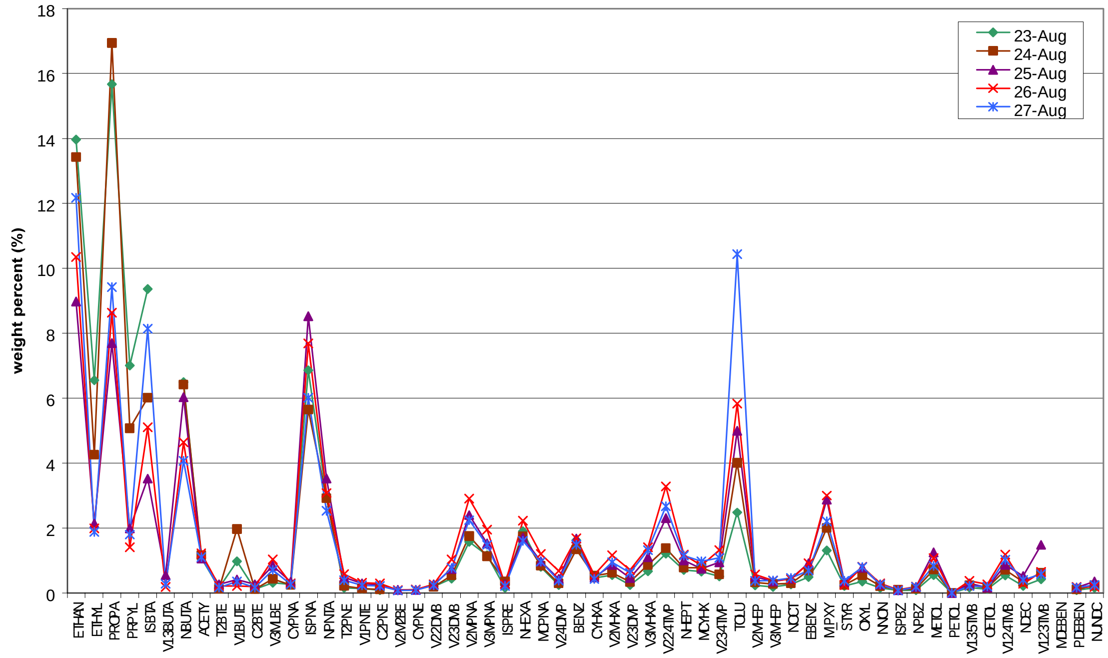

Figure 5-27. Median weight percents at Clinton, August 23-27, 2000 (0500-0700).

