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Analysis of Ambient VOCs Levels and Potential Sources in Windsor

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By

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ABSTRACT

Chemical Mass Balance (CMB), Positive Matrix Factorization (PMF), and Principal Component Analysis (PCA) were applied to investigate the major sources of Windsor ambient Volatile Organic Compounds (VOCs). The annual average total VOC concentrations declined from 2005 to 2006. Summer concentrations were higher than winter in both years. All three models results indicated that vehicle-related sources were the major contributors regardless of season in both years. Other major sources included Commercial Natural Gas and Industrial Refinery in winter; Architectural Coatings in summer. PMF provided profiles other than the ten sources for CMB: Adhesive & Sealant Coatings. PCA provided additional emitters: Adhesive and Sealant Coatings and Auto Paintings. Spatial patterns of source contribution indicated that there was a high correlation between the high All Vehicle, Industrial Refinery, and Commercial Natural Gas emissions with the Huron Church Road measurements.

DEDICATION

To my parents

ACKNOWLEGEMENT

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TABLE OF CONTENT

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1

INTRODUCTION

1.1 Background

Air pollution from transportation, industries, and other sources causes unbalance of the atmosphere in terms of the chemical composition. Air pollutants are harmful to living things (Environment Canada, 2013). Air pollutants are grouped into four categories. They are: criteria air contaminants, persistent organic pollutants (POPs), heavy metals, and toxic pollutants. There is overlap between toxics and the pollutants in the other three categories. Criteria air contaminants include Sulphur Oxides (SO_x), Nitrogen Oxides (NO_x), Particulate Matter (PM), Volatile Organic Compounds (VOCs), Carbon Monoxide (CO), and Ammonia (NH_3) (Environment Canada, 2013). Many air pollution problems including smog and acid rains are caused by the presence or the interactions of the criteria air contaminants.

VOCs are organic compounds that produce vapour at room temperature and pressure (Environment Canada, 2013). VOCs come from both indoor and outdoor sources. Indoor sources include the manufacture and use of everyday products and materials. The outdoor sources include transportation, the oil and gas industry, the use of paints and solvents, home firewood burning etc (Environment Canada, 2014). The reactive VOCs are primary precursors to the formation of ground-level ozone and particulate matter in the atmosphere. Ozone and PM are the main ingredients of the smog that have serious effects on living things. The health effects of VOCs include eye, nose, and throat irritation; headaches, coordination loss, nausea; damage to organs including liver, kidney, and central nervous system; and even cancer (Environment Canada, 2014).

Windsor, Ontario is polluted by various ambient air pollution sources. There are automobile industries including a Ford Engine Plant, and a Chrysler Assembly Plant. Huron Church Road is the corridor connecting traffic from Windsor to the busiest trade route in North America, the Ambassador Bridge. Transboundary pollution is another major source because Windsor is located in the airshed of Detroit, MI, and Ohio. Residents in Windsor may suffer the polluted air blowing from Detroit and Ohio. In order to address the air quality related problem caused by transboundary pollution, Canada and the USA unveiled an international agreement between Canada and United States known as the Border Air Quality Strategy (BAQS) (Environment Canada, 2003).

The pollutants from the emitters include PM, NO_x, and VOCs (Wheeler et al., 2011). Studying the ambient VOCs helps to understand and address the air pollution in Windsor. In order to control the VOCs levels, it is crucial to understand the emission sources contributing to the ambient VOCs.

Receptor models are useful for understanding the major sources of VOCs. Receptor models were developed to utilize the concentration measured at the receptor sites to determine the contributions of potential sources (US EPA, 2011). The common receptor models include Chemical Mass Balance (CMB) (US EPA, 2014a), Positive Matrix Factorization (PMF) (US EPA, 2014a), Unmix (US EPA, 2014a), and Principal Components Analysis (PCA) (Mathworks, 2014). The previous studies show that the receptor models have been applied to source apportionment in many places. The examples were application of PMF at Egbert, Ontario (Vlasenko et al., 2009); PMF in rural sites of British Columbia (Jeong et al., 2008); PCA in urban areas of Dalian, China (Wang et al., 2009); CMB in Windsor, Ontario (Templer, 2007).

Many studies conducted VOC source apportionment for multiple years. However, few of them compared the source contribution in different seasons due to the lack of measurement data or other reasons. Few studies applied three receptor models and compared the sources of different models, perhaps due to the lack of source profiles in the study region, lack of time, or other reasons. Learning the seasonal variation of the source contribution helps to understand the contributions of major sources in different seasons. Using different receptor models helps to identify the potential sources not provided by other models.

Few researchers studied the variation of ambient VOCs levels and the source contributions from different sources in different seasons of one year, and same season of two different years. Few studies conducted VOCs source apportionment by using three receptor models, and comparing their results.

VOC concentrations in both winter and summer in year 2005 and 2006 in Windsor were obtained in a study called “Windsor, Ontario Exposure Assessment” (WOEAS) (Wheeler et al., 2011). There were ten VOCs source profiles of Windsor prepared by Templer (2007). The CMB results of 2005 were obtained by Templer (2007). Therefore, these studies were prerequisites for carrying out VOCs source apportionment by using different receptor models.

1.2 Objectives

The overall objective is to study the seasonal variation of the ambient VOCs levels and source contributions in year 2005 and 2006, and annual variation in winter and

summer, respectively from 2005 to 2006 in Windsor, Ontario. By applying three receptor models, additional sources with low contribution to the VOCs levels other than the ten sources in Templer (2007) were expected to be found. The specific objectives are:

1) Compare the ambient VOC concentrations of the winter and summer in years 2005 and 2006, respectively, to see if there was seasonal trend; compare the annual concentration of year 2005 and 2006 to see the annual trend from year 2005 to 2006.

2) Run the CMB model with the VOCs concentration data of winter and summer 2006 to find out the major VOCs contributors

3) Compare the source contribution results of winter and summer in 2006 with that of 2005 from CMB model to see if the major sources in the same season were similar.

4) Use ArcGIS 10.1 software to compute the spatial source contribution distribution maps for each of the ten sources to see the spatial trends of different sources emissions.

5) Use the PMF model to analyze the potential sources of VOCs and the corresponding contributions for both winter and summer 2006. Identify the factors from the factor profiles based on the knowledge of source characteristics, literature reviews, and the potential sources in Windsor. Compare the sources in winter and summer to see the commonalities and differences.

6) Use the PCA model to analyze the potential sources of VOCs for both winter and summer 2006; identify the sources based on knowledge of source characteristics, literature reviews, and the potential sources in Windsor; compare the sources in winter

and summer to see the commonalities and differences.

7) Compare the sources input to CMB with those identified by PMF, and PCA to see the common sources and the additional sources from PMF or PCA over and above the source profiles for CMB.

CHAPTER 2

LITERATURE REVIEW

2.1 Volatile Organic Compounds

VOC are any organic compounds that can produce vapour under room temperature and pressure (Environment Canada, 2013). A number of individual VOCs including benzene and dichloromethane have been assessed to be toxic under the Canadian Environmental Protection Act (1999) (Environment Canada, 2013). Some highly toxic VOCs cause serious health problems including eye, nose, and throat irritation; headaches, loss of coordination, nausea; damage to liver, kidney, central nervous system, and even cancer. The level of the health effect depends on the extent of the exposure to the VOCs (US EPA, 2013).

Many VOCs react with sources of oxygen molecules such as NO_x and CO in the atmosphere in the presence of sunlight, and from ground-level ozone. Ozone is a constituent of photochemical smog. The outdoor VOC emissions are regulated by US EPA (US EPA, 2013b) in United States, and Environment Canada in Canada (Environment Canada, 2014).

The sources of VOCs include transportation, solvent use, industrial source, commercial fuel, and biogenic emission from deciduous trees. In 2012, VOC emissions in Canada reached 1768 kilotonnes (kt). The largest VOCs contributor was the oil and gas industry, with 34% (606 kt) of national emissions. The use of paints and solvents contributed 18% (323 kt) of national emissions, followed by the off-road vehicles, representing 14% (253 kt) of national emissions (Environment Canada, 2014).

2.2 Receptor Models

Receptor models help decision makers to control the VOC emissions. Different models have different functions. CMB is used for evaluating the source contributions when the potential sources profiles in an area are known. PMF and PCA are used for providing source profiles and their corresponding contributions. Similar as PMF, Unmix utilizes with the concentration put into the model to provide the profiles with the relative contributions, and a time-series of contributions (US EPA, 2014). There is a non-negative constraint for both source composition and contributions of Unmix, same as PMF. Unlike PMF or PCA, Unmix provides source profiles for every sample, because Unmix assumes that for each source, there are some samples contain very little or no contribution from that source (Norris et al., 2007). This restricts Unmix from identifying the infrequent or small sources (Kotchenruther and Wilson, 2003).

The fundamental of the receptor models is solving the mass balance equations as equation (1):

$$C_{ik}=\sum_{j=1}^{J} F_{ij} \times S_{jk} + e_{ik} \quad (1)$$

where C_{ik} is the concentration of the element i measured in sample k; F_{ij} is the mass fraction of the element i in source j for CMB and PMF, and loading of element i in factor j for PCA; S_{jk} is the contribution of the source j at sample k for CMB and PMF, and score of source j at sample k for PCA; and e_{ik} is the residuals between model calculation and measured data. C_{ik} is input data for all three models. F_{ij} is input data for CMB, but

output for PMF and PCA. S_{jk} and e_{ik} are outputs for all three models.

2.2.1 Chemical Mass Balance

CMB is applied to provide the source contribution of the sources when the source profiles in an area are known. The inputs include measurements of species concentration and source profile. Outputs include source contribution of each source. Source profiles are expressed as fractional abundances of common property in different emissions. To get the source profiles, the obtained samples from different emitters should be analyzed to determine the properties. The properties are then normalized (scaled) to some common property in the emissions from all sources by converting the measurements into ratio of fractional abundances. The sum of the percentage of individual species in a profile should be 100%. The species with high fractional abundance or the only measured species in the source could be identified as species markers for the emission (Watson et al., 2004).

Preparation of the source profiles is time consuming and costly. A more common method is to apply the available source profiles. However, users must be cautious when choosing the source profiles. The potential sources and the source profiles compositions for one place may not fit another. The source profiles should be a group of sources instead of several single emission sources. The “Collinearity” happens when there are two or more similar source profiles. Two or more CMB equations are redundant and the equations cannot be solved. This could cause one source contribution high; while another negative. In order to avoid this problem, similar source profiles should be grouped as one category (Watson et al., 2004). Source profile has to be normalized into a common

property that CMB model can accept. CMB protocol recommends using the sum of the 55 Photochemical Assessment Monitoring Stations (PAMS) target hydrocarbons as the common normalization standard for source profiles (Watson et al., 2004). The source contribution output could be positive or negative values. The negative source contributions could be replaced with zero in the post-processing.

CMB solves the equations on sample basis. It provides the source contribution solutions for each sample as output.

There are six fundamental assumptions for CMB model as in CMB protocol (Watson et al., 2004). They are:

1) The composition of the source profiles will not change in the process of transportation between sources and receptors

2) There is no chemical reaction between the compounds

3) Every potential source to the pollution at receptor sites in the area is identified and characterized.

4) Each identified source is independent with the others.

5) The number of the compounds is larger than that of the sources.

6) The uncertainties of the measurements are random, and with normal distributions.

For assumptions 1 and 2, the chemical composition of compounds measured at receptor sites should reflect the composition of the emission from sources. This is

because CMB apportions the measured compounds to the sources following the given proportion in the source profiles. CMB derives the best combination of the source contribution at each site to explain the measurements and the source profiles. This could be hardly achieved in reality because some reactive chemicals would react with others or decay in the process of transportation. For assumption 3 and 4, CMB assumes that there is no other source other than the provided source profiles in the area. Each source has nothing to do with the others. As a matter of fact, there could be more sources contributing to the receptors. The least squared solution requires random and uncorrelated uncertainties of the measured concentrations. However, the accurate distribution of the errors is hard to obtain.

The variance weighted least squared solution was applied to solve the mass balance equations to find out the best solution of S_{jk} explaining the concentration obtained at the receptor sites (Watson et al., 2004). The variance weighted least squared solution is described in equation (2) (Watson et al., 2004):

$$x_k{}^2 = \left(\frac{1}{i-j}\right) \sum_{i=1}^{I} \left[\frac{\left(e_{ik} - \sum_{j=1}^{J} F_{ij} S_{ik}\right)^2}{v_{ik}}\right] \qquad (2)$$

where $v_{ik} = \sigma_{e_{ik}}{}^2 + \sum_{j=1}^{J} (S_{ik})^2 \sigma_{F_{ij}}{}^2$

where $\sigma_{e_{ik}}{}^2$ is one standard deviation of the measured concentration of compound *i* in sample *k* and $\sigma_{F_{ij}}{}^2$ is one standard deviation of the fraction of compounds *i* in source *j*. The effective variance, v_{ik}, is constantly adjusted as the S_{ik} is refined.

Source contribution estimate, t-statistics (Tstat), R-square, Percent Mass Accounted (Mass %), and Chi-square are provided by the model to estimate model performance. Table 2.1 shows the meaning and the target of each measure.

Table 2.1CMB Performance Measures (Watson et al., 2004)

Output	**Abbreviation**	**Description**	**Target**
Source Contribution Estimate	SCE	Calculated concentration of the source emission	>0
t-Statistic	Tstat	SCE/Std Err. Higher the better.	> 2.0
R-square	R^2	Variance in ambient species concentrations explained by the calculated species concentrations. Range from 0 to 1.0. Higher the better.	0.8 - 1.0
Percent Mass Accounted	% Mass	Ratio of total calculated concentration and total measured concentration at sample.	100 ± 20%
Chi-square	χ^2	A large CHI SQUARE (>4.0) means that one or more calculated species concentrations differs from the measured concentrations by several uncertainty intervals.	0 -4.0

2.2.2 Positive Matrix Factorization

The fundamental of the PMF model is decomposing a matrix of speciated sample data into two matrices—factor contributions and factor profiles. “Positive” refers to the non-negative source composition and contribution output constraints. The factor profiles provided from PMF needs to be interpreted based on knowledge of the potential sources

in the study areas.

PMF model requires two input files including ambient concentrations and their uncertainties. Two types of uncertainty files are accepted: sample-specific and equation-based. The sample-specific uncertainty provides an estimate of the uncertainty for each sample of each species. The dimension of the specific uncertainty is the same as the concentration values. Another way to obtain concentration uncertainty is using equation (3) (Vedantham and Norris, 2008):

$$\text{Uncertainty}=\frac{5}{6}\times \text{MDL, if concentration}\leq\text{method detection limit (MDL)} \qquad (3)$$

$$\text{Uncertainty}=\sqrt{(\text{uncertainty percent}\times\text{concentration})^2+(\text{MDL})^2}$$

, if the concentration>MDL

PMF solves the mass balance equation (equation 1) by every species of each sample, and provides one profiles, and the source contributions of each source in every sample. The source contribution was given in the same order of factors. PMF operation consists of three steps; they are base model run, bootstrap run, and the Fpeak run. The follow up runs are based on the best run estimated in the previous one. Model is run multiple times as specified, and the best run will be selected automatically based on the Q (Robust) value of each run.

There are three kinds of outputs including Base model results, Bootstrap model results, and the Fpeak model results. The base run results include factor profiles containing species mass proportion in different factors; factor loadings for computing the

factor contributions, and residuals of the calculated concentrations for each species of samples.

The performance measures for PMF are shown in Base run outputs. The value of Q (robust), Q (true), and whether each run is converged were shown in a table. The best Goodness-of-fit run will be automatically marked with boldface in the Base Run report. Details of each output are listed in Table 2.2.

Table 2.2 Performance measures of PMF

Name	Description	Target
Q(robust)	Goodness-of-fit parameter calculated excluding outliers, defined as samples for which the scaled residual is greater than 4.	The lowest among all runs
Q(true)	Goodness-of-fit parameter calculated including all points, defined as samples for which the scaled residual is greater than 4. Q(true) is greater than 1.5 times Q(robust) indicate that peak events may be disproportionately influencing the model.	<=1.5 times Q(robust)
Convergence	Whether the run converged or not	Yes

Model outputs consist of factor profile tables, factor profile bar charts and pie charts by compounds. Factor contribution files contain tables, scatter plots, and G-space plots. The model performance was analyzed based on the residuals histogram charts, the observed and predicted scatter tables and charts, diagnostics (e.g. Q Robust in table), and G-space plots.

Both scaled and before scaled residuals are provided in PMF model outputs. Scaled residuals are between +3 and -3 on a histogram when they are normally distributed. Any skewed or bimodal residuals indicate that the model calculated concentration does not reproduce the observed concentrations well. The observed and predicted scatter plots show the one on one line and the model calculated concentration regression. The big bias between the predicted and the observed concentration also indicate the model does not reproduce the measurement data well. Observed and predicted time series is also on a line chart. The diagnostics table consists of the Q (Robust), Q (True), converged or not (Yes/No), number of steps of run. Both Q (Robust) and Q (True) indicate the goodness-of-fit parameter. Q (Robust) is calculated after excluding the samples with scaled residuals greater than 4, whereas Q (True) is calculated including all samples. The lowest Q (Robust) was highlighted to indicate the best goodness-of-fit run. The large range of the Q (Robust) among all runs is the implication of the poor stability between different runs. Aggregate contribution shows the boxplots of annually contribution of each factor. G-space plot shows the scatter plots of factor versus another factor. The desirable plot has all scatters distributing all over the space in between X and Y axis, while the poor one always shows two clear edges, indicating that the two factors are not independent with each other. Changing the number of factors could eliminate this problem.

The poor performance of measurements is the implication of poor input dataset reproduction. A second run is necessary. The model reproduction performance may be improved by changing the characteristics of species with poor performance to “weak” or “bad”, or using a different factor number (Norris and Vedantham, 2008).

2.2.3 Principal Component Analysis

PCA is used for proving the principal components that explain majority of the variance of the input measurements. PCA only requires concentration measurements as inputs. The outputs consist of coefficients containing loadings of each variable in every measurement, eigenvalues for each component, variance explained in percentage by descending order, and score. Each principal component is a linear combination of the variables with loadings and scores (Joliffe, 2002). “Coefficients” profile consists of the factor loadings.

Both loadings and scores have positive and negative values. Each component represents a new dimension of the measurement data constructed in a dimension of number of variables. Loadings represent the projection of the component vector on the variable axis. When the measurements of variables are in the same units, the different signs of the loadings of variables indicate the differences of the variables. The component is interpreted as the factor that reveals the differences among the variables with different signs. The higher the absolute loadings are, the greater the impacts the variables have on determining the components. When the absolute loadings of the variables are close to zero, the impact of the variables on the components is small. Similar to PMF, the components should be interpreted by users based on the loadings of variables, the knowledge of source characteristics, and the potential sources in the area.

The source contribution of each component to each species at a given sample is calculated by multiplying the value of score of component at the given sample with the loading of the component on the species. The summation of the source contribution of a

given component to every species at a given sample derives the source contribution of the component to the sample. The mean of the summations among all samples derives the average source contribution of a given component. The measurement of samples is reproduced by using the loadings and the scores profiles. Z score is applied when there are not enough components with eigenvalue greater than one, or the input measurements contain different units. Z score could be used to transform the original data by using the standard deviation and the mean value of the variables in a dataset. There could be more components with eigenvalues greater than one after applying Z score. However, Z score is not recommended to be applied as some of the characteristics of the original data would be lost. It is impossible to reproduce the measurements at samples when Z score is applied. This is because reproduction of the measurements requires the raw scores of data; however, Z score is a relative value, not an absolute value. For example, a low Z score of a data does not mean a low raw score, instead, it suggests that the raw score is among the lowest within that specific group (Gravetter and Wallnau, 2013).

Eigenvalues indicate the amount of the variance explained by each provided component. Singular value decomposition (SVD) theorem is used to find out eigenvalues. The components were ordered by eigenvalue of the factors, from high to low. Most studies chose one as eigenvalue cut off.

The components could be rotated in order to reveal the relationship between variables and components to the greatest extent without changing the relationship between the components. The rotation methods consist of orthogonal rotation which assumes that the given components are uncorrelated, and oblique rotation. The orthogonal rotation consists of equamax, orthomax, quartimax, and varimax rotations. The oblique

rotation assumes that the factors are correlated. The most widely used is varimax rotation (Brown, 2009).

2.3 VOC Source Characteristics

Source profiles are input for CMB and outputs for PMF and PCA. It is important to understand the potential sources of Windsor, Ontario and their chemical compositions. There were ten CMB sources profiles prepared by Templer (2007) for Windsor in year 2005. These source profiles could be applied if there is no major road or industries built or out of operation compared with year 2005. The ten sources were Gasoline Exhaust, Diesel Exhaust, Liquid Gasoline, Gasoline Vapour, Industrial Refinery, Architectural Coatings, Commercial Natural Gas, Liquid Petroleum Gas, Coke Oven, and Biogenic Emission. The source profiles consist of 55 non-methane hydrocarbons (NMHC) of PAMS, and other species summed as one species group named as other. The full source profiles are listed in Appendix A.

There are various compounds in different emission sources. Among the compounds, some of them are the ground-level ozone precursors. Among those species, 55 NMHC are the target species of Photochemical Assessment Monitoring Sites (PAMS). Most comprehensive VOC data derives from the PAMS. The sum of the 55 PAMS species are recommended to be the common normalization standard for source profiles (Watson et al., 2004).