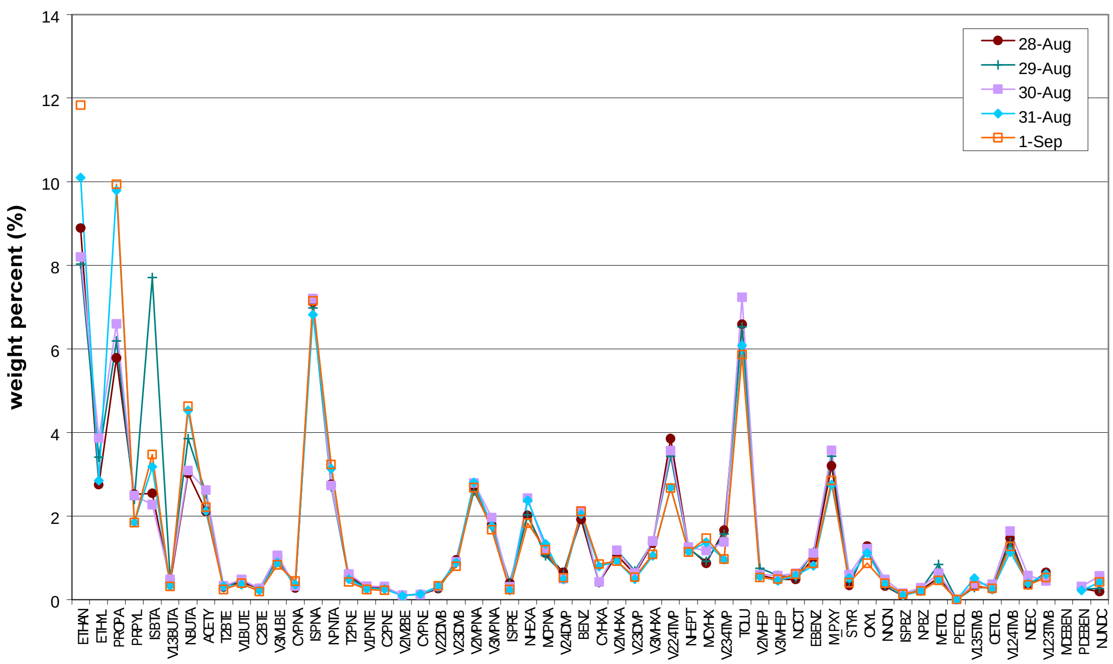

Figure 5-28. Median weight percents at Clinton, August 28-September 1, 2000 (0500-0700).

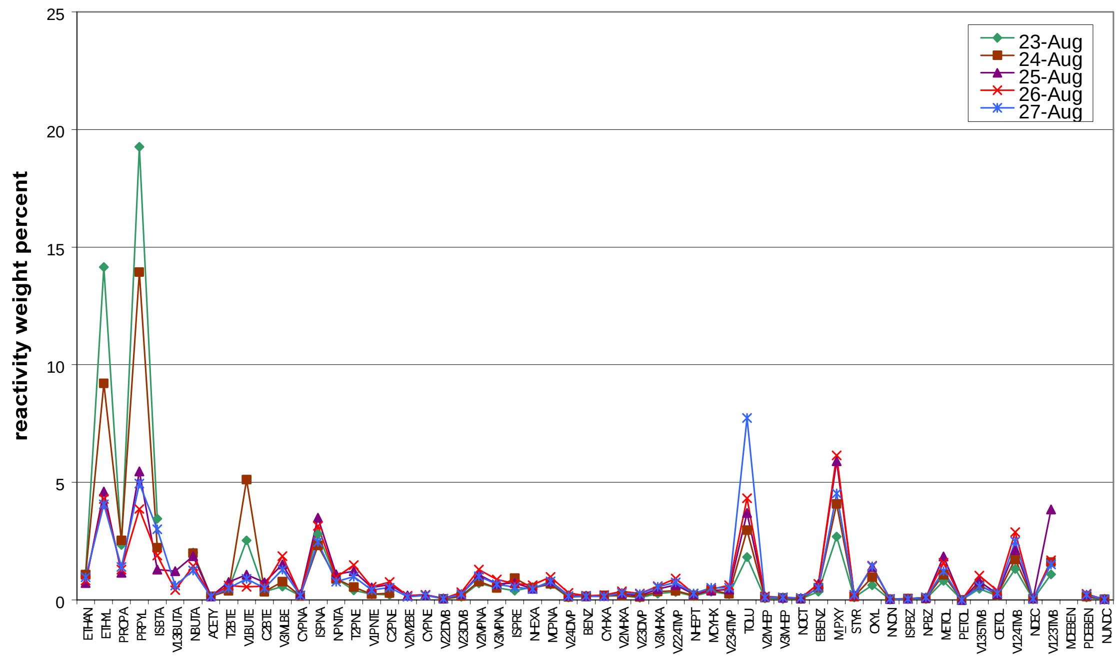

Figure 5-29. Median reactivity-weight percents at Clinton, August 23-27, 2000 (0500-0700).

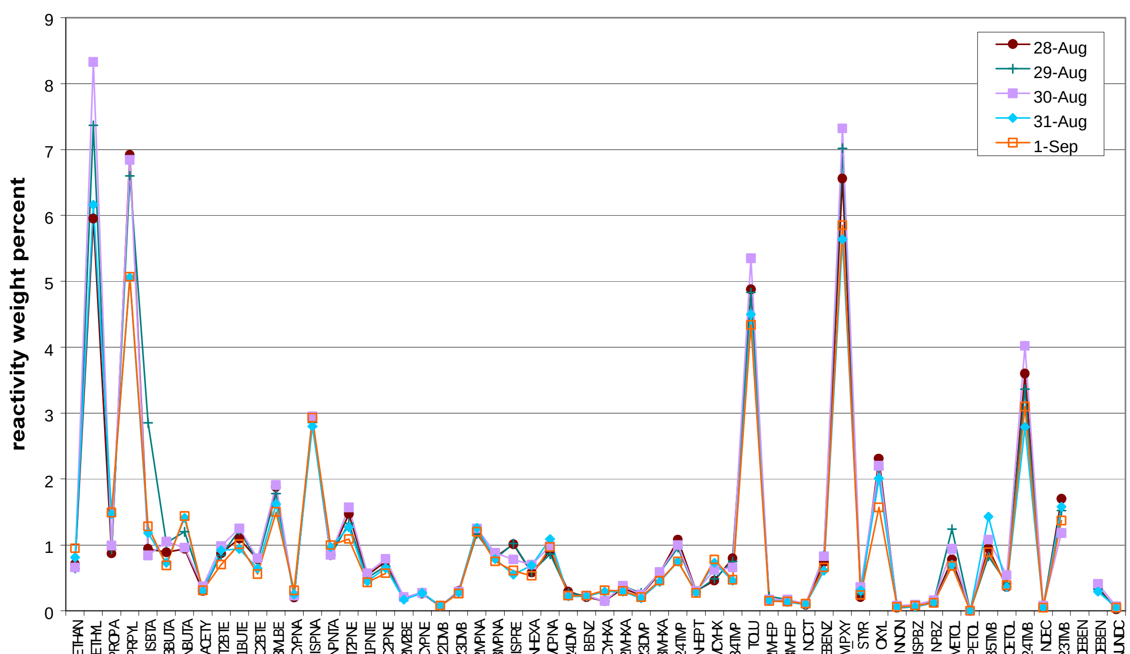

Figure 5-30. Median reactivity-weight percents at Clinton, August 28-September 1, 2000 (0500-0700).