Gasoline exhaust, diesel exhaust, liquid gasoline, gasoline vapour were all vehicle-related sources. Gasoline and diesel are two types of fuel derived from crude oil. The crude oil consists of up to 50% paraffins, 47% napthenes, and 3% aromatics (Simanzhenkov and Idem, 2005). Gasoline is the product of distillation, cracking, and treatment of crude oil refinery (Simanzhenkov and Idem, 2005). Finished gasoline consists mostly of hydrocarbons and additives with approximately 150 separate compounds. Additives are used to improve the performance and stability of the gasoline (ATSDR, 2014). Energy is produced by burning hydrocarbons. The hydrocarbons in gasoline are mostly with chain length between 4 to 12 carbon atoms (New Zealand Ministry for the Environment, 2014). Table 2.3 shows the detailed chemical composition of typical gasoline (ATSDR, 2014).

Table 2.3 Gasoline Composition (weight %) (ATSDR, 2014)

n-alkanes	**%**	**Branched alkanes**	**%**	**cycloalkanes**	**%**	**olefin**	**%**	**aromatics**	**%**
C_5 (e.g. n-pentane	3	C_4 (e.g. iso-butane)	2.2	C_6 (e.g. cyclohexane)	3	C_6 (e.g. hexene)	1.8	Benzene	3.2
C_6 (e.g. n-hexane)	11.6	C_5 (e.g. iso-pentane	15.1	C_7 (e.g. cyclo haptane	1.4			toluene	4.8
C_7 (e.g. n-haptane	1.2	C_6 (e.g. iso-hexane)	8	C_8 (e.g. cyclo octane)	0.6			xylene	
C_9 (e.g. n-nonane)	0.7	C_7 (e.g. iso-haptane)	1.9					ethylbenzene	1.4
C_{10-13} (e.g. n-decane, undecane, dodecane)	0.8	C_8 (e.g. iso-octane)	1.8					C_3-benzenes	4.2
		C_9	2.1					C_4-benzenes	7.6
		C_{10-13}	1					others	2.7
Total	17.3		32		5		1.8		30.5

According to ATSDR (2014), branched alkanes and aromatics accounted for most proportion of gasoline with 32% and 30.5%, respectively. Species n-alkanes also account for significant amount with 17.3%. The anti-knock additives include oxygenates such as ethers—methyl tertiary-butyl ether (MTBE), aromatic hydrocarbons and aromatic amines. The aromatic hydrocarbons include toluene, xylene, and benzene. The aromatic amines include m-toluidine, p-toluidine, p-tert-butylaniline, technical pseudocumidine, n-methylaniline, and cumidines; and organometallic compounds (carbonyls) such as methyl cyclopentadienyl manganese tricarbonyl, iron pentacarbonyl, and ferrocene (Groysman,

2014). The deflagration in the internal combustion engine could be adversely impacted by autoignition, leading a phenomenon called “engine knock”. The anti-knock additives provide high engine combustion ratio (octane rating) so that the gasoline combustion is at high efficiency. Diesel contains mostly hydrocarbons with chain length between 8 to 17 carbon atoms including octane, decane, undecane, and nonane (New Zealand Ministry for the Environment, 2014). Unlike gasoline engine, diesel engine does not rely on additives because the hydrocarbons of diesel are heavier and more stable. Larger hydrocarbons can be compressed to a high degree, creating high temperature that allows effective combustion (Kraus, 2011).

Gasoline exhaust and diesel exhaust were products of fuel combustion. The complete combustion of hydrocarbon results in carbon dioxide (CO_2) and water (H_2O); incomplete combustion results in CO and hydrocarbons. Among the hydrocarbons in the incomplete products, some of them are the evaporative unburned hydrocarbons; the others are hydrocarbons transformed from the ones in gasoline into another forms. Incomplete combustion could easily occur on hydrocarbons with higher amount of carbon atoms when the oxygen supply is not enough. For example, same amount of molecules of aromatics need more molecules of oxygen than isoalkanes do under the same environment conditions. One molecule of benzene, toluene, and xylene require 7.5, 9, and 10 molecules of oxygen, respectively; whereas, one molecule of isopentane/n-pentane requires only 6.5 molecules of oxygen. Thus, aromatics may not achieve complete combustion as isoalkanes do when the same amount of oxygen supply is provided. This happens particularly during the vehicle operation on idling or cold start. The oxygen catalyst has not reached the operation temperature (Nordin et al., 2011).

Gasoline exhaust consists of 71% nitrogen, 14% CO_2, 13% water, and 1-2% of CO, hydrocarbon, and 0.1% NO_x (ATSDR, 2014). Harley and Kean (2004) investigated the chemical compositions of non-methane organic carbon (NMOC) emitted from motor vehicles from 1991 and to 2001. Table 2.4 shows the percentage of the NMOC percentage in gasoline exhaust profile.

Table 2.4 Composition of motor vehicles NMOC emissions (weight %) (Harley and Kean, 2004)

(a) Hydrocarbons in tunnel emissions (weight %)

Species	1991	1994	1995	1996	1997	1999	2001	Average
n-alkanes	9	9	9	9	9	9	9	9.0
isoalkanes	28	23	24	26	25	29	29	26.3
cycloalkanes	5	3	4	5	7	5	5	4.9
alkenes	18	18	17	18	17	15	17	17.1
aromatics	35	39	37	27	27	29	23	31.0
acetylene	4	5	5	4	5	5	9	5.3
oxygenates	0	0	0	7	6	3	3	2.7
carbonyls	0	3	3	5	4	5	5	3.6
Total	100	100	100	100	100	100	100	100

(b) Aromatics hydrocarbons in tunnel emissions (weight %)

Species	1991	1994	1995	1996	1997	1999	2001	Average
benzene	6	6.5	6	4	4	5	4	5.1
toluene	8	10	10	9	8.5	10	9	9.2
m and p xylene	7	7.5	6	5	5.5	6.5	5	6.1
o-xylene	2	2.5	2	2	2	1	3	2.1
ethylbenzene	1	1.5	2	1	1	1	1	1.2
C_{9+} aromatics (1,2,4-trimethylbenzene, 1,3,5-trimethylbenzene, 1,2,3-trimethylbenzene)	13	11	11	6.5	7.5	8.5	7	9.2

According to Harley and Kean (2004), the composition of hydrocarbons in gasoline exhaust consists mostly of aromatics (31.0%), followed by 26.3% iso-alkanes, 17.1% alkenes, and 9.0% n-alkanes. Thus, aromatics and iso-alkanes are expected to be the dominant species with proportion of approximately 30% in gasoline exhaust. Toluene, C_9 aromatics, and xylenes are most abundant aromatics species in gasoline exhaust. The percentage of aromatics is slightly higher than the isoalkanes are.

Diesel exhaust consists of 67% nitrogen, 12% CO_2, 11% water, 10% oxygen, and only 0.3% of Sulfur dioxide, particulate matter, hydrocarbon, and CO (Volkswagen, 2014), and 0.1% NO_x,. Few detailed diesel exhaust VOCs composition is available. It consists of 75% of saturated alkanes including n-alkanes, iso-alkanes, and cycloalkanes; and 25% aromatics. The alkanes range from $C_{10}H_{20}$ to $C_{15}H_{28}$ (Diffen, 2014). Thus, there are less aromatic in diesel than in gasoline exhaust (approximately 31.0%). Heavier alkanes with chain length 10 to 15 carbon atoms are species markers for diesel exhaust.

Liquid gasoline and gasoline vapour are two unburned vehicle emission. They consist of the evaporative species from gasoline. Gasoline vapors are the releases of the fuel vapour from the engine and the fuel system during vehicle operation. Liquid gasoline is the migration of the fuel vapour from the evaporative canister, from leaks, and from fuel permeation through joints, seals, and polymeric components of the fuel system during the vehicle is resting (Harley and Kean, 2004). The resting losses process may due to the diurnal temperature changes where the temperature rises during the day; hot soak due to the high temperature after the engine is shut down for a short period (US EPA, 1994). In study of Harley and Kean (2004), composition of NMOC in liquid gasoline and gasoline vapour were detected. Table 2.5 shows the percentage of species in the profiles.

Table 2.5 Composition of NMOC in evaporative gasoline (weight %) (Harley and Kean, 2004)

(a) Composition of NMOC in Liquid Gasoline

Species	1995	1996	1999	2001 (Berkeley)	2001 (Sacramento)	Average
n-alkanes	9	6	7	9	9	8
isoalkanes	31	39	29	38	32	33.8
cycloalkanes	7	11	5	11	11	9
alkenes/dienes	9	2	15	2	5	6.6
aromatics	41	27	29	27	28	30.4
oxygenates	1	12	3	10	12	7.6
Others	2	3	5	3	3	3.2

(b) Composition of NMOC in headspace vapour (Harley and Kean, 2004)

Species	1995	1996	1999	2001 (Berkeley)	2001 (Sacramento)	Average
n-alkanes	23	16	20	20	20	19.8
isoalkanes	56	54	55	58	48	54.2
cycloalkanes	5	5	5	6	6	5.4
alkenes/dienes	11	5	2	6	5	5.8
aromatics	3	2	2	1	1	1.8
oxygenates	2	18	16	9	20	13

According to Harley and Kean (2004), the liquid gasoline samples were collected at service stations. The components were identified by gas chromatography on a Hewlett Packard Model 5890 II GC equipped with dual flame ionization detectors. The components analysis was done by using DB-1 capillary column, with co-eluting peaks resolved on a DB-5 column. The composition of headspace vapour was calculated by using vapor-liquid equilibrium theory for non-ideal ethanol-gasoline mixtures. Briefly,

the molecule fraction of different species in vapour phase is proportional with the liquid-phase molecules fraction with coefficient of species vapour pressure. In other words, given the same amount of molecules of species in liquid-phase, the higher the species vapour pressure is, the more amounts of molecules the species present in vapour phase (Harley and Kean, 2004).

The composition of the liquid gasoline is similar with gasoline with 33.8% iso-alkanes, 30.4% aromatics, 9% cycloalkanes, and 8% n-alkanes. Thus, isoalkanes and aromatics are the main species in liquid gasoline. In headspace vapour, isoalkanes accounted for over half of the total NMOC with 54.2%, followed by 19.8% n-alkanes. Gasoline vapour consists mostly of isoalkanes. This is because the vapour pressure of isopentane (77 kPa, 20°C) is much higher than that of the abundant aromatics in gasoline including benzene (10.1kPa, 20°C), toluene (2.7 kPa, 20°C), and xylene (0.9 kPa, 20°C) (CAMEO Chemicals, 2014). According to the vapor-liquid equilibrium theory for non-ideal ethanol-gasoline mixtures, the amount of the molecules of isopentane is much larger than that of the aromatics (Harley and Kean, 2004).

Petroleum refining is a series process of separation, conversion, and treatment. The hydrocarbons are separated by fractionation in atmospheric and vacuum distillation towers. Conversion is transforming the existing hydrocarbons into other forms of hydrocarbons. The air pollutants emitted from refinery process includes particulate matter (PM), metals, ammonia, CO2 (US EPA, 2011), sulphur dioxide, NO2, CO, hydrogen sulphide (H2S), PAHs, and hydrocarbons (Kraus, 2011).

The “Proposed Risk Management Approach for Petroleum and Refinery Gases” initiated by Health Canada and Health Canada compiled the main composition of petroleum and refinery gases. The results are listed in Table 2.6.

Table 2.6 Major components of the petroleum and refinery gases (Government of Canada, 2013)

*55 PAMS species

methane	cyclopentane	cyclopentadiene
ethane*	cyclopentene	ethyne (acetylene)*
propane*	1,2-propadiene	benzene*
n-butane*	1,2-butadiene	methanethiol
n-pentane*	1,3-butadiene	ethanethiol
2-methylpropane (isobutane) *	1,2-pentadiene	hydrogen sulphide
2-methylbutane	1-cis-3-pentadiene	ammonia
ethylene*	1-trans-3-pentadiene	hydrogen
1-propene*	1,4-pentadiene	nitrogen
1-butene*	2,3-pentadiene	carbon dioxide
2-butene* (cis-2-butene and trans-2-butene)	3-methyl-1,2-butadiene	carbon monoxide
2-methylpropene (isobutylene)	2-methyl-1,3-butadiene (isoprene) *	

The major gases of petroleum refinery emission are shown in Table 2.6. The PAMS species emitted from petroleum refinery are ethane, propane, n&iso-butane, n-pentane, ethylene, 1-propene, 1-butene, cis-2-butene and trans-2-butene, iso-butene, acetylene, isoprene, and benzene.

Coal is processed to become coke (pure carbon) at the coke oven batteries (US EPA, 2013). Coke oven emissions are a mixture of coal tar, coal tar pitch, volatiles, creosote, PAHs including benzo(a)pyrene, benzanthracene, chrysene, and phenanthrene; and metals. Coal tar volatiles include benzene, toluene, and xylenes (US EPA, 2013). Coke Oven gas contains hydrogen, methane, ethane, CO, CO_2, ethylene, propylene, butylene, acetylene, hydrogen sulfide, ammonia, oxygen, and nitrogen (U.S. Government, 2011).

According to (Totten et al., 2003), liquid petroleum gas refers to the mixture of ethane, propane, and butane that can exist under modest pressure at ambient temperature. The butane/propane mixture is commonly used as fuel (Totten et al., 2003). Propane accounted for at least 90% in the liquid petroleum gas (U.S. department of Energy, 2013). This is because liquid petroleum gas tank is always under pressure at normal operating temperature above the boiling point of -42 °C, and propane can be used from -40 °C to 45 °C; while and butane from 0 °C to about 110 °C. Thus, propane is more robust and reliable compared to butane.

Commercial natural gas consists mostly of methane (95%), followed by ethane (2.5%), propane (0.2%), n&iso-butane (0.06%), pentanes (0.02%), nitrogen (1.6%), CO_2 (0.7%), hydrogen sulphide (trace), water (trace) (Enbridge, 2014). Ethane, propane are the major NMHC in the Commercial natural gas.

Adhesives, painting and surface coatings are mixture of solids suspended in solvent or diluent (water). The solvents mainly consist of VOCs (Lambourne and Strivens, 1999). The solids bond to the substrate and the solvent will then evaporate. The

composition of the adhesives, painting and surface coatings depends on the solids, the substrate on which it is going to attach, and the conditions of the use (Lambourne and Strivens, 1999).

Architectural and industrial are two main uses of coatings. The solvents in architectural coatings contain mostly VOCs including toluene, styrene, and xylene (Lambourne and Strivens, 1999). Architectural coatings are applied under ambient temperature where the paint dries by atmospheric oxidation or the evaporation. The small polymer particles are expected to form as dispersion in water or an organic solvent so that a solid coating could be attached on the surface. This occurs when the temperature is above the polymer's glass transition temperature. However, adding the solvents containing VOCs could lower this property when the temperature is below the transition point. Industrial coatings include automotive paints; can coatings, coil coatings, furniture finishings and road-marking paints (IHS GlobalSpec, 2014). Many industrial finishing processes are under heat. The ‘thermosetting’ polymers mixed with alkyd combined with amino resin were often used in industrial coating processes. However, the composition of the industrial coatings is more diverse in terms of the requirements and factory conditions (Lambourne and Strivens, 1999).

Adhesives consist of sticky solids that make pieces of material stick together. One of the polymer-solvent systems is polychloroprene distributed in solvents mixed with a ketone or an ester, an aromatic and aliphatic hydrocarbon. The aliphatic hydrocarbon could be selected from naphtha, hexane, heptane, acetone, methyl ethyl ketone, benzene, xylene, and toluene (Wypych, 2000). Among the composition of solvent in the polymer-solvent systems, naphtha, hexane, heptane, methyl ethyl ketone, benzene, xylene, and

toluene are VOCs.

Biogenic emissions are released from trees and shrubs. They consist of isoprene and monoterpenes such as α-pinene and β-pinene (Lewandowski et al., 2013). The species are commonly found in mid-latitude regions including Canada (Bonn et al., 2004). The concentration of isoprene is higher in summer as there is much more leaves on the deciduous trees.

2.4 VOCs Source Apportionment Studies

2.4.1 CMB Studies

CMB has been applied to VOC source apportionment in places all over the world. Table 2.7 lists six studies applying CMB to VOC source apportionment.

Table 2.7 CMB VOCs source apportionment application

Location	**Sampling**	**Sources**	**Results**
Seoul, Korea (Na and Kimb, 2007)	Using 2-h integrated SUMMA canister collecting 18 samples from Sep. 8 to Sep. 13, 1998 in the morning, afternoon, and evening.	Vehicle Exhaust, Solvent Use, Gasoline Evaporation, Liquefied Petroleum Gas, and Liquefied Natural Gas	Vehicle Exhaust (52%) was the main source of VOCs in Seoul, followed by solvents (26%). Vehicle Exhaust is high in the morning and evening, and low in the afternoon. The contribution of Gasoline Evaporation and Solvent Usage is high in the afternoon and evening and low in the morning.
Delhi, India (Srivastava et al.,2005)	There were 360 four hourly samples collected at 15 locations during August 2001–July 2002. The measurements were taken during 8 am to 12 am, and 17 pm to 21 pm once a month.	Diesel Internal Combustion Engines, Composite Vehicle, Evaporative Emissions, Auto Repair, Degreasing and Dry-Cleaning, Natural Gas Combustion, Sludge, Consumer Products	Diesel Internal Combustion Engine was the dominant source. Vehicular Exhaust and Evaporative Emissions are another two main contributors.

Table 2.7 – continued 1

Helsinki and Ja¨rvenpa¨a¨, Finland (Helleän et al., 2006)	Using evacuated stainless steel canisters (6 L). The 24-hour concentration measurements were conducted in Helsinki in February, May, and September of 2004 on 16 different days and in Ja¨rvenpa¨a¨ in November and December of 2004 and in January of 2005 on 10 different days.	Traffic-Related, Wood Combustion, Commercial Natural Gas, Biogenic Hydrocarbon, Dry-Cleaning	Major source in urban site were traffic. At the residential site, Liquid Gasoline, and Wood Combustion made higher contributions than traffic sources. Biogenic compounds such as isoprene, also has significant anthropogenic sources such as Wood Combustion. Those compounds sometimes can be mistaken for traffic-related compounds (e.g., Benzene).
Urban area of Dunkerque, French (Badol et al., 2008)	Hourly data of 53 VOCs measured continuously during 1 year. There were 7000 samples collected.	Urban Sources: Urban Heating, Solvent Use, Natural Gas Leakage, Biogenic Emissions, Gasoline Evaporation and Vehicle Exhaust seven industrial sources: Hydrocarbon Cracking, Oil Refinery, Hydrocarbon Storage, Lubricant Storage, Lubricant Refinery, Surface Treatment and Metallurgy.	Vehicle Exhaust contribution in urban was 40%-55%. In industrial area, it was around 60% and could reach 80%. The Vehicle Exhaust contribution varies from 55% in winter down to 30% in summer.
Metropolitan area of Saitama in Tokyo, Japan (Morino et al., 2011)	Hourly concentration of C_2-C_8 non methane hydrocarbons (NMHCs) were measured throughout year of 2007. More than 6000 data were obtained.	Gasoline Vapour, Petroleum Refinery, Light-Duty Gasoline, Super-Light-Duty Gasoline, Diesel Vehicle, Liquefied Natural Gas, Liquefied Petroleum Gas, and Paint Solvent	Vehicle Exhaust, Gasoline Vapor, Liquefied Natural Gas and Liquefied Petroleum Gas, and other evaporative sources contributed 14%-25%, 9%-16%, 7%-10%, 49%-71%, respectively. This value agrees with the emission inventory except the LPG.

Table 2.7 - continued 2

Windsor, Canada (Templer, 2007)	SUMMA canister was set up in the backyards of 51 Windsor households for 24-h air sample collection for five consecutive days from January to March and from July to August of year 2005.	Diesel Exhaust, Gasoline Exhaust, Liquid Gasoline, Gasoline Vapour, Commercial Natural Gas, Liquefied Petroleum Gas, Industrial Refinery, Coke Oven, Architectural Coatings, and Biogenic Emissions	For the summer samples the major contributors were gasoline exhaust, gasoline vapour, architectural coatings and to a lesser extent industrial refineries, diesel exhaust and commercial natural gas. For the winter samples the major contributors were commercial natural gas, gasoline exhaust, industrial refineries and gasoline vapour. Spatial patterns of high and low source contributions were more apparent for the winter samples.

According to the six papers, CMB was applied for investigating the ambient VOCs in Europe, North America, and Asia. The data collection period ranged from a week to one year; and the number of samples collected ranged from 16 to thousands. Among the sources in the review, Diesel Exhaust, Gasoline Exhaust, Liquid Gasoline, Gasoline Vapour, Coke Oven, Architectural Coatings, Biogenic Emissions, Liquefied Petroleum Gas, and Industry Refinery were the sources included in this paper. The other sources were Liquefied Natural Gas, Auto Repair, Degreasing and Dry-Cleaning, Wood Combustion, Sludge, Consumer Products, Hydrocarbon Cracking, Hydrocarbon Storage, Lubricant Storage, Surface Treatment and Metallurgy, and Lubricant Refinery. The review showed that vehicle-related sources were the major VOC contributors in all VOCs source apportionment studies listed in Table 2.7. The VOC contributions from sources could vary during a day, and during different time of a year, according to Korea (Na and

Kimb, 2007), Badol et al. (2008), and Templer (2007).