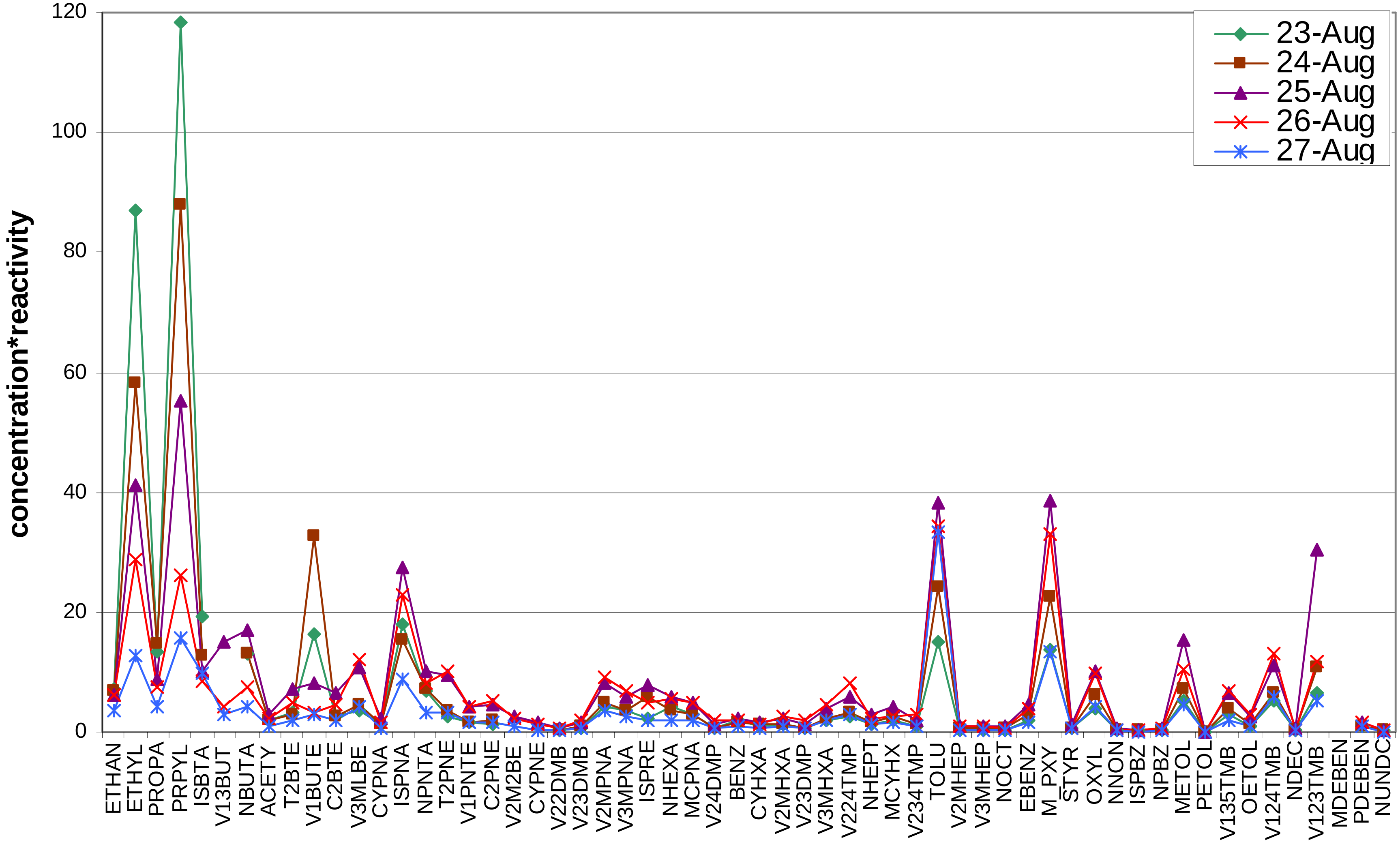

Figure 5-31. Median values of concentration*reactivity at Clinton, August 23-27, 2000 (0500-0700).

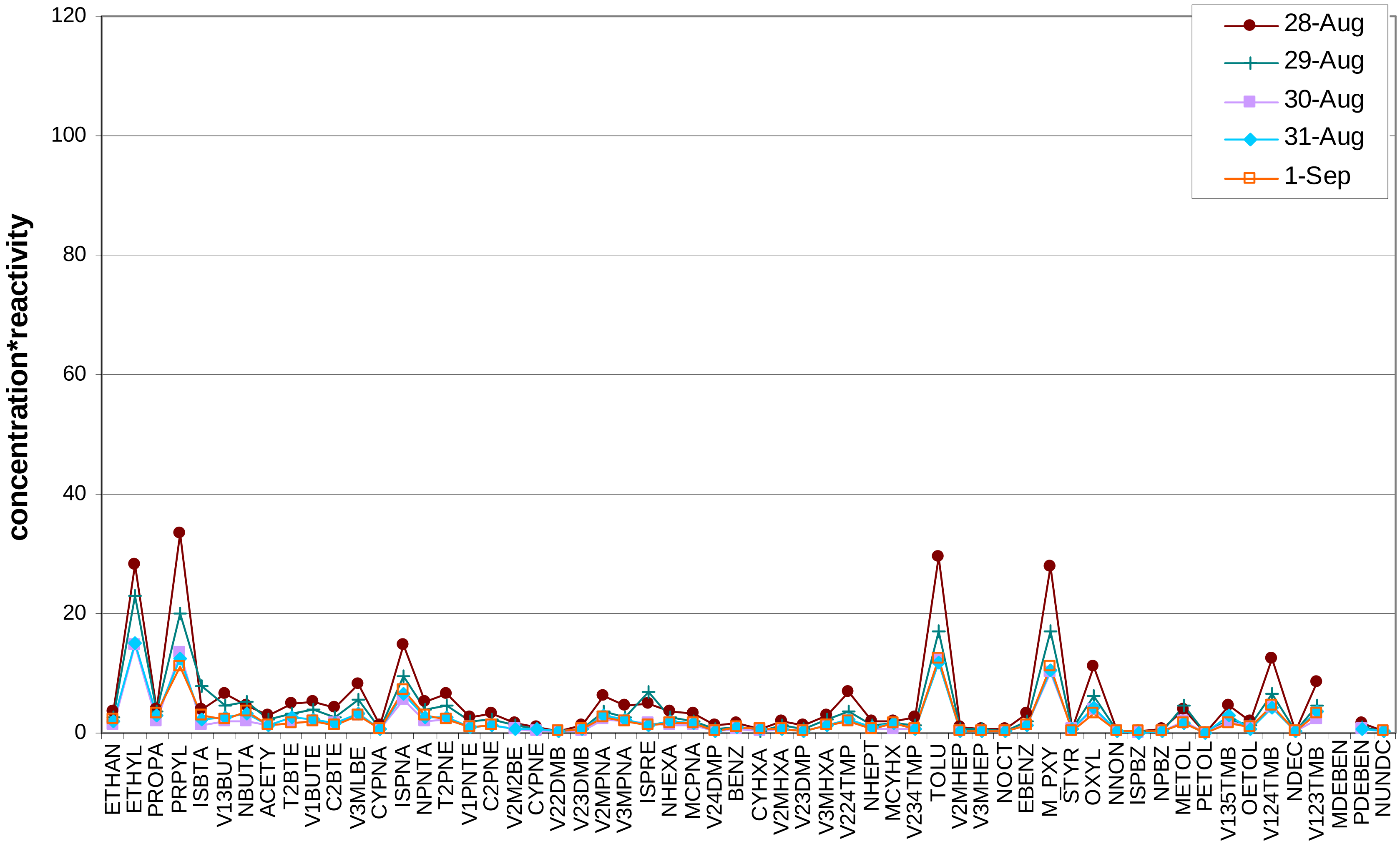

Figure 5-32. Median values of concentration*reactivity at Clinton, August 28-September 1, 2000 (0500-0700).

Further, there is no trend between the episode and non-episode days in terms of general categories such as total olefins, paraffins, aromatics and unidentified mass. **Table 5-2** details these sums for each day of the modeling period. Overall there appears to be no general trend between the episode and non-episode days during this period. Specific findings follow:

- Olefin fractions are actually highest on the non-episode days of August 23-24, which is surprising since olefins are very reactive and play a significant role in ozone formation.
- Aromatic hydrocarbon fractions (also significant contributors to ozone formation) are highest on August 27 and lowest on August 23, both of which are non-episode days.
- The unidentified mass fractions are somewhat higher on days of episodes, though the concentrations on the non-episode days of August 27-26 are fairly similar to concentrations on episode days.

Additional analyses of these dates with respect to wind quadrant will be performed.

Table 5-2. Ozone episode designation of median TNMOC (ppbC), percent of olefins, paraffins, aromatic hydrocarbons, and unidentified mass at Clinton for each day during from August 23 to September 1, 2000, at 0500-0900.

Date	Type of Episode	TNMOC	%Olefin	%Paraffin	%Aromatic	%Unidentified
8/23/2000	Non-episode	515	17	67	9	6
8/24/2000	Non-episode	513	15	66	13	7
8/25/2000	Episode	623	11	65	18	13
8/26/2000	Episode	581	8	63	16	10
8/27/2000	Non-episode	257	9	66	23	10
8/28/2000	Non-episode	393	11	57	19	12
8/29/2000	Episode	253	13	62	18	11
8/30/2000	Episode	155	14	56	20	10
8/31/2000	Episode	186	11	62	17	10
9/1/2000	Episode	180	8	69	18	13

5.6 OLEFIN TO NO_X RATIOS BY WIND DIRECTION

One indicator of ozone formation potential is a ratio between reactive olefin concentrations, such as ethylene, propylene and 1,3-butadiene, to NO_x. A higher ratio is thought of as "hot" or more reactive, thus leading to increased ozone formation. The Clinton site during July-August 2000 was selected to examine the variation of olefin to NO_x ratios based on wind direction. A detailed map of the area around the Clinton site (Figure 5-12) shows a dense area of industry to the east and southeast while to the west is a major freeway. Therefore, the olefin-to-NO_x ratios were compared between advection from the east (45-135 degrees) and from the west (225-315 degrees). These ratios were calculated on a strict ppb-to-ppb basis.