2.4.2 PMF Studies

There were 17 papers found involving the VOCs source apportionment by using PMF model, among them, nine papers included the source profiles from PMF. They are Wang et al. (2013), Cai et al. (2010), Wei et al. (2014), Song et al. (2008), Morino et al. (2011), Sauvage et al. (2009), Lam et al. (2013), Yuan et al. (2009), Song et al. (2007), and Chan et al. (2011). Out of the source profiles in nine papers, there were three Gasoline Exhaust profiles, two Liquid Gasoline profiles, three Diesel Exhaust profiles, three Gasoline Vapour profiles, eight paint and Solvent profiles, seven Liquid Petroleum Gas profiles, six Petrochemical sources profiles, and one Commercial Natural Gas profile. Coke Oven was not observed in any of the nine papers. The source profiles prepared in Templer (2007) were also included. The additional species other than the 55 PAMS species of CMB model were put at the end of each profile. The source profiles in concentration units were converted into percentage. The percentage of the species in each profiles were ranked in descending order. Table 2.8 shows any species with percentage of 6% or more in order to reveal the potential species markers in different profiles. The complete source profiles of each paper are listed in Appendix B.

Table 2.8 Gasoline Exhaust profiles from PMF in previous studies

(a) Previous studies 1

Song et al. (2008)		Yuan et al. (2009) (location 1)		Yuan et al. (2009) (Location 2)		Templer (2007)	
species	Per cent (%)	species	Per cent (%)	species	Per cent (%)	species	Per cent (%)
acetylene	16.8	toluene	18.3	benzene	30.5	other	24.6
propane	12	isopentane	15.2	toluene	27.3	toluene	7.7
isopentane	11.9	benzene	9.1	isopentane	10.5	isopentane	6.9
ethane	11.7	pentane	8.7	2-methylhexane	7.7	ethylene	6.5
ethylene	9.9	hexane	7.7	pentane	4.1	m and p-xylene	4.1
butane	8.4	2-methylpentane	5.6	butane	4	acetylene	3.7
toluene	6.6	3-methylpentane	4.7	3-methylpentane	3.2	2,2,4-trimethylpentane	3.5
isobutane	6.2	3-methylhexane	4.1	hexane	3	benzene	3.3

(b) Previous studies 2

Gasoline Exhaust (Wang et al., 2013)						
Car 1 Species	Mass per cent (%)	Car 2 Species	Mass per cent (%)	Car 3 Species	Mass per cent (%)	Average
ethylene	12.8	ethylene	11.4	ethylene	11.2	11.8
toluene	11.1	toluene	10.6	toluene	12.1	11.3
benzene	9.1	benzene	9.4	benzene	8.0	8.8
isopentane	6.7	isopentane	7.4	isopentane	5.8	6.6
propylene	5.4	alkyne ethyne	6.3	1,3-dimethylbenzene	5.4	

According to the Gasoline Exhaust profiles in Table 2.8, species including isopentane, toluene, and benzene are the common species markers (Song et al., 2008; Yuan et al., 2009; Templer, 2007; Wang et al., 2013). Species such as acetylene (Song et al.,2008; Wang et al., 2013) and ethylene (Song et al.,2008; Templer, 2007; Wang et al.,

2013), are another two species markers. Toluene and benzene were expected to be the species markers according to the vehicle emission study of Harley and Kean (2004). Ethylene is another significant species marker for gasoline exhaust. There were three Liquid Gasoline profile literature reviews. They are listed in Table 2.9.

Table 2.9 Liquid Gasoline profiles from PMF in previous studies

Liquid/evaporated/exhaust gasoline (Song et al., 2008)		Evaporated and Liquid Gasoline (Yuan et al., 2009)		Liquid Gasoline (Templer, 2007)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
isopentane	21.8	butane	21.1	toluene	14.9
acetylene	18.5	isopentane	19.5	m and p-xylene	9.8
ethylene	11.6	isobutane	14.6	isopentane	9.4
pentane	6.3	propane	8.7	pentane	6.3
toluene	5.8	benzene	8.1	other	4.6
MTBE	4.6	pentane	7.2	2-methylpentane	4.3

According to the Liquid Gasoline profiles in Table 2.9, species n&isopentane (28.1%, 26.7%, and 15.7%) is the common species marker for Liquid Gasoline (Song et al., 2008; Yuan et al., 2009; Templer, 2007). Toluene (5.8%, 4.5%) is another species marker according to Song et al. (2008) and Templer (2007). The large proportion of isopentane and toluene agree with the study of Harley and Kean (2004). In Harley and Kean (2004), the isoalkanes and aromatics are two dominant species classes with isoalkanes percentage slightly outweighing aromatics. There were five Diesel Exhaust profile literature reviews. They are listed in Table 2.10.

Table 2.10 Diesel Exhaust profiles from PMF in previous studies

(a) Previous studies 1

Lam et al. (2013)		Yuan et al. (2009) (Location 1)		Yuan et al. (2009) Location 2	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
toluene	19	toluene	11.9	isopentane	17.1
butane	15.6	isopentane	9.9	isobutane	15.7
hexane	11.5	m and p-xylene	7.8	propane	14.9
propane	10.9	benzene	7.1	pentane	10.1
acetylene	9.2	1,2,4-trimethylbenzene	6	toluene	9.6
isobutane	6.9	decane	5.9	1-butene	8.6
ethylbenzene	6.4	propane	5.2	butane	7.9
ethylene	5.6	hexane	5.2	iso-butene	6.8

(a) Previous studies 2

Song, et al. (2007)		Templer (2007)	
Species	Per cent (%)	Species	Per cent (%)
ethane	0.2	m and p-xylene	10
acetylene	0.2	other	9.2
ethylene	0.1	ethylene	8.9
decane	0.1	1,2,4-trimethylbenzene	6.8
isopentane	0.1	undecane	4.8
benzene	0	toluene	4.1
propane	0	3-ethyltoluene	3.8
toluene	0	propylene	3.6

According to the Diesel Exhaust profiles in Table 2.10, the species including decane (5.9%, 10%) (Yuan et al., 2009; Song, et al., 2007) and undecane (4.8%) (Templer, 2007) accounted for big proportion of Diesel Exhaust profile. Isopentane (17.1%, 10%) is

rich in Diesel Exhaust profile (Yuan et al., 2009; Song, et al., 2007). Aromatics including toluene (19%, 11.9%, and 4.1%) (Lam et al., 2013; Yuan et al., 2009; Templer, 2007), m and p-xylene (10%) and 1,2,4-trimethylbenzene (6%) (Templer, 2007; Yuan et al., 2009) are species markers. Species decane, undecane, and 1,2,4-trimethylbenzene could differentiate Diesel Exhaust from Gasoline Exhaust. There were four Gasoline Vapour profile literature reviews. They are listed in Table 2.11.

Table 2.11 Gasoline Vapour profiles from PMF in previous studies

Morino et al. (2011) Location 1		Morino et al. (2011) Location 2		Lam et al. (2013)		Templer (2007)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
butane	47.6	isopentane	42.8	butane	36.6	isopentane	28.5
isobutane	33.3	butane	23.3	propane	20.8	butane	23.8
propane	9.5	pentane	15.6	isobutane	19.6	pentane	12.2
toluene	9.5	isobutane	11.7	ethylene	11.1	toluene	4.4

Species n&iso-isopentane (Morino et al., 2011; Templer, 2007) and n&iso-butane (Morino et al., 2011; Lam et al., 2013; Templer, 2007) are species markers for Gasoline Vapour. Other species markers including propane and toluene accounted for relatively lower amount of the total percentage

There were eight Paint and Solvent related sources profiles literature review. They are listed in Table 2.12. Among all the nine Paint and Solvent-Related source profiles, the interpretation results from Cai et al. (2010), Yuan et al. (2009), Song et al., (2007), and

Templer (2007) indicated that toluene, m and p-xylene, ethylbenzene, and o-xylene were considered as the species markers of the Paint sources. This agreed with the characteristics of Paint sources discussed in section 2.3. Aromatics accounted for much larger fraction of the total mass compared with other species.

Table 2.12 Paint and Solvent related sources profiles from PMF in previous studies

(a) Previous studies 1

Paint solvent usage (Cai et al., 2010)		Adhesive & sealants (Lam et al., 2013)		Solvent (Lam et al., 2013)		Paint & varnish (Lam et al., 2013)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
toluene	19.4	isopentane	25.2	butane	17.8	acetylene	20.2
m and p-xylene	17.2	isobutane	22.7	acetylene	15.2	ethane	18.6
ethylbenzene	14.1	pentane	14.6	propane	11.4	butane	14.3
propane	13.9	propane	12.7	isoprene	10.2	propane	14
isopentane	5.9	butane	11.1	isobutane	10.2	ethylene	9.3
o-xylene	5	toluene	6	ethylene	9.2	isobutane	6.4

(b) Previous studies 2

Paint and Industrial Coating location 1 (Yuan et al., 2009)		Paint and Industrial Coating location 2 (Yuan et al., 2009)	
Species	Per cent (%)	Species	Per cent (%)
m and p-xylene	23.6	m and p-xylene	24.3
ethylbenzene	15.3	toluene	20.8
toluene	14.9	benzene	17.2
isobutane	8.6	ethylbenzene	16.8
o-xylene	7.4	o-xylene	9.3
butane	6.1	isopentane	2.4
benzene	5.7	butane	2.1

(c) Previous studies 3

Paint (Song et al., 2007)		Architectrual Coatings (Templer, 2007)	
Species	Per cent (%)	Species	Per cent (%)
m and p-xylene	0.3	other	66.9
ethylbenzene	0.1	toluene	25.9
o-xylene	0.1	o-xylene	2.9
toluene	0.1	m and p-xylene	2.7
pentane	0.1	2,4-dimethylpentane	1.1
r-pinene	0.1	ethylbenzene	0.5
benzene	0.1	benzene	0.1

There were eight Liquid Petroleum Gas profile literature reviews. They are listed in Table 2.13. The eight Liquid Petroleum Gas source profiles indicated that the most abundant species were propane, 18% in Song et al., (2008), 23.9% in Yuan et al. (2009), 38.4% Yuan et al. (2009), and 90.6% in Templer (2007). Other minor species include n&iso-butane (Cai et al., 2010; Song et al., 2008; Yuan et al., 2009), ethane (Morino et al., 2011; Lam et al., 2013), ethylene (Song et al., 2008), and propylene (Song et al., 2008; Templer, 2007). There were species including isobutene and propylene with comparable percentage with that of propane based on the reviews. This does not agree with the 90% of propane in Liquid Petroleum Gas reported in Liquid Petroleum Gas composition by U.S. department of Energy (2013). There could be differences between the source profiles and source composition.

Table 2.13 Liquid Petroleum Gas profiles from PMF in previous studies

(a) Previous studies 1

(Gasoline,LPG/LNG Leakage) Cai et al. (2010)		LPG (Song et al., 2008)		liquefied natural gas and liquefied petroleum gas (LPG) Morino et al. (2011)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
isopentane	21.8	propane	17.9	ethane	69.1
butane	12.2	isobutane	16	propane	10.6
isobutane	10.3	butane	14.2	butane	5.3
propane	7.1	1-butene	12.2	toluene	5.3
methylenechloride	4.6	ethylene	7.1	acetylene	4.3
propylene	4.2	propylene	7.1	benzene	2.7

(b) Previous studies 2

LPG usage & consumer product propellant (Lam et al., 2013)		LPG location 1 (Yuan et al., 2009)		LPG location 2 (Yuan et al., 2009)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
toluene	38.1	propane	23.9	propane	38.4
ethane	16	isobutane	22.4	butane	21.2
acetylene	12.5	butane	15.8	isobutane	17.2
benzene	6.2	toluene	9.6	isopentane	7.5
propane	6	isopentane	6.3	pentane	5.9
ethylene	3.8	hexane	3.5	benzene	5.4

(c) Previous studies 3

LPG (Song et al., 2007)		LPG (Templer, 2007)	
Species	Per cent (%)	Species	Per cent (%)
propane	0.2	propane	90.6
isobutane	0.2	propylene	5.1
butane	0.1	ethane	4.1
1-butene	0.1	isobutane	0.2
ethylene	0.1	ethylene	0
propylene	0.1	acetylene	0

There were six Petrochemical sources profile literature reviews. They are listed in Table 2.14. The n&iso-butane (Cai et al., 2010; Templer, 2007) and n&iso-pentane (Cai et al., 2010; Chan et al., 2011; Templer, 2007) accounted for large proportion of the Petrochemical source among all source profiles. Aromatics including toluene and benzene were also species markers for Industry Refinery Cai et al. (2010); Song et al. (2008); Chan et al., (2011). Species 2,4-dimethylpentane (Cai et al., 2010) and 2,3-dimethylbutane (Chan et al., 2011) were the species markers for petrochemical sources.

Table 2.14 Petrochemical sources profiles from PMF in previous studies

(a) Previous studies 1

Petrochemical sources Location 1 (Cai et al., 2010)		Petrochemical sources Location 2 (Cai et al., 2010)		Petrochemical sources (Song et al., 2008)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
propylene	13	2,4-dimethylpentane	12	m and p-xylene	20.9
isobutane	9	3-methylpentane	8.5	ethylene	17.4
butane	8	1-hexene	8	toluene	12.8
benzene	7.8	butane	7	ethylbenzene	9.1
3-methylpentane	7.5	pentane	7	o-xylene	8.7
isopentane	6	isopentane	6.5	acetylene	6
toluene	6	benzene	4.8	propylene	4.9

(b) Previous studies 2

Petrochemical sources Location 1 (Chan et al., 2011)		Petrochemical sources Location 2 (Chan et al., 2011)		Templer (2007)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
pentane	10	hexane	10	other	36.3
2,3-dimethylbutane	10	pentane	10	butane	22.9
m and p-xylene	5	2,3-dimethylbutane	10	isobutane	9.6
toluene	5	3-methylhexane	8	pentane	6.6
NO_2	5	styrene	8	propane	3.7
coarse particles	5	toluene	8	hexane	2.9

There were three Commercial Natural Gas profiles. They are listed in Table 2.15. Both source profiles from Song et al. (2008) and Templer (2007) showed that ethane was the dominant NMHC species in Commercial Natural Gas with 38.5% in Song et al.

(2008); and 68.9% in Templer (2007). Thus, the presence of approximately 35% to 69% of ethane indicates that the source being Commercial Natural Gas. This conclusion agreed with the major NMHC in Commercial Natural Gas, ethane, followed by propane.

Table 2.15 Commercial Natural Gas profiles of NMHC from PMF in previous studies

Song et al. (2008) (Using source profiles of Song et al. (2007)		Song et al. (2007)		Templer (2007)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
ethane	38.5	ethane	38.5	ethane	68.9
acetylene	9.5	acetylene	9.5	propane	21.1
toluene	9.4	toluene	9.4	butane	3.1

2.4.3 PCA Studies

There were six papers showing the PCA source profiles. Among them, five did not apply Z score or not mentioned (Duan et al., 2008; Guo et al., 2007; Huang et al., 2012; Wang et al., 2006; Lai et al., 2013); while the other one applying Z score (Chang et al, 2015). Only the species with loadings equal or greater than 0.5 were listed in the six papers. Table 2.16 lists the five solvent source profiles of PCA.

Table 2.16 Solvents profiles from PCA in previous studies

(a) Previous studies 1

Solvent usage/LPG Location 1 (Guo et al., 2007)		Solvent usage/LPG Location 2 (Guo et al., 2007)		Solvent usage/LPG Location 3 (Guo et al., 2007)	
Species	Loadings	Species	Loadings	Species	Loadings
o-xylene	0.9	o-xylene	0.92	1,2,3-trimethylbenzene	0.86
m-xylene	0.89	m-xylene	0.87	1,2,4-trimethylbenzene	0.85
ethylbenzene	0.88	1,3,5-trimethylbenzene	0.86	1,3,5-trimethylbenzene	0.82
p-xylene	0.88	p-xylene	0.85	propene	
1,2,3-trimethylbenzene	0.84	ethylbenzene	0.84	iso-butane	
1,2,4-trimethylbenzene	0.81	1,2,4-trimethylbenzene	0.83	n-butane	
toluene	0.76	1,2,3-trimethylbenzene	0.72	toluene	
1,3,5-trimethylbenzene	0.73	toluene	0.64	ethylbenzene	
n-butane	0.59	propene		m-xylene	
propene	0.57	iso-butane		p-xylene	
iso-butane	0.53	n-butane		o-xylene	

(b) Previous studies 2

Solvent Usages (Huang et al., 2012)		Solvent-related (Duan et al., 2008)	
Species	Loadings	Species	loadings
1,2-dichloroethane	0.98	xylenes	0.78
trichloroethene	0.96	trimethylbenzenes	0.78
chloroform	0.95	n-hexane	0.76
1,1,2-trichloroethane	0.94	ethylbenzene	0.75
1,2-dichloropropane	0.94	i/n-butane	0.53
cyclohexane	0.92	% variance	9.25
isopentane	0.9	Eigenvalue	1.3
1,1-dichloroethene	0.88		
trans-1,2-dichloroethene	0.88		
pentane	0.87		
hexane	0.86		
chloromethane	0.86		
chloroethene	0.86		
1,1-dichloroethane	0.85		
2,2-dimethylbutane	0.83		
2-butanone	0.83		
2-methylpentane	0.81		
2,3-dimethylbutane	0.8		
dichloromethane	0.8		
cis-1,2-dichloroethene	0.79		
3-methylpentane	0.78		
isobutane	0.73		
cis-2-pentene	0.73		
1-pentene	0.72		
carbon disulfide	0.72		
acetone	0.72		
1-hexene	0.58		
toluene	0.58		
2,2,4-trimethylpentane	0.5		
%Total variance	33.29		
Eigenvalue	21.97		

Among all the source profiles in Table 2.16, the common species with high loadings include m, p-xylenes (Guo et al., 2007; Duan et al., 2008), o-xylene (Guo et al., 2007), ethylbenzene, trimethylbenzenes (Guo et al., 2007; Duan et al., 2008), and toluene (Guo et al., 2007; Huang et al., 2012). Toluene was among the top species with high loadings, but lower than the other top species. Additional species with high loadings included n&iso -butane (Guo et al., 2007; Huang et al., 2012; Duan et al., 2008).

As there was no percentage of species in the profiles provided by PCA, the approach of identification of PCA is different from the profiles provided by PMF. However, the acknowledged abundant species in different sources are consistent regardless from PMF or PCA. For PCA, the species markers in PMF profiles are expected to have high loadings in the component of the same source. In adhesive Sealant Coating profiles, other than the aromatics including m and p-xylenes, o-xylene, ethylbenzene, trimethylbenzenes, and toluene, hexane and heptane are expected to have high loadings as well (Wypych, 2000).

The auto painting source profile of PCA is listed in Table 2.17. Among the source profiles in Table 2.17, the auto painting profiles from Huang et al. (2012) indicated that the aromatics species including n-ethyltoluene, benzene, toluene, ethylbenzene, xylene, and propylbenzene had the highest loadings. Species n-ethyltoluene and propylbenzene differentiate Auto Painting from Adhesive and Sealant Coatings, and Architectural Coatings.

Table 2.17 Auto Painting profiles from PCA in previous studies

Species (Huang et al., 2012)	Loadings
m/p-xylene	0.88
p-ethyltoluene	0.85
o-ethyltoluene	0.84
o-xylene	0.83
ethylbenzene	0.82
m-diethylbenzene	0.82
m-ethyltoluene	0.8
p-diethylbenzene	0.8
toluene	0.78
n-propylbenzene	0.76
3-methylheptane	0.7
n-octane	0.66
benzene	0.65
%Total variance	16.39
Eigenvalue	10.82

Six Industrial Refinery profiles of PCA from literature review are listed in Table 2.18. Among all the Industrial Refinery source profiles of PCA in Table 2.18, there were some common high loading species; they were alkenes including 1-butene (Guo et al., 2007; Huang et al., 2012), cis/trans-butene (Huang et al., 2012), propene (Chang et al., 2009; Guo et al., 2007), and ethylene (Guo et al., 2006). Other species with high loadings in Industrial Refinery profiles include propane (Guo et al., 2006), ethane (Chang et al., 2009), heptane (Huang et al., 2012; Guo et al., 2006), and aromatics including toluene, benzene (Chang et al., 2009; Guo et al., 2006), and styrene (Chang et al., 2009).

Table 2.18 Industrial Refinery profiles from PCA in previous studies

(a) Previous studies 1

Petrochemical Plants and Solvent Usage (Chang et al., 2009)		Industrial source Location 1 (Guo et al., 2007)		Industrial source Location 2 (Guo et al., 2007)	
Species	Loadings	Species	Loadings	Species	Loadings
styrene	0.85	1-butene	0.84	iso-butene	0.92
propene	0.74	iso-butene	0.8	1-butene	0.84
benzene	0.62	propene	0.7	propene	0.75
ethane	0.53				
toluene	0.48				
variance of explained %	4.56				
Eigenvalue	2.01				

(b) Previous studies 2

Oil refineries and storage leaks (Huang et al., 2012)		Industrial emissions 1 (Guo et al., 2006)		Industrial emissions 2 (Guo et al., 2006)	
Species	Loadings	Species	Loadings	Species	Loadings
propene	0.96	ethylbenzene	0.89	ethylbenzene	0.9
1-butene	0.86	o-xylene	0.86	tetrachloroethene	0.86
2-methoxy-2-methyl-propane	0.85	p-xylene	0.84	n-hexane	0.85
trans-2-butene	0.84	m-xylene	0.81	n-heptane	0.85
cis-2-butene	0.82	tetrachloroethene	0.79	toluene	0.82
1,3-butadiene	0.77	n-hexane	0.78	ethyne	0.66
isoprene	0.76	n-heptane	0.76	n-octane	0.65
2-methylheptane	0.65	benzene	0.69	iso-butane	0.57
trans-2-pentene	0.65	n-octane	0.64	benzene	0.57
butane	0.55	ethyne	0.58	n-butane	0.56
heptane	0.52	iso-butane	0.56	iso-pentane	0.55
1-hexene	0.5	toluene	0.56	propane	0.52
%Total variance	24.8	ethene	0.53	ethene	
Eigenvalue	16.37	n-butane	0.51	o-xylene	
		propane	0.5	m-xylene	
		iso-pentane		p-xylene	
		% of variance	68.99	% of variance	8.72
		Eigenvalue	15.18	Eigenvalue	1.83

There were two Liquid Petroleum Gas profiles from PCA literature reviews. They are listed in Table 2.19. According to the Liquid Petroleum Gas source profiles in Table 2.19, the loadings of propane and n&iso-butane were the highest. The loadings of other species including ethylene, n&iso-pentane, and aromatics were also high on Liquid Petroleum Gas (Guo et al., 2006; Chang et al., 2009).

Table 2.19 Liquid Petroleum Gas profiles from PCA in previous studies

liquefied petroleum gas (Chang et al., 2009)		Commercial/domestic LPG/NG use (Guo et al., 2006)	
Species	Loadings	Species	Loadings
isobutane	0.86	n-butane	0.76
n-butane	0.85	propane	0.72
ethene	0.83	iso-butane	0.71
cyclohexane	0.71	propene	0.61
propane	0.7	% of variance	6.53
n-pentane	0.62	Eigenvalue	1.44
n-hexane	0.5		
o-xylene	0.49		
ethane	0.47		
toluene	0.47		
m and p-xylene	0.47		
n-heptane	0.44		
ethylbenzene	0.44		
isopentane	0.43		
benzene	0.43		
n-octane	0.42		
3-methylpentane	0.41		
% of variance explained	7.27		
Eigenvalue	3.2		

Two Gasoline Exhaust source profiles of PCA are listed in Table 2.20. According to the Gasoline Exhaust source profiles in Table 2.20, the common species with high loadings in Gasoline Exhaust profile were 2,2,4-trimethylpentane, iso-butane, and n-pentane. Other high loading species include ethylene, n-pentane, n-heptane, 2,3-dimethylbutane, 1-butene, benzene, propene, 2-methylpentane.

Table 2.20 Gasoline Exhaust profiles from PCA in previous studies

Lai et al., 2013 (Summer)		(Autumn)	
Species	Loadings	Species	Loadings
2,2,4-trimethylpentane	0.96	n-heptane	0.98
iso-butane	0.84	n-hexane	0.91
ethylene	0.81	2,2,4-trimethylpentane	0.84
n-hexane	0.72	2,3-dimethylbutane	0.8
n-pentane	0.68	1-butene	0.8
benzene	0.45	iso-butane	0.73
ethane	0.42	benzene	0.67
m and p-xylene	0.42	propene	0.62
n-heptane	0.32	2-methylpentane	0.54
acetylene	0.31	isoprene	0.53
2-methylpentane	0.29	o-xylene	0.49
1-butene	0.27	3-methylpentane	0.42
isoprene	0.2	acetylene	0.42
n-butane	0.19	n-butane	0.36

Table 2.20 - continued

iso-pentane	0.14	ethylene	0.25
propene	0.12	n-pentane	0.23
n-propane		iso-pentane	0.23
2,3-dimethylbutane		n-propane	0.17
3-methylpentane		m and p-xylene	0.14
toluene		toluene	0.12
o-xylene		ethane	
%Total variance	10.99	%Total variance	12.82
Eigenvalue	2.42	Eigenvalue	2.82

Two Diesel Exhaust profiles are listed in Table 2.21. According to Diesel Exhaust profile in Lai et al. (2013) in Table 2.21, the common species with high loadings included propene, styrene, benzene, and 2-methylpentane. Among these species, the loadings of propene, benzene were higher than that of 2-methypentane. Other species with high loadings but not as high as the species mentioned above included toluene, m and p-xylene, ethane, 1-butene, n-propane, acetylene, n-heptane, and 2,2,4-trimethylpentane.

Table 2.21 Diesel Exhaust profiles from PCA in previous studies

Lai et al. (2013)	Summer	Lai et al. (2013)	winter
Species	Loadings	Species	Loadings
propene	0.96	o-xylene	–0.15
toluene	0.92	styrene	0.85
m and p-xylene	0.89	benzene	0.82
ethane	0.8	n-heptane	0.77
styrene	0.75	propene	0.73
1-butene	0.7	3-methylpentane	0.54
benzene	0.7	2,2,4-trimethylpentane	0.53
n-propane	0.67	iso-pentane	0.49
o-xylene	0.66	2,3-dimethylbutane	0.39
acetylene	0.65	isoprene	0.19
2-methylpentane	0.44	toluene	0.16
n-butane	0.41	ethane	0.13
ethylene	0.38	2-methylpentane	0.12
iso-pentane	0.37	ethylene	0.12
iso-butane	0.36	%Total variance	12.07
n-hexane	0.32	Eigenvalue	2.66
isoprene	0.27		
3-methylpentane	0.2		
n-pentane	0.17		
%Total variance	14.5		
Eigenvalue	3.19		

Two Gasoline Evaporation profiles of PCA are listed in Table 2.22. Based on the profiles in both Guo et al. (2007) and Wang et al. (2006), the loadings of n&iso-pentane were the highest among all the species. The other species with high loading consisted of n&iso-butane (Guo et al., 2007), and toluene (Wang et al., 2006). The Gasoline evaporation profile in Wang et al. (2006) explains only 4.67% per cent of the variance of the measurements, indicating the insignificance of this source. The sources explaining the remaining 95.33% variance were not shown.

Table 2.22 Gasoline Evaporation (Liquid Gasoline/Gasoline Vapour profiles from PCA in previous studies

Gasoline evaporation (Guo et al., 2007)		Gasoline evaporation (Wang et al., 2006)	
Species	Loadings	Species	Loadings
n-pentane	0.77	iso-pentane	0.98
iso-pentane	0.72	n-pentane	0.77
n-butane	0.57	toluene	0.77
iso-butane	0.55	Variance Explained (%)	4.67
		Eigenvalue	1.03

There was a research applying CMB, PMF, and PCA models to 14 ambient VOCs source apportionment of from 1980 to 1984 in New Jersey, U.S. (Anderson et al., 2002). Table 2.23 shows the source profiles and their corresponding source contributions of CMB model, PMF factors and contributions, and PCA principal components with loadings and contributions. The source contribution is within the range of uncertainty.

Table 2.23 Source profiles and source contributions (Anderson et al., 2002)

(a) Source profiles and source contributions from CMB model (Mass Percentage %)

Species	**Automobile Exhaust**	**Insecticide**	**Deodorizers**	**Dry cleaning**	**Tap Water**	**Tailgas Scrubber**
benzene	25	0	0	0	0	58
carbon tetrachloride	0	0	0	0	20	0
chlorobenzene	0	0	0	0	0	37
chloroform	0	0	0	0	22	0
1,4-dichlorobenzene	0	0	100	0	0	5
1,2-dichlorobenzene	0	0	0	0	0	5
ethylbenzene	15	0	0	0	0	0
styrene	5	0	0	0	0	0
tetrachloroethylene	0	0	0	100	19	0
1,1,1-trichloroethane	0	95	0	0	20	0
trichloroethylene	0	0	0	0	19	0
o-xylene	20	0	0	0	0	0
m and p-xylene	40	5	0	0	0	0
Source contributions (%)	43% ± 19%	19%± 19%	13% ± 20%	9%±11%	15%± 10%	2% ± 3%

(b) Factors and contributions from PMF model (Mass percentage %) (Anderson et al., 2002)

	Factor 1	**Factor 2**	**Factor 3**	**Factor 4**	**Factor 5**	**Factor 6**
benzene	60	0	0	0	0	1
carbon tetrachloride	3	0	0	0	0	1
chlorobenzene	1	0	0	0	0	0
chloroform	13	0	1	0	0	1
1,4-dichlorobenzene	1	0	0	100	0	0
1,2-dichlorobenzene	1	0	0	0	0	0
1,2-dichloroethane	2	0	0	0	0	0
ethylbenzene	3	20	1	0	0	1
styrene	6	1	0	0	0	0
tetrachloroethylene	2	0	0	0	95	1
1,1,1-trichloroethane	1	0	96	0	5	10
trichloroethylene	1	0	0	0	0	85
o-xylene	1	20	1	0	0	0
m and p-xylene	6	60	1	0	0	0
Source contributions (%)	21%± 14%	32%± 19%	20%± 18%	13%± 21%	9%± 10%	5%± 8%

(c) Principal Components and loadings from PCA (Anderson et al., 2002)

	PC1	**PC2**	**PC3**	**PC4**	**PC5**
benzene	0.28	0.02	0.05	0	0.03
carbon tetrachloride	-0.01	0.01	0.04	0.03	0
chlorobenzene	0.02	0	0.01	0	0
chloroform	0.1	-0.01	0	0	0
1,4-dichlorobenzene	0.04	0.01	0.18	0.95	-0.09
1,2-dichlorobenzene	0	0	0	0.03	0
1,2-dichloroethane	0	0	0.02	0	0
ethylbenzene	0.06	0.26	0.02	0.02	0.01
styrene	0.1	0.01	-0.01	-0.01	-0.02
tetrachloroethylene	0.06	0.01	0.03	0.03	0.48
1,1,1-trichloroethane	0.16	0.02	0.58	-0.1	0.19
trichloroethylene	-0.01	0.01	0.04	-0.01	0.33
o-xylene	0.04	0.18	0	0	0.02
m, p-xylene	0.15	0.48	0.04	0	0.06
Source contributions (%)	33%± 28%	17%±20%	28%± 25%	13%±27%	8%± 15%

The Automobile Exhaust profiles in CMB profiles consist of abundant benzene, ethylbenzene, and xylenes. There was large proportion of benzene in profile 1 of both PMF and PCA, respectively. The second profile of both PMF and PCA were dominated by ethylbenzene and xylenes. The first two profiles were both identified as Automobile Exhaust. There was abundant 1,1,1-trichloroethane, and 1,4-dichlorobenzene in profile 3 and profile 4 in PMF and PCA, respectively. According to the CMB source profiles, profile 3 and profile 4 could be Insecticide and Deodorizers, respectively. There was a factor in PMF that was dominated by trichloroethylene. Factor 5 in PCA was rich on both trichloroethylene and tetra-chloroethylene. The contributions of the two sources to the

total VOCs concentration are small (5%±8%, and 8%±15%). Table 2.23 (a) shows that none of the source profiles in CMB had large proportion of trichloroethylene, trichloroethylene, or tetra-chloroethylene. Thus, PMF and PCA provided small sources with low source contributions other than the six sources of CMB (Anderson et al., 2002). The source and contributions from different models are listed in Table 2.24.

Table 2.24 Source profiles of different models and source contribution estimates (SCE) (Anderson et al., 2002)

Major compounds	**CMB**		**PMF**		**PCA**	
	Profile	SCE (%)	Profile	SCE (%)	Profile	SCE (%)
benzene, ethylbenzene, xylenes	Automobile Exhaust	43±14				
benzene			1P	21±14	1PA	33±28
ethylbenzene, xylenes			2P	32±19	2PA	17±20
1,1,1-trichloroethane	Insecticide	19±19	3P	20±18	3PA	28±25
1,4-dichlorobenzene	Deodorizers	13±20	4P	13±21	4PA	13±27
tetrachloroethylene	Dry Cleaning	9±11	5P	9±10		
trichloroethylene			6P	5±8		
trichloroethylene, tetra-chloroethylene					5PA	8±15
carbon tetrachloride, chloroform, tetrachloroethylene, 1,1,1-trichloroethane, trichloroethylene	Tap Water	15±10				
benzene, chlorobenzene	Tail Gas Scrubber	2±3				

According to Table 2.24, there were four common sources of all three models. They were Automobile sources, Insecticide, Deodorizers, and Dry Cleaning. The source contribution of Automobile Exhaust calculated from CMB (43%) and from PMF (53%) indicated that Automobile Exhaust was the major contributor among all the other sources. Neither PMF nor PCA identified Tail Gas Scrubber with low contribution source included in CMB profile. Both PMF and PCA provided profiles of an additional source Tap Water which was not included in CMB profiles. PMF and PCA provided most of the sources in CMB model. They both provide additional sources with low contributions (Anderson et al., 2002). The errors of source contributions of Insecticide, Deodorizers, Dry Cleaning, and Tail Gas Scrubber from CMB model; Deodorizers and Dry Cleaning from PMF; and Deodorizers from PCA exceed the SCE values. The large errors indicate the great uncertainties of the source contribution estimates of those sources. When the errors of the source contribution are larger than the source contribution, the source identification is difficult.

2.5 Comparison of the CMB, PMF, and PCA

Each receptor model has advantages and disadvantages. Based on the review of fundamentals of each receptor model and source apportionment applications, the advantages and disadvantages of each of three receptor model are listed in Table 2.25.

Table 2.25 Advantages and disadvantages of CMB, PMF, and PCA

	CMB	**PMF**	**PCA**
Advantages	• Straight forward to analyze the source contributions from model outputs.	• There is no need to prepare the source profiles. • Can choose the number of required sources. • Model provides scatter plots, bar charts, linear regression, and pie charts for visualizing the reliability of input data, model performance in terms of the stability, the calculations, the outputs, and the reliability of the outputs at both data preparation and results stages. • Providing small sources with low contributions	• There is no need to prepare the source profiles. • Easy to prepare the input data • Providing sources in addition to the compiled profiles

Table 2.25 - continued

Disadvantages	• The process of source profiles preparation could be tedious and time consuming. • The negative source contribution in the source contribution estimation is hard to explain. • The results highly rely on the sources profiles. If the source profile does not fully explain the species composition at the receptor sites, the model may not provide actual results.	• The process of source identification could both be tedious.	• The number of Components is not selectable. • The source contribution could not be computed if Z score is used. • Source identification could be tedious and time consuming. • The source identification highly rely on the species markers loadings. Once the species markers are not included in measurements, model would not provide the associated source profiles.

CHAPTER 3

METHODOLOGY

3.1 Data collection and preparation

3.1.1 Data collection

The ambient VOCs monitoring sites were selected by University of Windsor and Health Canada. The air samples of year 2005 and 2006 were collected by Health Canada and University of Windsor. The results of CMB of 2005 were used in this study. There were 49 sites, 47 in winter and 45 in summer, respectively in the year 2006. Among the 47 sampling sites in winter 2006, four of them did not do in summer; instead, two additional households were recruited for summer sampling. The 24-h air samples of year 2005 and 2006 were collected by using 6-L SUMMA canisters set up in the backyards of residential households in Windsor for five consecutive days at each site. The VOCs concentration measured at National Air Pollution Surveillance Program (NAPS) during the period overlapped with the sampling dates in this study were also included.

The NAPS program provides the long term air quality information across Canada. It had 286 measurement sites in 203 communities located in territory in year 2013 (Environment Canada, 2013). The site located at College and South St., Windsor collects 24-h samples every six days (Environment Canada, 2013). The monitoring equipment and methodology are similar with Templer's study (Templer, 2007). There were eight samples in winter and eight in summer, respectively, measured on dates that overlapped with those of this study. All 16 samples were included in this study. The NAPS sampling dates of winter and summer for 2006 are listed in Table 3.1. The collected VOC samples were sent to the Environment Canada laboratory for analysis.

Table 3.1 Sampling dates of winter and summer of year 2006

	Date of sampling	**NAPS sampling dates overlapped with this study**
Winter	Jan. 23rd to Mar. 10th Mar. 20th to Mar. 24th	Jan. 23rd, Jan. 29th, Feb. 10th, Feb. 16th, Feb. 22nd, Feb. 28th, Mar. 6th, Mar. 24th
Summer	July 3rd to Aug. 25th	Jul. 4th, Jul. 10th, Jul. 22nd, Jul. 28th, Aug. 3rd, Aug. 9th, Aug.15th, Aug. 21st

In 2005, sampling sites were set up in the backyards of 51 residential households (Figure 3.1) in Windsor. The 24-h air samples collection were conducted for 5 consecutive days during winter and in summer 2005. The sampling sites of both years 2005 and 2006 are shown in Figure 3.

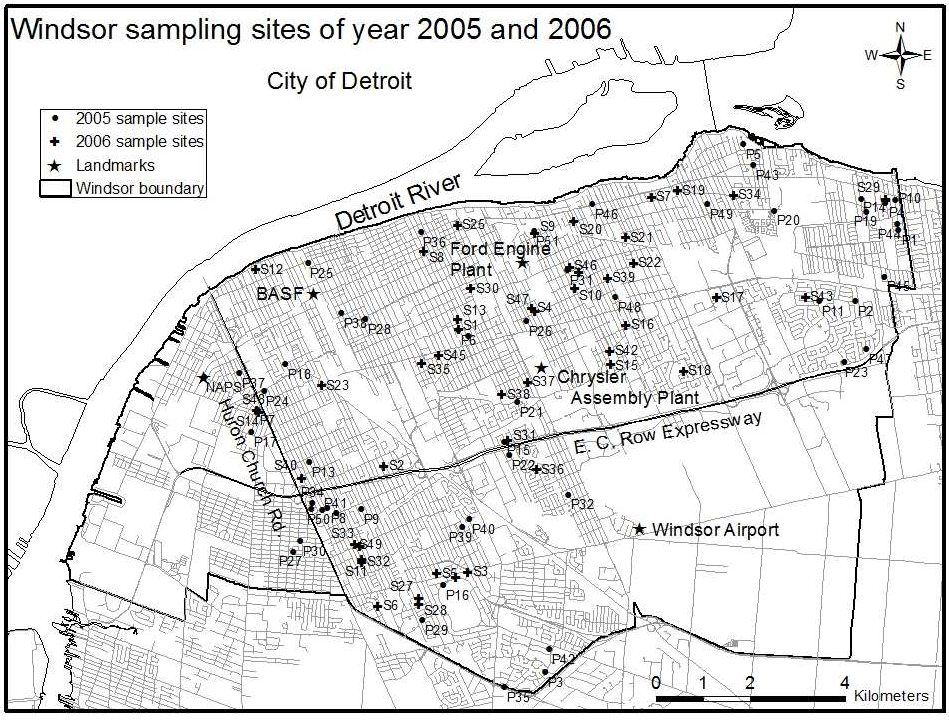

Figure 3.1 Sampling sites for 2005 and 2006

3.1.2 Data processing

In winter and summer of both years, 240 samples were planned to be deployed. However, the actual number of the deployed samples was less than 240. Not all analyzed samples were included for analysis. The number of planned samples, deployed samples, the samples included in analysis, and the retained per cent are listed in Table 3.2.

Table 3.2 Sampler retrieval and retention rates in year 2005 and 2006

Year	**Season**	**Samples planned**	**Samples deployed**	**Included for analysis**	**Retained (%)**
2005	Winter	240	239	201	84
	Summer	240	228	225	99
	Annual	480	467	426	91
2006	Winter	240	232	214	92
	Summer	240	228	214	94
	Annual	480	460	428	93

There were 84% and 99% samples included in analysis out of the total deployed samples in winter and summer 2005, respectively. The year 2005 annual retained percentage of year 2005 was 91% (Templer, 2007). In year 2006, 92% and 94% samples were retained in winter and summer, respectively; and the annual retained rate was 93%. Overall, the retained rate in summer was higher than that of winter; and higher in year 2006 compared to year 2005.

Not all sites obtained the samples for all five consecutive days. Table 3.3 shows the percentage of sites with different number (1, 2, 3, 4, and 5) of samples obtained in each season, and year 2006.

Table 3.3 Percentage of sites with different number of samples obtained in each season and annual of 2005 and 2006

(a) Year 2006

Number of samples obtained at one site	**Winter (%)**	**Summer (%)**	**Annual (%)**
5	66	76	72
4	28	20	24
3	2	2	2
2	4	0	2
1	0	0	0

(b) Year 2005

Number of samples obtained at one site	**Winter (%)**	**Summer (%)**	**Annual (%)**
5	71	87	79
4	13	11	12
3	9	2	6
2	2	0	1
1	5	0	2

There were 66% and 76% sites with five samples in winter and summer of year 2006, respectively. For year 2006, 72% sites obtained five samples. There were 28% and 20% sites with four samples collected in winter and summer, respectively. There were 24% sites with four samples in the year 2006. The percentage of the sites with three samples was 2% in both seasons of year 2006. There were 4% of sites with only two samples obtained in winter 2006. There was no site with one or zero samples obtained in either season. All samples were retained for further analysis. This was to keep as many samples as possible, following (Templer, 2007).

There were 71% and 87% sites with five samples in winter and summer of year 2005, respectively. There were 12% sites obtaining four samples in year 2005, followed by 6% sites with three samples, 1% with two samples, and 2% with only one sample. There were 91% sites obtaining five or four samples, indicating that the samples represented the overall VOC concentrations in Windsor. The samples of year 2005 were all retained for the further analysis.

The collected air samples were sent to the Environmental Technology Centre, Environment Canada for analysis. Among the 188 VOCs analyzed, only the 112 NMHC species were included in this study, leaving the other 76 excluded from this study. However, in this case, some species markers including MEK for Coatings were excluded. Among the 112 NMHC species, only 55 PAMS species are components of the source profiles, according to the CMB protocol (Waston et al., 2004). Thus, the 57 species other than the PAMS were summed as one species named “Others”. There were 32 species (Table 3.4) named as “fitting species” participating in CMB model calculation. The fitting species are species with low reactivity, and are the species markers in one or more source profiles. The only exception is isoprene as it has high reactivity but serve as the only species marker for Biogenic Emissions.