(Hydrocarbons are generally reported in ppbC; to convert to ppb the concentration needs to be divided by the number of carbons in the hydrocarbon, i.e. 2 ppbC ethylene = 1 ppb ethylene.)

Preliminary findings are that

- Olefin-to-NO_x ratios were generally below 2, with median values ranging from 0.03 to 0.32.
- Olefin-to-NO_x ratios were two to eight times higher with advection from the east during the morning, and three to seven times higher from the east during all hours. This observation indicates that the industrial emissions from the east have a greater ozone formation potential than the lower ratios found in emissions from the west.
- There was generally little difference in olefin-to-NO_x ratios between episode and non-episode days by wind direction.

6. REFERENCES

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Fehling, D. (January 14, 2002) "What's really to blame for Houston's bad air?", KHOU Channel 11 News, archived at <http://www.khou.com/news/upclose/khou020114_ds_UpCloseOzone.18832f8a.html>.

Main H. H. and Roberts P. T. (2000) PAMS Data Analysis Workbook: Illustrating the use of PAMS data to support ozone control programs. Prepared for the U.S. Environmental Protection Agency, Research Triangle Park, NC by Sonoma Technology, Inc., Petaluma, CA, STI-901070-2071-FR, May.

Main H.H. and O'Brien T. (2001) Statistical summary of PAMS data collected in the Northeast and Mid-Atlantic states. Report prepared for NESCAUM, Boston, MA by Sonoma Technology, Inc., Petaluma, CA, STI-900860-2045-FR2, June.

Stoeckenius T. E., Ligocki M. P., Cohen B. L., Rosenbaum A. S., and Douglas S. G. (1994) Recommendations for analysis of PAMS data. Final report prepared by Systems Applications International, San Rafael, CA, SYSAPP94-94/011r1, February.

APPENDIX A

MISSING AUTO-GC DATA, JULY-SEPTEMBER 1998-2000, AND AUGUST-OCTOBER 2001

Table A-1. Times and dates of missing auto-GC data during July-September 1998-2000, and August-October 2001.

Site	Year	Dates	Comments
Aldine	00	9/2-9/4, 9/14-9/18	All Data Missing
Bayland	00	7/16 0700-7/18 1600 7/21: 000-1500 8/2 1500-8/4 1300	All Data Missing
		7/1-7/14	No Propylene
Bayland	99	7/6:900-1700 7/8 1300-7/9 1200 7/18 1100-7/19 1300 7/21: 600-1600 7/27 600-7/28 1500 8/12 1500-8/16 1200 8/19: 200-1300 8/20 1600-8/24 1200 8/31 1300-9/1 1300 9/3 1700-9/7 1300 9/10 1700-9/13 1600 9/15: 1000-1400 9/30: 800-1200	All Data Missing
Bayland	98	7/1-7/10	No Propylene
		7/16 700-7/18 1600 7/21: 000-1500 7/23-8/8 8/12: 0500-1100 8/13: 1300-1700 8/15 700-9/1 2300 9/3: 700-1500 9/8 1200-9/9 1700 9/20 000-9/24 1600	All Data Missing
		9/2-9/3	No TNMOC
Channelview	01	8/17 100-8/21 1100 8/22-8/27 900 9/4 500-1300 9/12 1500-9/13 1700 9/18 1000-9/19 1500 9/24 1700-9/25 1300 9/26 000-1100 9/27-10/1 1000 10/12 10/16 900-1200	All Data Missing
		8/16 8/21 8/27	No Propylene
		10-1 1000-10/3 1200	No TNMOC
Clinton	01	8/30 1200-9/2 400 9/5 800-1200 9/18 000-900 9/21 1200-9/24 1200 10/8 000-1000 10/27 300-10/29 1300	All Data Missing

Table A-1. Times and dates of missing auto-GC data during July-September 1998-2000, and August-October 2001.