Table 3.4 55 PAMS species and fitting species (marked with *) (Templer, 2007)

PAMS Species	Fitting Species	PAMS Species	Fitting Species
acetylene	*	methylcyclopentane	*
benzene	*	2-methylhexane	*
n-butane	*	3-methylhexane	*
1-butene		2-methylheptane	*
c-2-butene		3-methylheptane	*
t-2-butene		2-methylpentane	*
cyclohexane	*	3-methylpentane	*
cyclopentane	*	2-methyl-1-pentene	
n-decane	*	n-nonane	*
1,3-dimethylbenzene		n-octane	*
1,4-diethylbenzene		n-pentane	*
2,2-dimethylbutane	*	1-pentene	
2,3-dimethylpentane	*	c-2-pentene	
2,3-dimethylbutane	*	t-2-pentene	
2,4-dimethylpentane	*	n-propane	*
ethane	*	propene	
ethene		n-propylbenzene	
ethylbenzene		styrene	
2-ethyltoluene		1,2,3-trimethylbenzene	
3-ethyltoluene		1,2,4-trimethylbenzene	
4-ethyltoluene		1,3,5-trimethylbenzene	
n-heptane	*	2,2,4-trimethylpentane	*
n-hexane	*	2,3,4-trimethylpentane	*
isobutane	*	toluene	*
isopentane	*	n-undecane	*
isoprene	*	m and p-xylene	
iso-propylbenzene		o-xylene	
methylcyclohexane	*		

The concentrations of each of the 47 and 45 site in winter and summer 2006 were averaged as one sample. The weekly mean, standard deviation, skewness, kurtosis, and number of the obtained samples at each site was computed and listed in Supplementary Information. The general statistics including mean, standard deviation, coefficient of

variance, minimum, maximum, median, interquartile range, skewness, and kurtosis of each compound among all the sampling sites in year 2006 were computed by using Minitab 16 (Minitab, 2010). The results are listed in Appendix C. The eight samples measured at the NAPS site in each season were averaged as one sample for winter and summer, respectively, in order to not overemphasis the sample in this location (Templer, 2007).

The method detection limit (MDL) of each measured species is listed in Appendix D. MDL is the minimum concentration that can be measured and reported with 99 percent confidence that the concentration is greater than zero. The concentration cannot be detected accurately if the actual concentration is equal or below this value. The species with concentrations below the MDL and the percentage in winter and summer 2006 are listed in Table 3.5. For CMB, any concentration below MDL was replaced with the species MDL value; for PMF, the seven species in winter and three in summer having 60% or more samples below MDL were excluded from input data. For PCA, all species were kept for the initial run.

Table 3.5 Percentage of the species concentration below MDL

(*Fitting species)

Winter 2006		**Summer 2006**	
Species	Per cent (%)	Species	Per cent (%)
iso-propylbenzene	100	trans-2-butene	100
1-hexene/2-methyl-1-pentene	100	iso-propylbenzene	68.9
1-pentene	100	1-hexene/2-methyl-1-pent	66.7
trans-2-butene	100	1,3-diethylbenzene	48.9
1,3-diethylbenzene	100	1-pentene	24.4
2,2-dimethylbutane*	89.4	cis-2-butene	22.2
1,4-diethylbenzene	74.5	styrene	8.9
cis-2-butene	31.9	1,4-diethylbenzene	6.7
styrene	23.4		
cis-2-pentene	14.9		
1,2,3-trimethylbenzene	4.3		
1-butene	2.1		
n-propylbenzene	2.1		
trans-2-pentene	2.1		
isoprene*	17		

3.2 Receptor Model Simulation

The receptor models source apportionment in this study was based on some assumptions. They are:

1) The measurements obtained at each of the 49 sites in winter and summer 2006, and 51 sites in winter and summer 2005 represented the VOCs levels in city of Windsor, respectively. This is because the sampling sites were set up all over the Windsor city.
2) The chemical composition of species at receptor sites reflected the emission source composition.

3) The species markers for every potential source were included in the measurements. For CMB, the species markers account for a large proportion of the profile, this assumption makes sure the calculation is correct. For PMF/PCA, the high percentage/loadings of species markers help to identify the potential source.

3.2.1 CMB Source Apportionment

The concentrations measured at receptor sites, uncertainties of the concentration, and the source profiles are required as inputs for CMB. The uncertainty for the CMB was assumed to be 15% of the concentration of each species following CMB protocol (Watson et al., 2004), because there were no measured errors provided for this study. CMB is sensitive to uncertainty because CMB uses effective variance weighted least squares solutions. The solution gives greater influence to the species with lower uncertainties in both source contributions and calculated concentration than to the ones with higher uncertainties. Thus, the measured uncertainties for species were preferred. However, 15% of the concentration was used due to the lack of measured errors in this study.

The ten source profiles compiled in Templer (2007) were used as CMB input in this study. This study assumed that those ten sources were the only VOC emitters in Windsor, and any pollutants measured at receptor sites were emitted from one or more of the ten sources. The species markers for every source were included in the measurements. The outputs include the source contribution estimates ($\mu g/m^3$), indicating how much each source contributes to the ambient VOCs concentration. The performance measures at

each sampling site were also provided. Table 3.6 lists the model inputs and outputs for CMB.

Table 3.6 Inputs and outputs for CMB

Inputs	**Outputs**
Ambient concentration Dimension: winter 56 species × 48 sampling sites; summer 56 species×46 sampling sites	Source contribution estimates from each source at each site (winter 10 sources×48 sites; summer 10 sources×46 sites)
10 source profiles	Contribution of the species at each site Calculated total concentrations at each site
Uncertainty of ambient concentration: 15% of the concentration	Performance measures: % Mass at each site Chi-Square t-Statistic R-Square

Any negative contributions were replaced with “zero”, resulting in the corresponding amount of total calculated concentration increase for samples. On average, the model overestimated the concentrations in winter with 5.4%, whereas in summer with 31.2% year 2006. In year 2005, CMB model underestimated the concentration with 2.8%; while overestimated in summer with 16.7%.This could influence the season trends of source contributions. Thus, each of the source contribution estimate values for winter and summer in both years were scaled to the measured values. The contribution from each source in the sample was assumed as overestimated in the same level, and scaled back with the same percentage. The scaling was done for each receptor site, year and season by following the equation (4) as:

$$\text{Scaled concentration} = \text{Calculated concentration} \times \frac{\text{total measured concentration of sample}}{\text{total calculated concentration of sample}} \quad (4)$$

In order to study the contribution from the vehicle-related sources, the sum of source estimate contribution of Diesel Exhaust, Gasoline Exhaust, Liquid Gasoline, and Gasoline Vapour were named as “All vehicles”. The percentage of the contribution of each source including the All-Vehicle among all ten sources was computed for both seasons of year 2005 and 2006.

The averages, medians, standard deviation, and the coefficient of variation of the source contribution from each of the ten sources in four seasons were computed, respectively. The percentage of the source contribution of each source among the site concentrations was calculated for both seasons of year 2005 and 2006.

3.2.2 PMF Source Apportionment

PMF assumes non-negative source compositions and contributions. PMF model requires species concentration and the uncertainties as input data, and provides factor contributions and the factor profiles as the outputs. It is suggested by PMF manual that the species with 60% or more samples having concentration below MDL need to be excluded from the input dataset (Norris and Vedantham, 2008). This is because species with large portion of concentrations below MDL could affect apportionment of other species because PMF model needs to take the species with below MDL concentrations into considerations. Thus, model will not likely to provide the species with large amount

of unreliable concentrations with reasonable results. Among the 55 PAMS species, seven and three species (Table 3.5) had 60% or more samples with concentrations below MDL in winter and summer, respectively. Among the seven species in winter, 2,2-dimethylbutane is a fitting species. It was kept for model simulation to be consistent with CMB model inputs. The other six species were excluded. The three species in summer were all excluded.

The equation-based uncertainty file included species names, MDL and the uncertainty. The uncertainty 15% of concentration when the concentration is greater than the MDL; whereas the uncertainty is 5/6 MDL when the concentration is less or equal than the MDL. The equation was described as:

Uncertainty= 5/6 ×MDL, if concentration≤ MDL;

Uncertainty=$\sqrt{(\text{uncertianty percent} \times \text{concentration})^2 + (\text{MDL})^2}$,

if concentration>MDL (5)

The concentration and the uncertainty were put into the PMF model for the input data analysis. Species with noticeable step changes or extreme events were checked on the concentration time series. The noticeable step changes indicate the changes of sampling or analytical methods. As the sampling in winter and summer took place three months apart, there was little chance for sampling or analytical methods dramatic changes to happen. There were five extreme events. However, they were kept because they reflect the real concentration spatial patterns. All samples were kept for model

simulations for both winter and summer 2006.

Model was run with the concentration of 50 species and 53 species and their uncertainties for winter and summer, respectively. Model simulation set-up is listed in Table 3.7.

Table 3.7 PMF model inputs and outputs of year 2006

Items	**Set-up**
Inputs	1) Species concentration data in winter(50 species×47 sites) and summer (53 species×45 sites)2006, separate runs 2) Equation-based uncertainties
Runs (number)	20
Factors (number)	13
Seed (Random/fixed number)	Fixed: 25
Extra modeling uncertainty (Up to 25% beyond 15% of concentration)	Did not apply
Species characteristics (Strong, Weak or Bad)	Strong
Outputs	1) Factor profiles 2) Factor loadings 3) Diagnostics 4) Residuals 5) Observed and predicted plots 6) Aggregate contribution 7) G-space plots

The default value of the number of runs is 20. The number of factors for PMF was specified as 13 because PMF was expected to identify three sources in addition to the ten sources used in CMB. By defining the number of runs as 13, it was assumed that there

were 13 potential sources in Windsor. However, if this model set up changes, the results could be different from the ones derived from 13 sources. Fixed seed 25 was used as suggested in the PMF demo to ensure the outputs from two separate runs are exactly the same. The extra modeling uncertainty could be introduced to add the same percentage uncertainty to all species beyond the provided uncertainties in inputs when the runs are not stable. It was not used in this study because the initial solution was stable. For the initial run, all species' characteristics were left as strong. The model performance in terms of species reproduction is shown the diagnostics.

3.2.3 PCA Source Apportionment

PCA with Varimax rotation was conducted by using Matlab 2013 (Mathworks, Inc., 2014) for both winter and summer 2006. There were 20 principal components requested, because PCA was expected to explore additional factors other than the ten sources prepared for CMB. Any components provided by PCA with eigenvalue equal or greater than one were retained for the varimax rotation, in order to keep as many principal components as possible. The inputs and outputs are listed in Table 3.8.

Table 3.8 Inputs and Output of PCA

	Winter	**Summer**
Input	Concentration matrix of winter 2006 with 51 species Dimension: 51 species×48sites	Concentration matrix of summer 2006 with 52 species dimension: 52 species×46 sites
Output	Loading matrix with coefficients dimension: 20 Components×56 species	Loading matrix with coefficients dimension: 20 Components×56 species
	Principal Component score dimension: 20 Components×56 species	Principal Component score dimension: 20 Components×56 species
	Latent i.e., the eigenvalues dimension: 1×20 Components	Same as winter
	Percentage of variance explained by each Component dimension: 1×20 Components	Same as winter

Among the components with eigenvalue greater than one, there were only 14, and 15 compounds with absolute factor loadings greater than 0.1 in any of the components in winter and summer, respectively. More components with eigenvalues greater than one with more than one high loadings species were expected to show up. Thus, the data was transformed by using the Z score function. The data matrix was normalized by using mean and standard deviation of each column of the matrix (Mathworks, 2014). The mean and the standard deviation used to calculate the Z score for each species are based on the values from all sampling sites. The individual Z score is different from each site.

In winter, there were 4 non-fitting species including 1,3-diethylbenzene, 1,4-diethylbenzene, iso-propylbenzene, and others that did not have loadings greater than 0.25 in any components. Among these four compounds, 1,3-diethylbenzene, 1,4-diethylbenzene, iso-propylbenzene were with a large percentage of concentration below

MDL, 100%, 74%, and 100%, respectively as shown in Table 3.5. Thus, they were excluded from the inputs as they may not help to explain the variance of the dataset. In summer, there were six non-fitting species including 1,3-diethylbenzene, 1,4-diethylbenzene, 1-butene, ethylene, iso-propylbenzene, trans-2-butene with loadings less than 0.25 in any components. However, ethylene is the species marker for Diesel Exhaust in the source profiles used in CMB, thus, it was kept. Among the other five species, the percentage of the below MDL concentration of iso-propylbenzene, and trans-2-butene was 68.9% and 66.7%, respectively as shown in Table 3.5. The five non-fitting species with the exception of ethylene were excluded from the summer 2006 input to PCA.

3.3 Factor/Component Interpretations

PMF and PCA provide factors and components as source profiles, respectively. Factors consist of the mass percentage of the species. Components are a linear combination of variables with loadings and scores on the components (Mathworks, 2014). As the profiles given by the two models are in two different forms, it is beneficial to summarize the interpretation approaches for them individually.

3.3.1 PMF Factor Interpretations

According to study by Harley and Kean (2004) in Chapter 2, the vehicle-related sources could be differentiated by the proportion of different species classes including n-alkanes, isoalkanes, cycloalkanes, alkenes, aromatics, oxygenates, carbonyls, and

unidentified species in the profiles. Among the eight classes, oxygenates, carbonyls, and unidentified species were not included in this study. In this study, there is an species class: isoprene. Thus, the species were classified into six species classes, and the sum concentrations of each class were calculated. Table 3.9 lists the species in each class.

Table 3.9 The species classification of six classes

aromatics	**isoalkanes**	**n-alkanes**
toluene	isopentane	butane
benzene	isobutane	decane
1,2,4-trimethylbenzene	2-methylpentane	ethane
3-ethyltoluene	3-methylpentane	heptane
m and p-xylene	2,2,4-trimethylpentane	hexane
1,3,5-trimethylbenzene	3-methylhexane	nonane
2-methylhexane	2,3,4-trimethylpentane	octane
4-ethyltoluene	2,3-dimethylbutane	pentane
2-ethyltoluene	3-methylheptane	propane
1,2,3-trimethylbenzene	2-methylheptane	trans-2-butene
n-propylbenzene	2,3-dimethylpentane	undecane
o-xylene	2,2-dimethylbutane	
ethylbenzene	2,4-dimethylpentane	
styrene		
1,4-diethylbenzene		
1,3-diethylbenzene		
iso-propylbenzene		

Table 3.9-continued

alkene	**cycloalkane**	**isoprene**
ethylene	methylcyclohexane	isoprene
propylene	cyclopentane	
1-butene	cyclohexane	
trans-2-pentene	methylcyclopentane	
cis-2-butene		
cis-2-pentene		
1-pentene		
1-hexene/2-methyl-1-pentene		
trans-2-butene		

Based on the literature review, a flow chart for PMF source identification was created to identify sources, these steps were followed: 1) Group species into n-alkanes, isoalkanes, aromatics, cycloalkanes, alkenes, isoprene, and acetylene category. The species in each class has been listed in Table 3.9. 2) Adding up the percentage of the species in each species class. The identification procedures are compiled in the flow chart. Figure 3.2 and Figure 3.3 show the identification procedures of sources from PMF. The component with highest absolute loading of ethane among the factors was identified as Commercial Natural Gas. The component with highest absolute loading of isoprene among the factors was identified as Biogenic Emission.

It should be noted that the identification procedure has not been tested with the published paper to verify if it applies to the source profiles. There could be large uncertainties of the identification results.

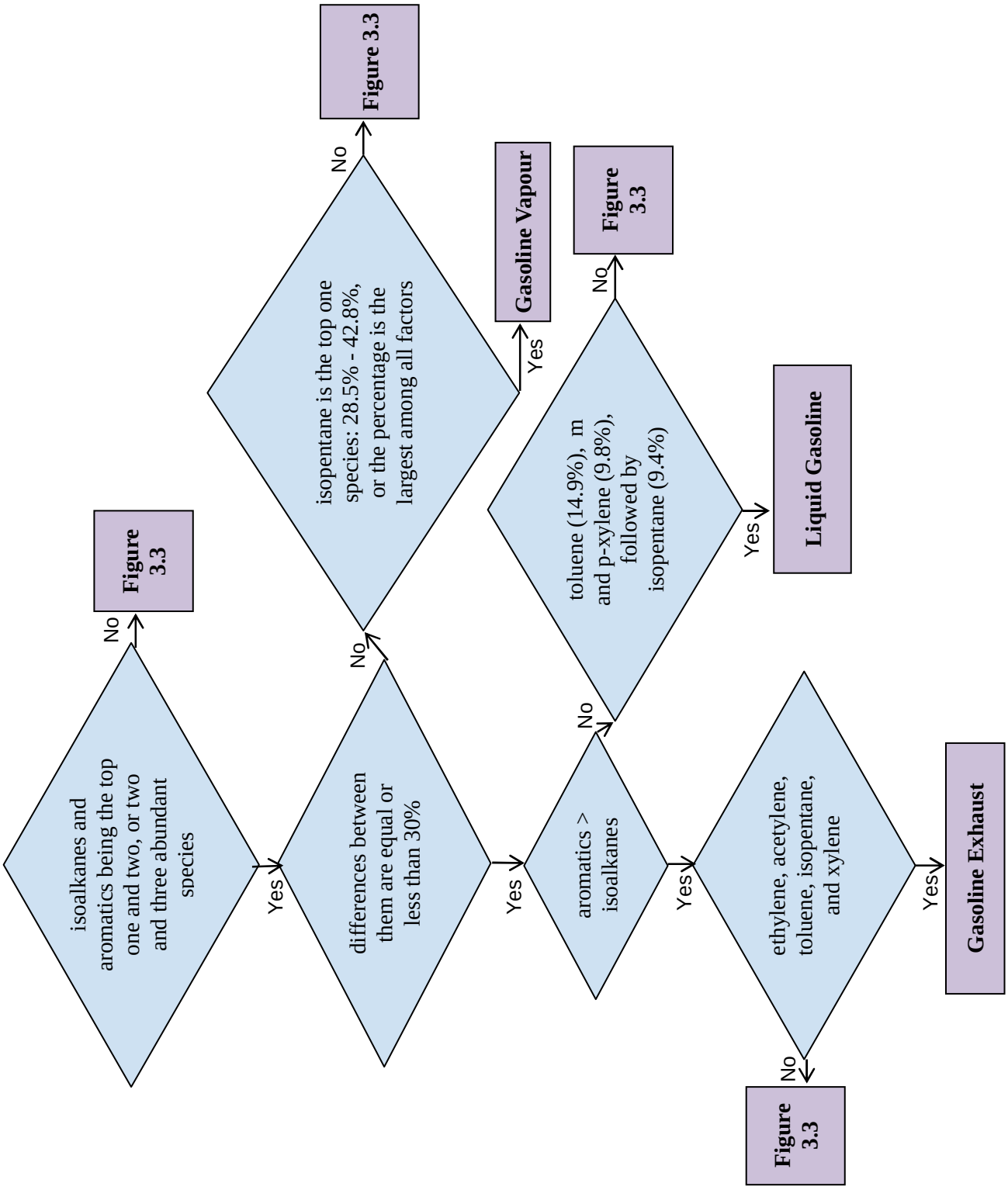

Figure 3.2 Gasoline-related sources from PMF identification procedures

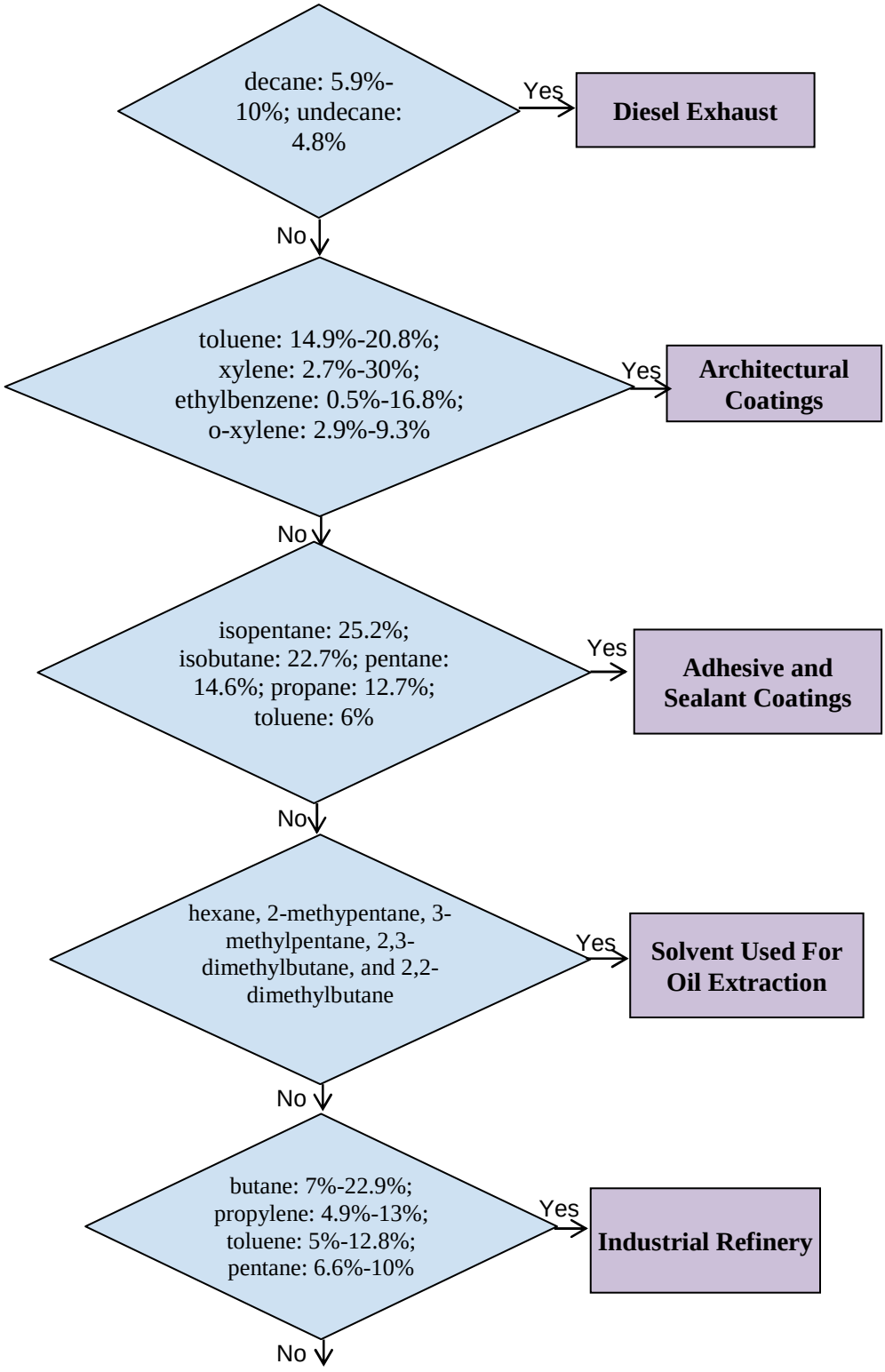

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Figure 3.3 Sources other than gasoline-related sources from PMF interpretation procedures

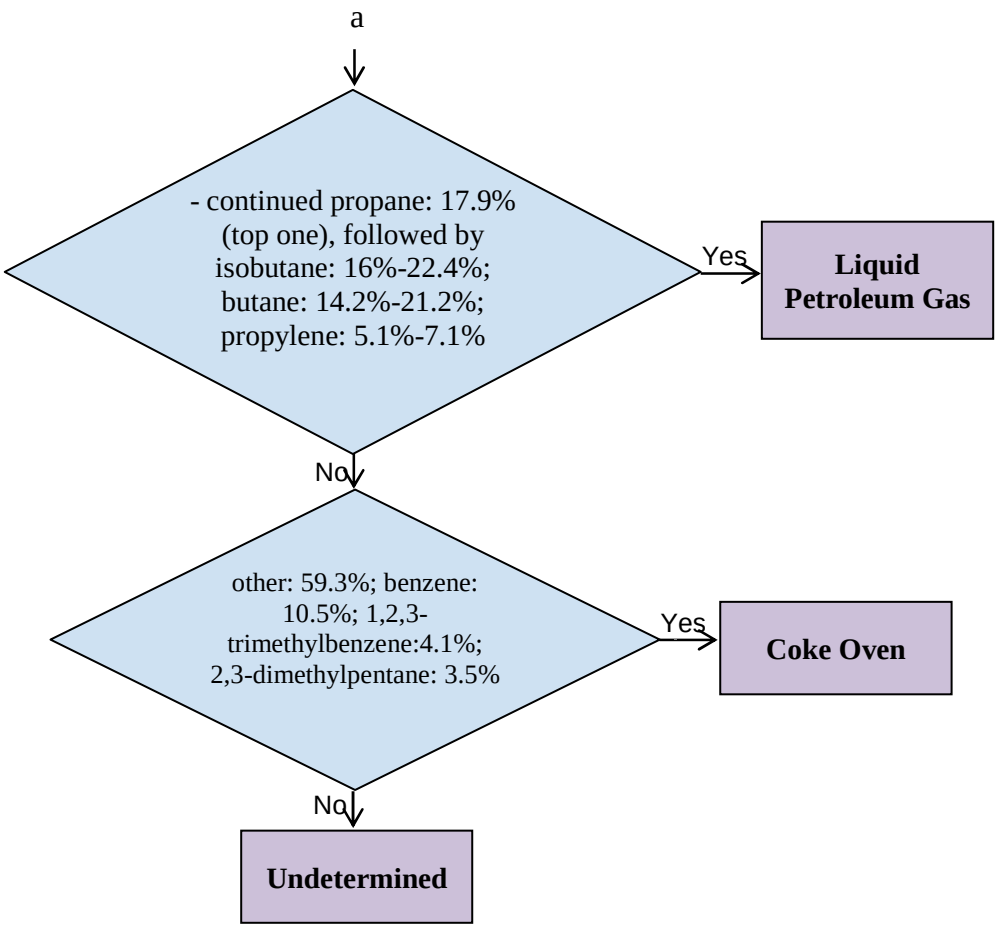

Figure 3.3 - continued

Gasoline Exhaust consists mostly of aromatics (31.0%), followed by 26.3% iso-alkanes. Species including ethylene, toluene, and isopentane were the species markers of Gasoline Exhaust (Wang et al., 2013; Templer, 2007; Yuan et al., 2009; Song, et al., 2007). Thus, if the percentage of the total isoalkanes and aromatics is the highest, and the aromatics account for larger proportion than isoalkanes; meanwhile, ethylene, acetylene, toluene, xylene, and isopentane accounted for big proportion, it indicates that the source could be Gasoline Exhaust. Isoalkanes and aromatics could be the second and the third places if they are not the most abundant two species classes in any profiles.

Liquid Gasoline consists mostly of 33.8% iso-alkanes and 30.4% aromatics (Harley and Kean, 2004). Therefore, if the percentage of the total isoalkanes outweighs aromatics do, and the aromatics account for higher proportion, the source could be Liquid Gasoline.

In Gasoline Vapour profile, iso-alkanes account for 54.2% of the profile (Harley and Kean, 2004). Isopentane is a specie marker for Gasoline Vapour (Morino et al., 2011; Templer, 2007). If the percentage of isoalkanes is the top one abundant species with 28.5% to 42.8%, this profile could be Gasoline Vapour (Harley and Kean, 2004). If there is no profile with isoalkanes as top one species class, the profile with the highest percentage of isopentane among all profiles could be Gasoline Vapour as well.

The Diesel Exhaust profile consists of large proportion of undecane (Templer, 2007) and decane (Yuan et. al, 2009; Song, et al., 2007). Thus, if a profile contains large proportion of undecane and n-decane, the source could be Diesel Exhaust. If there is no profile containing decane or undecane with percentage 6% or more, the profile with the

highest percentage of either of them could be Diesel Exhaust as well.

According to Lambourne and Strivens (1999), toluene, styrene, and xylene are the species markers for the Architectural Coatings. The studies of Cai et al. (2010), Yuan et al. (2009), and Song et al. (2007), and Templer (2007) indicated that toluene and xylene accounted for 10% to 25%, and 17% to 30%, respectively. Templer (2007) indicated that toluene and xylene are two most abundant species in Architectural Coatings profile. Study of Song et al. (2008), Yuan et al. (2009), and Templer (2007) indicated that propane is the most abundant species in Liquid Petroleum Gas profile, followed by species including n&iso-butane and propylene.

According to Wypych (2000), the common PAMS VOC composition of Adhesive and Sealant Coatings is hexane, heptane, xylene, benzene, and toluene. The study of Lam et al. (2013) indicated that Adhesive and Sealant Coatings consists of 25.2% of isopentane, 22.7% of isobutene, 14.6% of pentane, 12.7% of propane, and 6% of toluene. Thus, those species are the species markers for Adhesive and Sealant Coatings.

According to the report from Government of Canada (2009), hexane is widely use in a variety of products as a extraction solvent in food processing, and as solvent-carrier in adhesives, sealants, binders, fillers, lubricants, various formulation components, fuel components, laboratory reagent and solvent. According to the National Pollutant Release Inventory and Air Pollutant Emission Summaries and Trends Datasets (2006) reported by Environment Canada, n-hexane is the speciated chemical of facility ADM Agri-Industries-ADM Windsor, categorized as Grain and Oilseed Milling sector. In Windsor, hexane and its isomers, 2-methypentane, 3-methylpentane, 2,3-dimethylbutane, and 2,2-

dimethylbutane are the only pollutants of this facility. ADM Agri-Industries-ADM Windsor is the only facility emitting hexane. Few studies including source profiles with n-hexane being the top one species were found. Therefore, the source profile of Solvent Used for Oil Seed Extraction consists of hexane and its isomers, 2-methypentane, 3-methylpentane, 2,3-dimethylbutane, and 2,2-dimethylbutane.

In Industrial Refinery profiles, the percentage of and butane could be 7% to 22.9% (Cai et et al., 2010; Templer, 2007). The study of Cai et et al. (2010), Song et al. (2008) indicated that propylene accounted 4.9% to 13% of the profile. Toluene accounts for 5% to 12.8% in Industrial Refinery profiles according to studies of (Cai et et al. (2010); Chan et. al. (2011), and Song et al. (2008). The studies of Cai et et al. (2010), Chan et. al. (2011), and Templer (2007) indicated that pentane accounts for 6.6% to 10% of Industrial Refinery profiles. Coke Oven profile consists of abundant benzene, toluene, xylenes, ethane, ethylene, propylene, butene, acetylene (US EPA, 2013; U.S. Government, 2011) and 1,2,4-trimethylbenzene (US EPA, 1994). The presence of 35% to 69% of ethane, followed by up to 10% of other species including propane, acetylene and aromatics indicates that the source being Commercial Natural Gas (Song et al., 2008; Templer, 2007). Biogenic VOCs emissions are released from trees and shrubs. They consist of isoprene and monoterpenes such as α-pinene and β-pinene, commonly found in forested areas (Lewandowski et al., 2013).

The sources with the same names identified from winter and summer were compared to see the commonalities and differences of their chemical compositions. The sources were expected to be similar because the main industries, streets, and facilities in Windsor did not have major changes from winter to summer. However, there could be slight differences between the chemical compositions of factor profiles in winter and summer as the volatility and reactivity of different VOCs vary at different levels when temperature changes.

For all sources identified from winter and summer factor profiles, the same sources were placed next to each other, and the species accounted for 6% or more in each source in winter and summer were listed in descending orders. The species and their percentage were compared to see the similarities and the variations.

3.3.2 PCA Factor Interpretations

Based on the profiles interpretations in studies of Chang et al. (2009), Duan et al. (2008), Huang et al. (2012), Wang et al. (2006), and Lai et al. (2013), Solvent has high loading of m, p-xylenes, o-xylene, ethylbenzene, trimethylbenzenes, toluene, and hexane. Study of Lambourne and Strivens (1999) indicated that toluene, styrene, and xylene are the main content of solvent used for Architectural Coatings. Thus, toluene, styrene, and xylene have high loadings in Architectural Coatings.

According to Wypych (2000), Adhesive and Sealant Coatings are rich on aromatics including toluene, benzene, and xylene; and aliphatic hydrocarbon including hexane, heptane. Thus, toluene, benzene, xylene, hexane and heptane have high loadings

in Adhesive and Sealant Coatings profile. Auto Paints has high loadings of aromatics species including n-ethyltoluene, benzene, toluene, ethylbenzene, xylene, propylbenzene (Huang et al., 2012).

Industrial Refinery has high loadings of alkenes including 1-butene (Guo et al., 2007; Huang et al., 2012), cis/trans-butene (Huang et al., 2012), propylene (Chang et al., 2009; Guo et al., 2007; Huang et al., 2012), and ethylene (Guo et al., 2006). Species including propane (Guo et al., 2006), ethane (Chang et al., 2009), heptane (Huang et al., 2012) and toluene (Chang et al., 2009; Guo et al., 2006), benzene (Chang et al., 2009; Guo et al., 2006), and styrene (Chang et al., 2009) could also have high loadings in Industrial Refinery profile.

The loading of propane, n&iso-butane is the highest on Liquid Petroleum Gas. Ethylene, n&iso-pentane, and aromatics also have high loadings in Liquid Petroleum Gas profile (Guo et al., 2006; Chang et al., 2009). Species 2,2,4-trimethylpentane, iso-butane, and n-pentane, 2,3-dimethylbutane, n-heptane, 1-butene, propylene (Lai et al., 2013;), ethylene, benzene (Lai et al., 2013; Song et al., 2008; Templer, 2007; Wang et al., 2013), and 2-methylpentane (Yuan et al., 2009; Lai et al., 2013) were loading high on Gasoline Exhaust.

Diesel Exhaust has high loadings on propylene, styrene (Lam et al., 2013), benzene (Lam et al., 2013; Yuan et al., 2009), followed by 2-methylpentane, toluene (Lam et al., 2013; Yuan et al. (2009), m and p-xylene (Lai et al., 2013; Yuan et al., 2009), ethane, 1-butene, n-propane (Lai et al., 2013; Lam et al., 2013; Yuan et al., 2009), acetylene (Lai et al., 2013; Lam et al., 2013; Song, et al., 2007), and 2,2,4-

trimethylpentane (Lai et al., 2013; Yuan et al., 2009). According to studies Guo et al. (2007) and Wang et al. (2006), profiles of Gasoline evaporation including Liquid Gasoline and Gasoline Vapour have high loadings of n&iso-pentane, and toluene. Biogenic Emission contains high loadings of isoprene (Templer, 2007; Lewandowski et al., 2013). The identification procedures of PCA are shown in Figure 3.4. The Italic font in the Figure stands for the species with high loadings in components. The component with highest absolute loading of ethane among the factors was identified as Commercial Natural Gas. The component with highest absolute loading of isoprene among the factors was identified as Biogenic Emission. The component with highest absolute loading of propane among the factors was identified as Liquid Petroleum Gas.

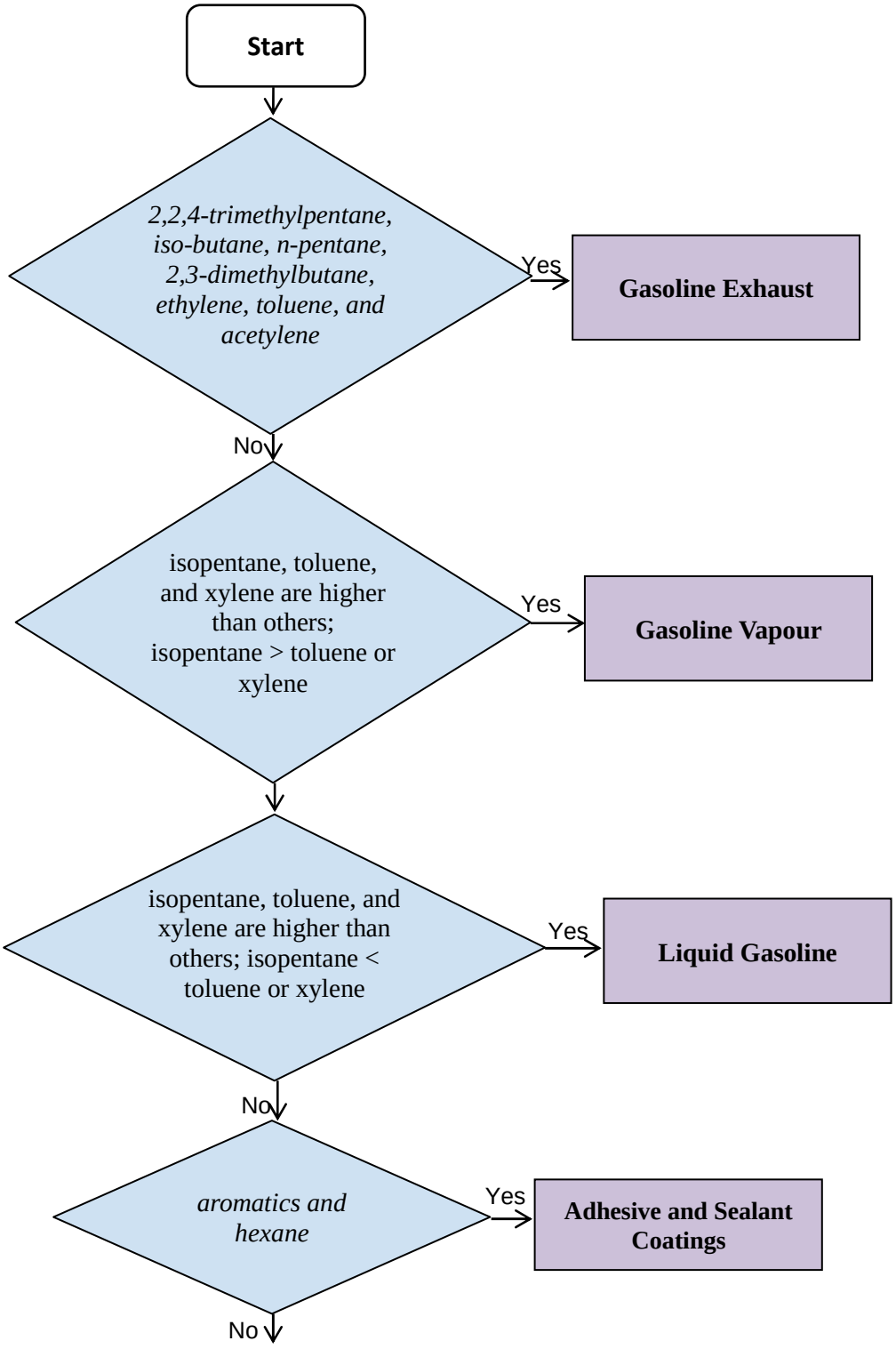

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Figure 3.4 PCA sources identification procedures

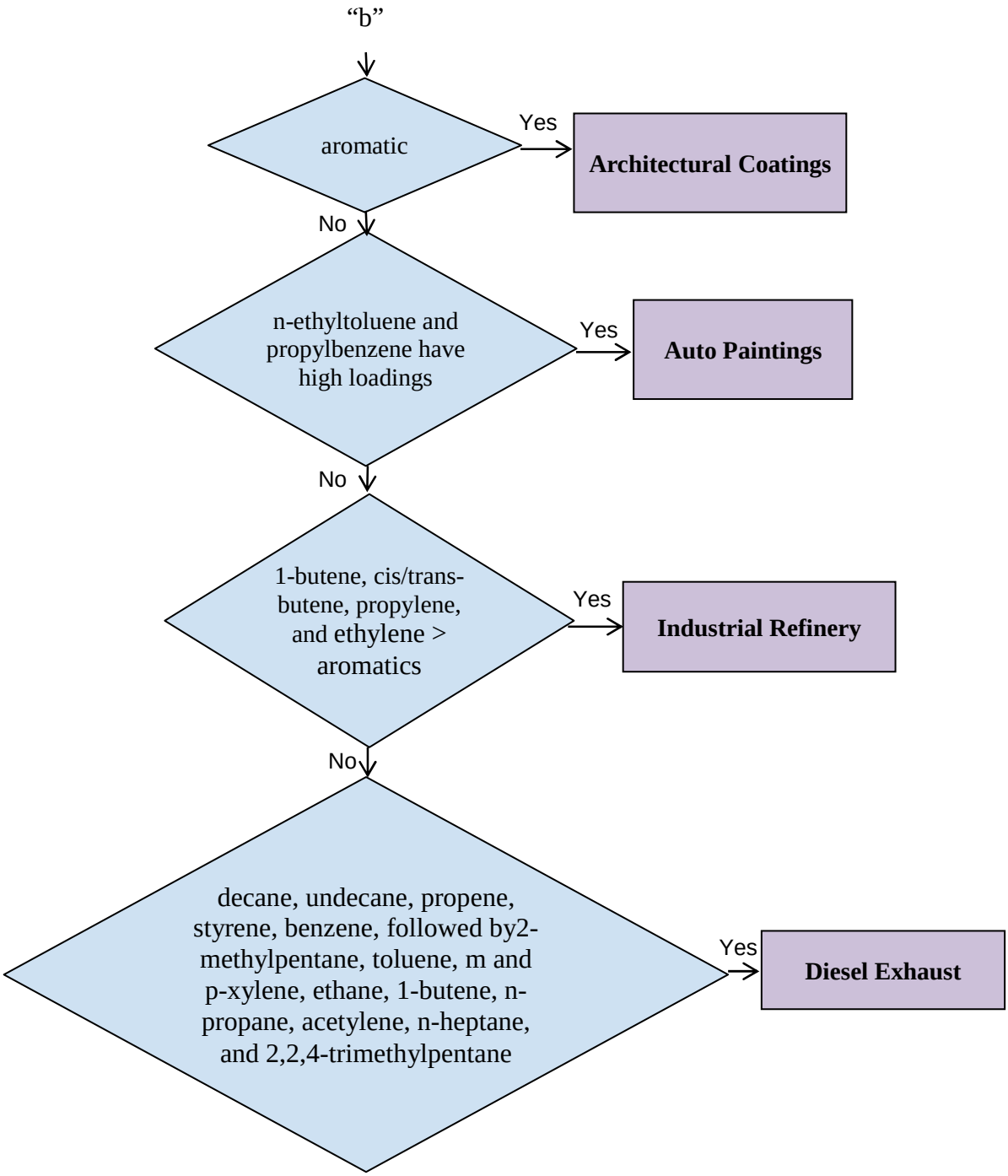


Figure 3.4 - continued

The sources with the same names identified from winter and summer, were placed next to each other, and compared to see the commonalities and differences of their profiles. Although many previous studies chose 0.5 as the loading cut off for source identification; however, species with loadings equal or greater than 0.26 in one or more components were used for source identification in this study. This was to keep four or more species for source identification. The species with loading equal or greater than 0.26 in each component were ranked in descending orders. The species and their corresponding loadings were compared.

Compare with the identification procedure of PMF, PCA relies more on the species markers of each source because only the loadings of the species were provided as outputs. PCA finds the components explaining the variance of the majority of the measurements.

3.3.3 Procedures of Comparison of CMB, PMF, and PCA Results

The sources of PMF and PCA were compared with the ten sources prepared for CMB, respectively in the same season and both seasons. The identified factors from PMF and components from PCA were compared mutually by season and both seasons to see if there were any commonalities and differences. Table 3.10 lists the detailed comparison procedures.