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Site	Year	Dates	Comments
Clinton	00	7/5 1300-1600 7/14 900-1200 7/19 1500-1800 7/27 600-900 7/31 1100-8/1 1000 8/2 000-1800 8/3 000-0900 8/7 1000-1500 8/14 1200-1500 8/16 1200-1500 8/23 1900-2300 8/28 900-1200	All Data Missing
		9/1-9/30	No Ethylene
Clinton	99	7/13: 900 7/24 700-7/26 1000 8/28-8/30 8/31 1300-9/1 1200 9/4-9/7 9/15 1100 9/30 800-1400	All Data Missing
		9/16-9/19 000	No TNMOC
Clinton	98	7/14:000-1200 8/26 800-8/27 700 8/28: 400-1400 9/14:1000-1600 9/15:000-1600 9/18 1100-9/20 1700 9/28: 600-1700	All Data Missing
		7/1-7/2 7/6-7/10 7/15-8/3 8/7 8/14-8/22 8/24-8/25 9/7-9/9	No TNMOC
Deer Park	01	8/7 000-1300 8/15 900-1200 9/5 600-900 9/9 900-1200 9/25-10/1 100 10/4-10/5 900 10/13-10/14 1200 10/14:1300-2300 10/15 0-800 10/16 800 10/18-10/22 1200	All Data Missing
		10/1-10/2 1300 10/14-10/16 0900 10/22 900-10/23 1200	No TNMOC

Table A-1. Times and dates of missing auto-GC data during July-September 1998-2000, and August-October 2001.

Site	Year	Dates	Comments
Deer Park	00	7/12 000-7/13 900 7/19 1000-2300 7/23 1300-1700 7/28 000-8/6 0200 8/7 500-800 8/10 000-8/11 800 8/13 1000-8/15 1400 8/23 -9/21	All Data Missing
		7/1-7/22 9/21-10/1	No TNMOC
Deer Park	99	7/9 000-7/13 1000 7/15 2000-7/16 1000 7/20 900-1400 8/12 1200-8/13 1100 9/13 400-9/14 1300 9/18 000-9/20 1800 9/29 1500-9/30 1700	All Data Missing
Deer Park	98	9/18 700-9/21 600 9/22 000-1200	All Data Missing
		7/1-9/10 9/24-10/1	No TNMOC
HRM-3 – Haden Rd.	01	8/30 700 9/2 1200 9/5 1100,1300 9/6 000-9/11 200 9/14 1900 9/17 1300 9/20 800-1500 9/21 1500-9/24 1500 9/25 2000 9/26 1500 9/27 1000 10/2 1100-1700 10/18 1000,1200-1500 10/23 000-900	All Data Missing
		8/21-8/28 0600 9/5 9/24 1400-9/26 1900 10/22-10/24 1200	No TNMOC

Table A-1. Times and dates of missing auto-GC data during July-September 1998-2000, and August-October 2001.

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Site	Year	Dates	Comments
HRM 7 – Baytown	01 01	8/28 700,900 8/31 1100-1600 9/1-9/5 400 9/5 1300 9/6 800 9/18 1200-1700 9/19 500-800 9/20 1800-2300 9/21 900-1900 9/26 700 10/6 2000-2300 10/11	All Data Missing
		8/27 8/29 10/12-10/13 0900	No TNMOC

APPENDIX B

SPECIES ABBREVIATIONS USED IN THIS REPORT

Table B-1. AIRS code, abbreviation, hydrocarbon name, and species group (O=olefin, P=paraffin, A=aromatic).

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AIRS code	Abbreviation	Hydrocarbon	Species Group
43206	acety	Acetylene	O
43203	ethyl	Ethylene	O
43202	ethan	Ethane	P
43205	prpyl	Propylene	O
43204	propa	Propane	P
43214	isbta	Isobutane	P
43280	1bute	1-Butene	O
43212	nbuta	n-Butane	P
43216	t2bte	trans-2-Butene	O
43217	c2bte	cis-2-Butene	O
43282	3mlbe	3-Methyl-1-Butene	O
43221	ispna	Isopentane	P
43224	1pnte	1-Pentene	O
43220	npnta	n-Pentane	P
43243	ispre	Isoprene	O
43226	t2pne	trans-2-Pentene	O
43227	c2pne	cis-2-Pentene	O
43228	2m2be	2-Methyl-2-Butene	O
43244	22dmb	2,2-Dimethylbutane	P
43283	cypne	Cyclopentene	O
43234	4mlpe	4-Methyl-1-Pentene	O
43242	cypna	Cyclopentane	P
43284	23dmb	2,3-Dimethylbutane	P
43285	2mpna	2-Methylpentane	P
43230	3mpna	3-Methylpentane	P
43246	2m1pe	2-Methyl-1-Pentene	O
43231	nhexa	n-Hexane	P
43289	t2hex	trans-2-Hexene	O
43290	c2hex	cis-2-Hexene	O
43262	mcpna	Methylcyclopentane	P
43247	24dmp	2,4-Dimethylpentane	P
45201	benz	Benzene	A
43248	cyhxa	Cyclohexane	P
43263	2mhxa	2-Methylhexane	P
43291	23dmp	2,3-Dimethylpentane	P
43249	3mhxa	3-Methylhexane	P
43250	224tmp	2,2,4-Trimethylpentane	P
43232	nhept	n-Heptane	P
43261	mcyhx	Methylcyclohexane	P
43252	234tmp	2,3,4-Trimethylpentane	P
45202	tolu	Toluene	A

Table B-1. AIRS code, abbreviation, hydrocarbon name, and species group (O=olefin, P=paraffin, A=aromatic).

AIRS code	Abbreviation	Hydrocarbon	Species Group
43960	2mhep	2-Methylheptane	P
43253	3mhep	3-Methylheptane	P
43233	noct	n-Octane	P
45203	ebenz	Ethylbenzene	A
45109	m/pxy	m/p-Xylene	A
45205	mxyl	m-Xylene	A
45206	pxyl	p-Xylene	A
45220	styr	Styrene	A
45204	oxyl	o-Xylene	A
43235	nnon	n-Nonane	P
45210	ispbz	Isopropylbenzene	A
45209	npbz	n-Propylbenzene	A
43256	apine	alpha-Pinene	O
45207	135tmb	1,3,5-Trimethylbenzene	A
45208	124tmb	1,2,4-Trimethylbenzene	A
43257	bpine	beta-Pinene	O
45211	oetol	o-Ethyltoluene	A
45212	metol	m-Ethyltoluene	A
45213	petol	p-Ethyltoluene	A
45218	mdeben	m-diethylbenzene	A
45219	pdeben	p-diethylbenzene	A
45225	123tmb	1,2,3-trimethylbenzene	A
43238	ndec	n-Decane	P
43954	nundc	n-Undecane	P
43102	tnmoc	Total Non-Methane Organic Compounds	
43502	form	Formaldehyde	C
43503	aceta	Acetaldehyde	C
43551	acet	Acetone	C
43218	13buta	1,3-butadiene	O
43225	2m1bte	2-methyl-1-butene	O
43295	3ethex	3-ethylhexane	P
43955	25mhex	2,5-dimethylhexane	P
43293	hex24m	2,4-dimethylhexane	P
43294	hex23m	2,3-dimethylhexane	P
43222	propa22m	2,2-dimethylpropane	P
43270	ibute	Isobutene	O
43240	mcpne	Methylcyclopentene	O
43395	4mhpte	4-Methylheptane	P
43000	pamshc	Sum PAMS Target Species	