Table 3.10 Procedures of comparison among sources of CMB, PMF, and PCA

Table generation	• Listing the sources of PMF as the number of them was the largest that of all three models, the contribution from each source by concentration and mass percentage, and the total model calculated contribution. • Placing the sources of CMB next to the same ones from PMF, leave the units blank if any sources only belonged to PMF but not to CMB. • Placing the sources from PCA next to the same sources from CMB or PMF or both, leave the units blank if any sources do not belong to any of CMB or PMF. • Summarizing the common sources of all three models in each season.
PMF vs. CMB	• To see if all the ten sources prepared for CMB were included in PMF for each season, if not, explain the potential reasons behind it. • Checking out the major sources from PMF based on the source contribution in each season; compare them with that of CMB to see the commonalities and the differences. • To see if there are additional sources other than the ten for CMB. • To see if there is any commonalities in two seasons.
PCA vs. CMB	• To see if all the ten sources prepared for CMB were included in PCA for each season, if not, explain the potential reasons behind it. • To see if there are additional sources other than the ten for CMB. • To see if there is any commonality in two seasons.
PMF vs. PCA	• Summarizing the common sources of the two models in each season. • Comparing the sources in addition to that of CMB of two models in each season, to see if there is any commonality. • To see if there is any commonality in both seasons. • Analyzing the advantages and disadvantages of PMF and PCA.

3.4 Spatial Trends of Source Contribution by CMB

In order to study the spatial distribution of the source contribution from different emission sources in winter and summer 2006, ArcGIS 10.1 (ESRI Canada, 2014) was applied to generate the concentration maps. Inverse Distance Squared Weighted Interpolation method was applied to generate the maps. Inverse Distance Weighted uses the measured values surrounding the prediction location to predict the locations without

measurements. The measurements take place closest to the prediction location give more influence on the prediction than those further away. The input data includes coordinates of each measurement location, and the corresponding concentrations.

Table 3.11 ArcGIS inputs

Inputs
The coordinates of sites and CMB source contributions in winter and summer 2005 and 2006 The map of every source was generated separately
Method: Inverse Distance Weight Interpolation
Power (The higher the power is, the lower the measurements in distance would have on the predicted locations): 2 (Default)
Neighborhood (How many measurements in surroundings are considered in prediction of the unmeasured locations): Maximum 15; Minimum 10
Windsor mainland shapefile
Essex streets shapefile of

The total measured concentration at site; total CMB modeled source contributions (Without scaling) were plotted. Those sources are All Vehicle, Commercial Natural Gas, Industrial Refinery, and Architectural Coatings in winter and summer 2005 and 2006. CMB source contributions of Liquid Petroleum Gas in winter 2005 and 2006, and Biogenic Emissions in summer 2005 and 2006 were also plotted. In total, there were 24 maps of spatial distribution of contributions from different sources in two seasons of both 2005 and 2006. Table 3.11 shows the inputs of ArcGIS.

There were similarities among the maps of different sources observed in each of the four seasons. The similarities could be due to the correlations among the sources. In order to study the correlations among different sources in the same season, correlation matrices of the contribution from different sources were generated by using Minitab 16 software (Minitab, 2010). The absolute values of correlation coefficient equal or greater than 0.8 and less or equal to 1 indicate a strong relationship between the two variables; greater than 0.5 and less than 0.8 indicate a moderate relationship between the two variables; and less or equal to 0.5 and equal or greater than zero indicate a weak relationship between the two variables. The total measured VOC and the source contributions results of All Vehicle and all the ten sources obtained from CMB were used for computing the internal relationships among each pair of them.

CHAPTER 4

RESULTS AND DISCUSSIONS

4.1 Ambient Concentration Analysis

The mean concentration of the 56 VOCs and the total NMHC VOC concentrations and 56 VOCs (55 PAMS species and other) in winter and summer of year 2005 and 2006 are shown in Table 4.1. The ratio of winter and summer concentration in each of the two years, in the same season but different years, and the concentration ratio of year 2006 and 2005 in same season are listed in Table 4.2.

Table 4.1 The mean concentration of the species of all sampling sites in winter and summer of year 2005 and 2006 (*fitting species)

Species		MDL ($\mu g/m^3$)	Winter 2005 ($\mu g/m^3$)	Summer 2005 ($\mu g/m^3$)	Annual 2005 ($\mu g/m^3$)	Winter 2006 ($\mu g/m^3$)	summer 2006 ($\mu g/m^3$)	Annual 2006 ($\mu g/m^3$)
1,2,3-trimethylbenzene		0.04	0.05	0.24	0.15	0.07	0.18	0.12
1,2,4-trimethylbenzene		0.06	0.25	1.25	0.75	0.32	0.84	0.58
1,3,5-trimethylbenzene		0.04	0.08	0.38	0.23	0.09	0.22	0.16
1,3-diethylbenzene		0.04	0.02 (<MDL)	0.04	0.03	0.04	0.04	0.04
2011,4-diethylbenzene		0.08	0.06 (<MDL)	0.13	0.10	0.08	0.14	0.11
1-butene		0.15	0.30	0.29	0.30	0.24	0.30	0.27
1-hexene/2-methyl-1-pent		0.08	0.05 (<MDL)	0.06 (<MDL)	0.06	0.08	0.08	0.08
1-pentene		0.06	0.04 (<MDL)	0.07	0.06	0.06	0.08	0.07
2,2,4-trimethylpentane	*	0.04	0.26	0.31	0.29	0.17	0.25	0.21
2,2-dimethylbutane	*	0.07	0.07	0.12	0.10	0.07	0.15	0.11
2,3,4-trimethylpentane	*	0.02	0.10	0.10	0.10	0.06	0.09	0.07
2,3-dimethylbutane	*	0.01	0.12	0.22	0.17	0.09	0.24	0.17
2,3-dimethylpentane	*	0.04	0.15	0.22	0.19	0.10	0.16	0.13
2,4-dimethylpentane	*	0.02	0.07	0.10	0.09	0.05	0.09	0.07
2-ethyltoluene		0.04	0.07	0.30	0.19	0.08	0.19	0.14
isopentane	*	0.06	2.49	4.51	3.50	1.99	4.17	3.08
2-methylheptane	*	0.03	0.09	0.11	0.10	0.06	0.13	0.10
2-methylhexane	*	0.02	0.31	0.46	0.39	0.23	0.36	0.29
2-methylpentane	*	0.05	0.64	1.06	0.85	0.49	1.26	0.87
3-ethyltoluene		0.03	0.18	0.73	0.46	0.19	0.46	0.32
3-methylheptane	*	0.02	0.09	0.16	0.13	0.07	0.12	0.09
3-methylhexane	*	0.04	0.33	0.51	0.42	0.24	0.42	0.33
3-methylpentane	*	0.06	0.54	0.82	0.68	0.44	0.86	0.65

Table 4.1 - continued

4-ethyltoluene		0.02	0.09	0.36	0.23	0.09	0.23	0.16
acetylene	*	0.00	2.09	0.71	1.40	1.18	0.54	0.86
benzene	*	0.04	1.04	0.86	0.95	0.85	0.80	0.82
butane	*	0.18	4.39	3.28	3.84	3.69	2.31	3.00
cis-2-butene		0.04	0.06	0.07	0.07	0.05	0.06	0.05
cis-2-pentene		0.01	0.03	0.06	0.05	0.02	0.05	0.04
cyclohexane	*	0.02	0.09	0.11	0.10	0.07	0.13	0.10
cyclopentane	*	0.02	0.11	0.23	0.17	0.09	0.28	0.18
decane	*	0.02	0.11	0.55	0.33	0.11	0.34	0.23
ethane	*	0.00	8.20	3.72	5.96	4.47	3.24	3.85
ethylbenzene		0.04	3.19	1.46	2.33	0.37	0.74	0.55
ethylene		0.00	0.42	0.75	0.59	1.68	1.19	1.44
heptane	*	0.09	0.24	0.32	0.28	0.18	0.34	0.26
hexane	*	0.07	1.10	0.91	1.01	0.64	1.00	0.82
isobutane	*	0.11	1.53	1.34	1.44	1.26	1.34	1.30
isoprene	*	0.02	0.04	0.59	0.32	0.03	0.64	0.34
iso-propylbenzene		0.04	0.02 (<MDL)	0.05	0.04	0.04	0.04	0.04
m and p-xylene		0.07	1.10	2.17	1.64	1.08	2.18	1.63
methylcyclohexane	*	0.02	0.09	0.12	0.11	0.07	0.13	0.10
methylcyclopentane	*	0.02	0.29	0.35	0.32	0.18	0.38	0.28
nonane	*	0.02	0.09	0.19	0.14	0.08	0.17	0.12
n-propylbenzene		0.04	0.07	0.24	0.16	0.07	0.16	0.12
octane	*	0.04	0.12	0.26	0.19	0.09	0.16	0.12
o-xylene		0.04	0.35	0.70	0.53	0.32	0.67	0.49
pentane	*	0.06	1.38	2.77	2.08	1.31	2.83	2.07
propane	*	0.16	4.03	3.97	4.00	3.29	3.59	3.44
propylene		0.09	0.56	0.52	0.54	0.46	0.47	0.46
styrene		0.04	0.05	0.07	0.06	0.05	0.06	0.05
trans-2-butene		0.33	0.07 (<MDL)	0.08 (<MDL)	0.08	0.33	0.33	0.33
trans-2-pentene		0.02	0.06	0.14	0.10	0.04	0.12	0.08
toluene	*	0.07	4.31	5.96	5.14	2.67	5.34	4.00
undecane	*	0.03	0.10	0.31	0.21	0.12	0.40	0.26
Total PAMS			34.61	35.25	35.00	24.41	32.24	28.32
other			1.20	2.79	2.00	1.07	3.00	2.04
Total NMHC			35.81	38.04	37.00	25.48	35.24	30.36

Table 4.2 The season and year concentration ratio (*fitting species)

		Winter/Summer Year 2005	Winter/Summer Year 2006	Annual 2006/2005	Winter 2006/2005	Summer 2006/2005
1,2,3-trimethylbenzene		0.2	0.4	0.8	1.4	0.7
1,2,4-trimethylbenzene		0.2	0.4	0.8	1.3	0.7
1,3,5-trimethylbenzene		0.2	0.4	0.7	1.2	0.6
1,3-diethylbenzene		0.5	0.9	1.3	1.8	1.1
1,4-diethylbenzene		0.5	0.6	1.1	1.4	1.1
1-butene		1.0	0.8	0.9	0.8	1.0
1-hexene/2-methyl-1-pent		0.8	0.9	1.4	1.6	1.4
1-pentene		0.6	0.8	1.1	1.5	1.1
2,2,4-trimethylpentane	*	0.8	0.7	0.7	0.6	0.8
2,2-dimethylbutane	*	0.6	0.5	1.1	1.0	1.2
2,3,4-trimethylpentane	*	1.0	0.7	0.7	0.6	0.9
2,3-dimethylbutane	*	0.5	0.4	1.0	0.8	1.1
2,3-dimethylpentane	*	0.7	0.6	0.7	0.7	0.7
2,4-dimethylpentane	*	0.7	0.5	0.8	0.7	0.9
2-ethyltoluene		0.2	0.4	0.7	1.2	0.6
isopentane	*	0.6	0.5	0.9	0.8	0.9
2-methylheptane	*	0.8	0.5	1.0	0.7	1.2
2-methylhexane	*	0.7	0.6	0.8	0.7	0.8
2-methylpentane	*	0.6	0.4	1.0	0.8	1.2
3-ethyltoluene		0.2	0.4	0.7	1.0	0.6
3-methylheptane	*	0.6	0.6	0.7	0.7	0.7
3-methylhexane	*	0.6	0.6	0.8	0.7	0.8
3-methylpentane	*	0.7	0.5	1.0	0.8	1.0
4-ethyltoluene		0.3	0.4	0.7	1.0	0.6
acetylene	*	2.9	2.2	0.6	0.6	0.8

Table 4.2 - continued

benzene	*	1.2	1.1	0.9	0.8	0.9
butane	*	1.3	1.6	0.8	0.8	0.7
cis-2-butene		0.9	0.8	0.7	0.8	0.8
cis-2-pentene		0.5	0.4	0.7	0.7	0.9
cyclohexane	*	0.8	0.6	1.0	0.8	1.2
cyclopentane	*	0.5	0.3	1.1	0.8	1.2
decane	*	0.2	0.3	0.7	1.0	0.6
ethane	*	2.2	1.4	0.6	0.5	0.9
ethylbenzene		2.2	0.5	0.2	0.1	0.5
ethylene		0.6	1.4	2.4	4.0	1.6
heptane	*	0.8	0.5	0.9	0.7	1.1
hexane	*	1.2	0.6	0.8	0.6	1.1
isobutane	*	1.1	0.9	0.9	0.8	1.0
isoprene	*	0.1	0.0	1.1	0.7	1.1
iso-propylbenzene		0.4	1.1	1.0	2.0	0.8
m and p-xylene		0.5	0.5	1.0	1.0	1.0
methylcyclohexane	*	0.8	0.5	0.9	0.8	1.1
methylcyclopentane	*	0.8	0.5	0.9	0.6	1.1
nonane	*	0.5	0.5	0.9	0.9	0.9
n-propylbenzene		0.3	0.4	0.7	1.0	0.7
octane	*	0.5	0.5	0.7	0.7	0.6
o-xylene		0.5	0.5	0.9	0.9	1.0
pentane	*	0.5	0.5	1.0	0.9	1.0
propane	*	1.0	0.9	0.9	0.8	0.9
propylene		1.1	1.0	0.9	0.8	0.9
styrene		0.7	0.8	0.9	1.0	0.9
trans-2-butene		0.9	1.0	4.1	4.7	4.1
trans-2-pentene		0.4	0.4	0.8	0.7	0.8
toluene	*	0.7	0.5	0.8	0.6	0.9
undecane	*	0.3	0.3	1.3	1.2	1.3
total PAMS		1.0	0.8	0.8	0.7	0.9
others		0.4	0.4	1.0	0.9	1.1
total NMHC		0.9	0.7	0.8	0.7	0.9

The annual concentration of PAMS species decreased from 35μg/m^3 in year 2005 to 28.3μg/m^3 in year 2006. Concentration of 112 NMHC declined from 37μg/m^3 to 30.4μg/m^3. Between the two seasons, The averaged ambient VOCs levels averaged among all sites increased from winter to summer with 49 out of 55 PAMS species in year 2005, and 52 out of 55 in year 2006, so did the total NMHC in both years.

Among the species that decreased from winter to summer, acetylene had winter concentrations more than doubled that of the summer; for ethane, the winter/summer ratios was 2.2 and 1.4 in 2005 and 2006, respectively. The concentrations of benzene, butane, and hexane were slightly higher in winter (ratio: 1.2-1.3). These five compounds are all fitting species. Thus, the contributions of sources that have any of the above listed compounds as major species could decrease from winter to summer of both 2005 and 2006. Non-fitting species ethylbenzene decreased from winter to summer (ratio: 2.2) only in year 2005; ethylene (ratio: 1.4) only in year 2006. For annual averaged concentrations of summer and winter, 50 out of 55 PAMS species deceased from year 2005 to 2006, also did total NMHC. The exceptions included non-fitting species 1,3-diethylbenzene, 1-hexene/2-methyl-1-pent, fitting species undecane with 2005/2006 ratio of 1.3-1.4; and non-fitting species ethylene, trans-2-butene with high ratios of 2.4 and 4.1, respectively. All five species increased from 2005 to 2006 for both seasons. The concentration of several species increased in one season but decreased in another. However, their annual concentration still decreased from year 2005 to 2006 (1,2,3-trimethylbenzene, 1,2,4-trimethylbenzene, 1,3,5-trimethylbenzene, 2-ethyltoluene) or didn't change between the two years (2-methylheptane, 2-methylpentane, cyclohexane, cyclopentane, and iso-propylbenzene).

4.2 CMB Source Apportionment Results

4.2.1 Performance Measures

According to the CMB Protocol, the PAMS species should account for 80% or more of the ambient NMHC in urban areas (Watson et al., 2004), to be high enough to represent the total NMHC species. In this study, the range of the percentage of PAMS species among all NMHC species was 82%to 98% in year 2006, and the mean value was 95%. Thus, the concentrations of the 55 PAMS species could represent that of the total NMHC species concentration.

Samples with performance measures out of range are listed as Tables 4.3 and Table 4.4. For winter output, Chi-Square of 13 samples was greater than 4; there were 2 samples with Mass percent greater than 120%; R-square of 3 samples is out of range (0.8-1). For summer output, only one sample was found with Chi-Square greater than 4; all 45 samples were found with mass percent lower than 120%, and higher than 80%.

Table 4.3 Number of performance measures out of range in winter 2006 out of 47 sites

	SCE<0	**Tstat <2**	**Tstat <1.5**	**Tstat <1**
Tu_MchHD	0	0	0	0
Exh_Lin1	0	7	2	0
WA_LIQ	18	47	46	43
WA_VAP	0	0	0	0
CNG	0	0	0	0
LPG	0	5	3	2
Ind_Ref	0	1	0	0
Coke_Ovn	0	1	0	0
Arc_Coat	0	17	3	1
Biogenic	0	29	3	1

Table 4.4 Number of performance measures out of range in summer 2006 out of 45 sites

	SCE<0	**Tstat <2**	**Tstat <1.5**	**Tstat <1**
Tu_MchHD	0	0	0	0
Exh_Lin1	0	8	3	2
WA_LIQ	4	36	33	28
WA_VAP	0	1	0	0
CNG	0	0	0	0
LPG	0	9	3	1
Ind_Ref	0	2	1	1
Coke_Ovn	5	44	33	19
Arc_Coat	0	24	4	1
Biogenic	0	0	0	0

There were 18 out of 47 and 4 out of 45 samples with negative source contribution from Liquid Gasoline in winter and summer, respectively. There were 18 out of 45 samples with negative source contributions from Coke Oven in summer 2006. The negative contributions of Liquid Gasoline indicated that it may have collinearity with the other sources. Liquid Gasoline was also observed with 43 out of 47; and 28 out of 45 samples with Tstat values less than one in winter and summer, respectively. There were 5 out of 45 samples with Tstat values of Coke Oven less than one. The majority of Tstat lower than one indicated that most of the contribution estimates outputs were not reliable because their uncertainties were even higher than the source contribution values. CMB model overestimated summer ambient concentration with Percent Mass (%) of 45 over 120%. CMB outputs are listed in Appendix F.

4.2.2 Comparison of Source Apportionment Results from Different Seasons and Years

The source contribution estimates and the source contribution mass percentage results for winter and summer in both years are shown in Table 4.5. The average source contributions ($\mu g/m^3$) and their mass percentage were calculated. They are listed in Table 4.5.

Table 4.5 Source contribution estimates and percentage for year 2005 and 2006

(a) Year 2005 source contribution estimates ($\mu g/m^3$)

Source	**Summer**				**Winter**				
	Mean	Median	SD	CV (%)	Mean	Median	SD	CV (%)	S/W
Diesel Exhaust	5.1	3.3	6.6	130.8	2.0	1.4	2.1	107.2	2.5
Gasoline Exhaust	9.7	9.5	4.2	43.9	8.2	5.7	8.4	102.9	1.2
Liquid Gasoline	2.0	1.1	2.7	139.6	1.8	1.3	1.6	93.9	1.1
Gasoline Vapour	9.8	8.5	5.7	57.7	6.2	5.0	4.3	70.5	1.6
Commercial Natural Gas	4.3	4.2	1.6	36.6	10.3	9.0	4.5	43.5	0.4
Liquefied Petroleum Gas	2.5	2.4	1.0	39.4	2.1	1.8	1.2	57.8	1.2
Industrial Refinery	5.4	5.2	2.3	42.1	7.4	5.4	6.5	88.3	0.7
Coke Oven	1.2	1.2	0.7	54.9	2.4	2.0	1.4	58.7	0.5
Architectural Coatings	7.7	6.8	4.2	54.3	3.7	3.3	2.2	57.8	2.1
Biogenic Emissions	0.5	0.3	0.5	88.0	0.0	0.0	0.0	95.8	13.1
All vehicles	26.5	24.2	11.3	42.4	18.1	14.4	13.1	72.4	1.5
Total calculated mean	48.2				44.0				1.1
Annual calculated mean	46.1								

(b) Year 2006 source contribution estimate ($\mu g/m^3$)

Source	**Summer**				**Winter**				
	Mean	Median	SD	CV (%)	Mean	Median	SD	CV (%)	S/W
Diesel Exhaust	6.1	5.4	3.1	50.6	2.1	1.9	0.8	35.6	2.9
Gasoline Exhaust	6.6	6.4	2.5	37.7	5.1	4.8	2.1	41.6	1.3
Liquid Gasoline	2.5	1.2	2.9	115.4	0.5	0.2	1.0	204.1	4.9
Gasoline Vapour	8.3	7.1	3.9	47.0	5.0	4.9	1.8	35.2	1.7
Commercial Natural Gas	3.4	3.3	0.8	22.6	5.4	5.3	0.9	16.8	0.6
Liquefied Petroleum Gas	2.0	1.3	3.3	162.0	2.0	2.1	0.8	39.6	1.0
Industrial Refinery	5.5	4.8	3.1	56.3	5.4	5.2	1.7	30.7	1.0
Coke Oven	0.8	0.7	0.6	68.5	1.7	1.7	0.3	19.4	0.5
Architectural Coatings	5.5	4.6	3.3	59.8	3.3	3.1	1.6	48.0	1.7
Biogenic Emissions	0.5	0.4	0.4	75.4	0.0	0.0	0.0	20.8	17.3
All vehicles	23.5	21.0	8.2	34.7	12.7	12.5	4.1	32.6	1.9
Total calculated mean	41.2				30.5				1.4
Annual calculated mean	35.8								

(c) Year 2005 mass percentage estimate (%)

Source	**Summer**				**Winter**				
	Mean	Median	SD	CV (%)	Mean	Median	SD	CV (%)	S/W
Diesel Exhaust	10.1	7.7	9.3	92.3	4.4	3.8	2.6	58.8	2.3
Gasoline Exhaust	20.2	22.1	6.2	30.8	17.3	16.6	4.1	23.7	1.2
Liquid Gasoline	4.0	2.3	4.9	122.4	4.4	4.3	3.5	79.9	1.0
Gasoline Vapour	19.8	19.5	5.9	29.9	13.7	12.9	3.5	25.6	1.4
Commercial Natural Gas	9.1	8.8	2.9	32.3	24.7	25.4	4.5	18.1	0.4
Liquefied Petroleum Gas	5.4	5.4	1.8	34.1	4.9	4.5	1.8	37.2	1.1
Industrial Refinery	11.7	11.5	4.0	34.4	16.1	15.7	3.4	21.1	0.7
Coke Oven	2.7	2.8	1.2	45.0	5.6	5.6	1.1	20.2	0.5
Architectural Coatings	15.8	15.2	5.0	31.6	8.9	9.1	3.1	34.8	1.8
Biogenic Emissions	1.1	0.8	0.9	84.4	0.1	0.1	0.0	37.1	13.0
All vehicles	54.2	53.0	6.0	11.1	39.7	38.2	4.7	11.7	1.4
Total Calculated	100.0				100.0				

(d) Year 2006 mass percentage estimate (%)

Source	**Summer**				**Winter**				
	Mean	Median	SD	CV (%)	Mean	Median	SD	CV (%)	S/W
Diesel Exhaust	14.9	14.1	4.6	31.0	7.1	6.8	2.2	30.7	2.1
Gasoline Exhaust	16.6	16.8	5.3	31.9	16.2	16.3	3.7	22.8	1.0
Liquid Gasoline	5.6	3.5	5.5	98.9	1.6	0.4	2.6	166.7	3.5
Gasoline Vapour	20.1	20.3	5.3	26.2	16.2	15.6	3.9	24.0	1.2
Commercial Natural Gas	8.9	8.6	2.6	28.9	18.0	18.1	2.6	14.7	0.5
Liquefied Petroleum Gas	4.4	3.8	3.8	86.7	6.8	6.4	2.6	38.0	0.7
Industrial Refinery	13.2	13.1	3.5	26.9	17.8	17.8	3.4	18.9	0.7
Coke Oven	2.2	2.1	1.5	67.0	5.6	5.6	1.0	18.2	0.4
Architectural Coatings	12.7	12.5	3.8	29.6	10.6	10.5	3.6	33.8	1.2
Biogenic Emissions	1.4	1.0	1.3	93.9	0.1	0.1	0.0	17.7	14.3
All vehicles	57.2	56.9	6.8	12.0	41.0	41.0	5.0	12.2	1.4
Total calculated	100.0				100.0				

There were similarities in the same seasons of two years, and also both years. The discussion of the results is listed in Table 4.6.

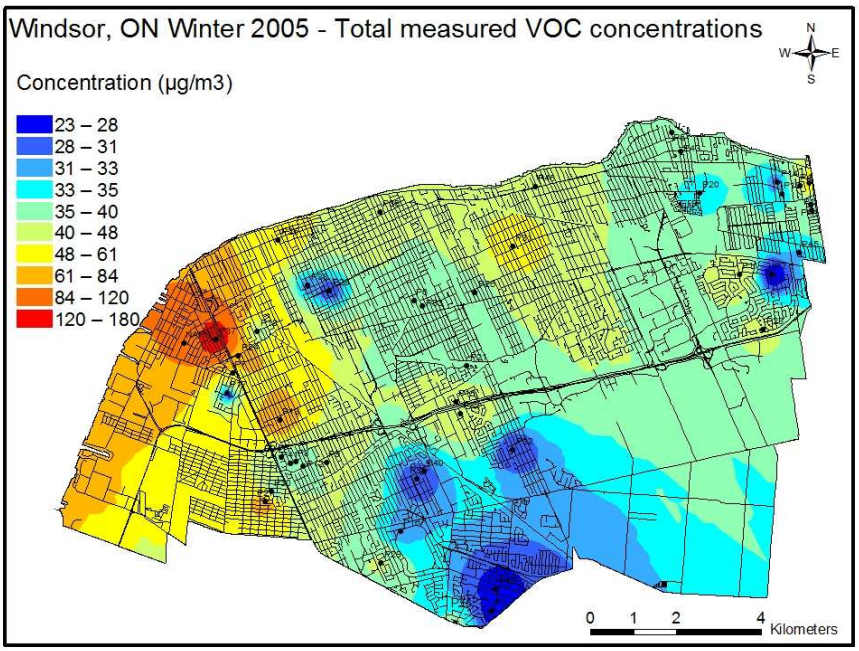
Table 4.6 Discussion of the source contributions results for winter and summer in both years

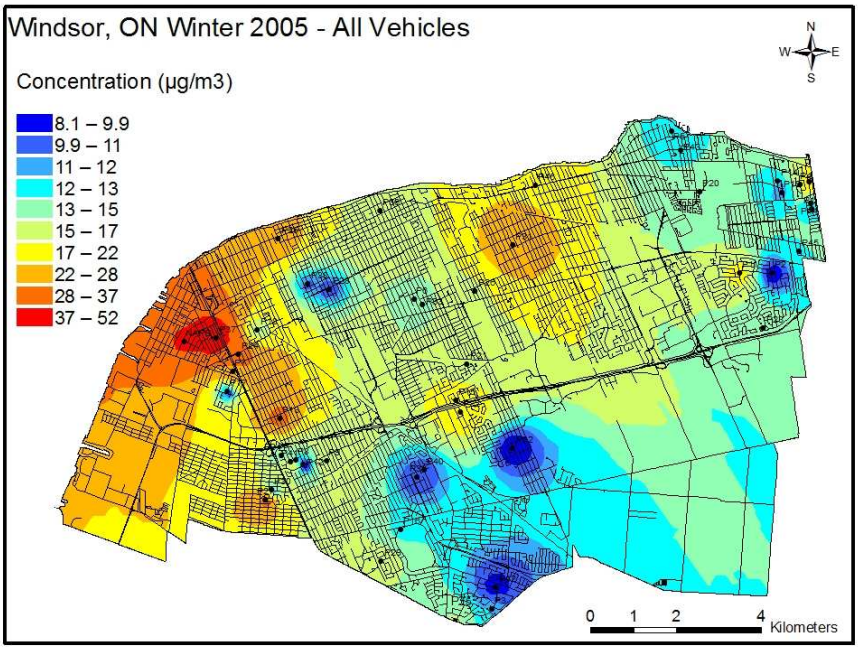
Year 2005	**Year 2006**
Gasoline Exhaust and Gasoline Vapour were the common dominant emission contributors in both seasons (20.2%, 19.8 % respectively in summer, and 17.3 %, 13.7 % respectively in winter).	Gasoline Exhaust, Gasoline Vapour, and Industrial Refinery were the common dominant emission contributors in both seasons (16.6%, 20.1% and 13.2% respectively in summer, and 16.2%, 16.2% and 17.8% respectively in winter).
Architectural Coatings (15.8%) was another main emission source in summer, and Commercial Natural Gas (24.7%) and Industrial Refinery (16.1%) were the dominant contributors other than Gasoline Exhaust and Gasoline Vapour in winter.	Diesel Exhaust (14.9%) and Architectural Coatings (12.7%) were another two main contributors in summer; Commercial Natural Gas (18.0%) was another dominant contributor in winter.
The percentage mass of Commercial Natural Gas, Industrial Refinery and Coke Oven in winter were higher than the ones in summer.	The percentage mass of Commercial Natural Gas, Liquefied Petroleum Gas, Industrial Refinery and Coke Oven in winter were higher than the ones in summer.
In summer, over half of the emission came from all vehicles (54.2%), while in winter, less than half of emission came from them (39.7%).	Same as 2005

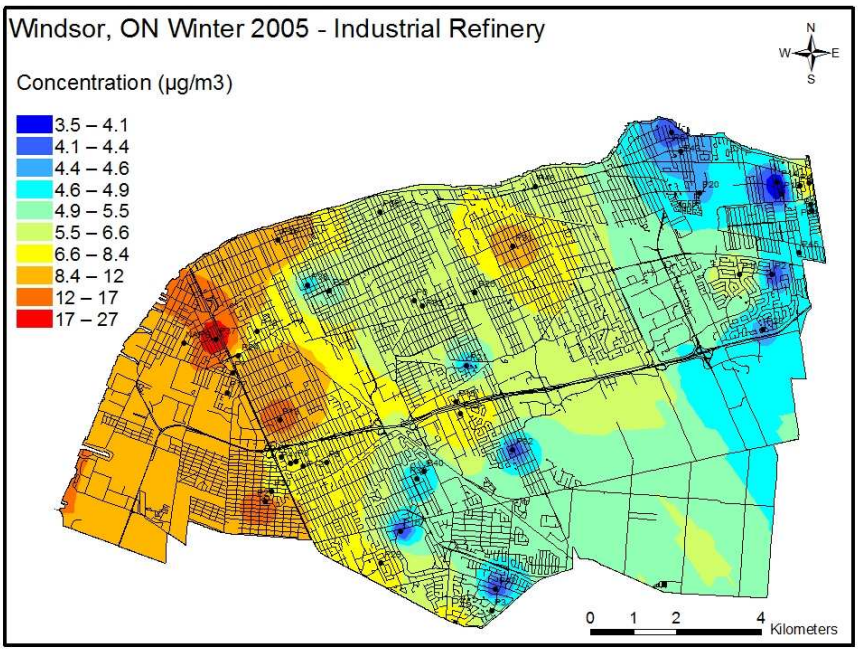
According to Table 4.6, Gasoline Exhaust, Gasoline Vapour, Commercial Natural Gas and Industrial Refinery were the biggest VOCs emitters in winter of both two years. Over half of the VOCs concentration was attributed to all vehicles in summer (54% and 57% for year 2005 and 2006, respectively), while in winter, less than half of emission came from them for both two years (38% and 41%) for year 2005 and 2006, respectively). The percentage mass of Commercial Natural Gas, Industrial Refinery and Coke Oven in winter were higher than the ones in summer for both two years. Gasoline Exhaust, Gasoline Vapour and Architectural Coatings were the main emission sources in summer in both two years. Diesel Exhaust and Architectural Coatings were other two big emitters in summer for year of 2006. The much anticipated large contributions from diesel Exhaust did not show in the results. This could be due to the lack of measurements and source profile of PAHs and Sulfur Dioxide, the species markers of Diesel Exhaust.

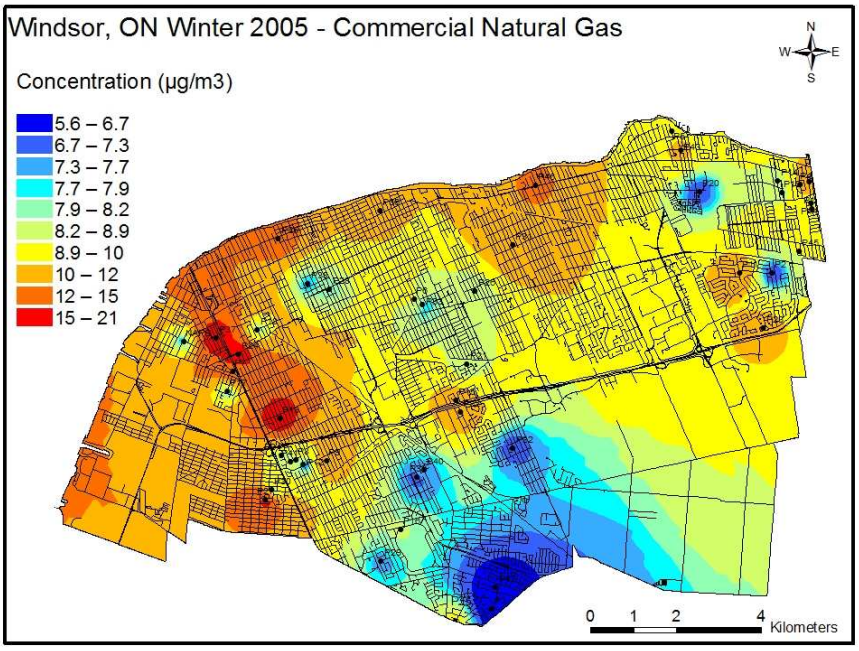
4.2.3 Spatial Trends of the Source Contribution

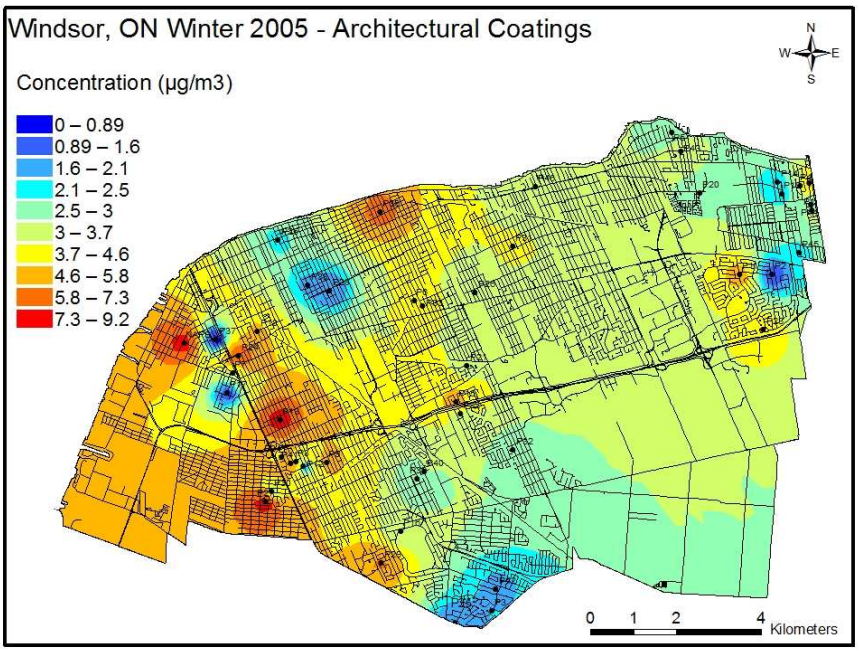
The spatial trends of total measured VOC concentrations, source contribution of All Vehicle, Industrial Refinery, Architectural Coatings, Liquid Petroleum Gas, and Biogenic Emission in winter and summer of each of 2005 and 2006 were generated by using ArcGIS 10.1 software (ESRI Canada, 2014). The results are shown in Figure 4.1.


Windsor, ON Winter 2005 - Total measured VOC concentrations
N
W
E
S
Concentration (µg/m3)
23 – 28
28 – 31
31 – 33
33 – 35
35 – 40
40 – 48
48 – 61
61 – 84
84 – 120
120 – 180
0 1 2 4
Kilometers


Windsor, ON Winter 2005 - All Vehicles
N
W
E
S
Concentration (µg/m3)
8.1 – 9.9
9.9 – 11
11 – 12
12 – 13
13 – 15
15 – 17
17 – 22
22 – 28
28 – 37
37 – 52
0 1 2 4
Kilometers


Windsor, ON Winter 2005 - Industrial Refinery
Concentration (µg/m3)
3.5 – 4.1
4.1 – 4.4
4.4 – 4.6
4.6 – 4.9
4.9 – 5.5
5.5 – 6.6
6.6 – 8.4
8.4 – 12
12 – 17
17 – 27
N
W
E
S
0 1 2 4
Kilometers


Windsor, ON Winter 2005 - Commercial Natural Gas
Concentration (µg/m3)
5.6 – 6.7
6.7 – 7.3
7.3 – 7.7
7.7 – 7.9
7.9 – 8.2
8.2 – 8.9
8.9 – 10
10 – 12
12 – 15
15 – 21
N
W
E
S
0 1 2 4
Kilometers



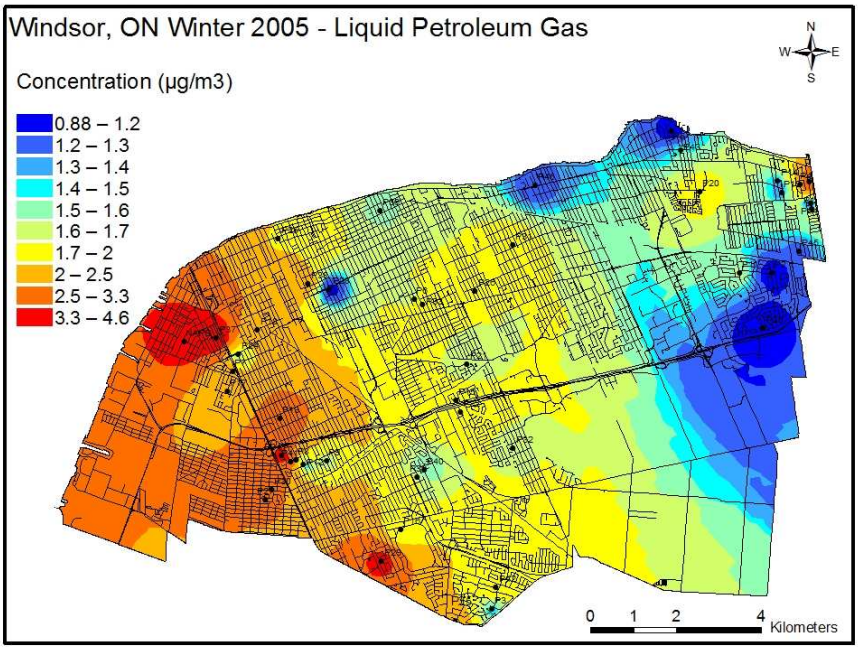
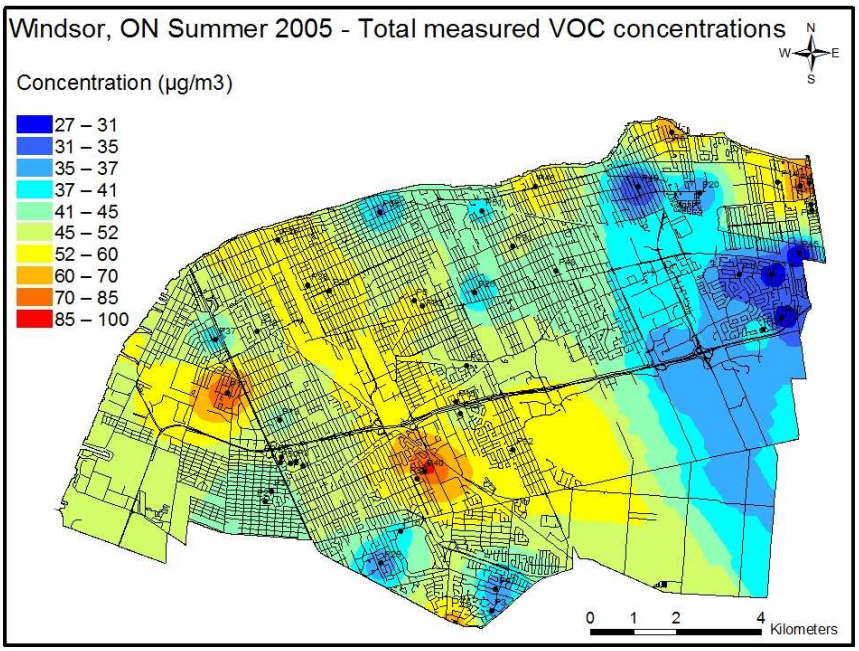
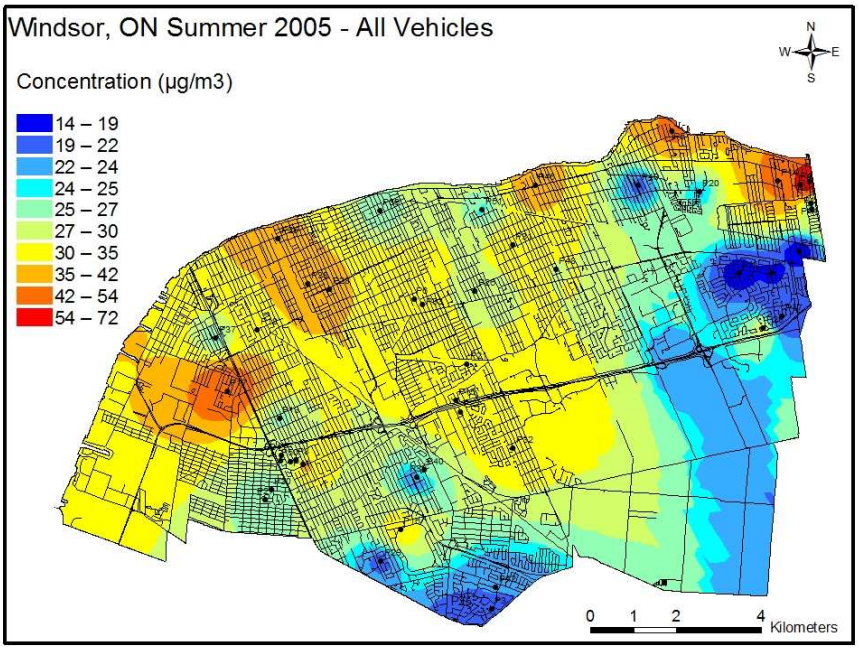


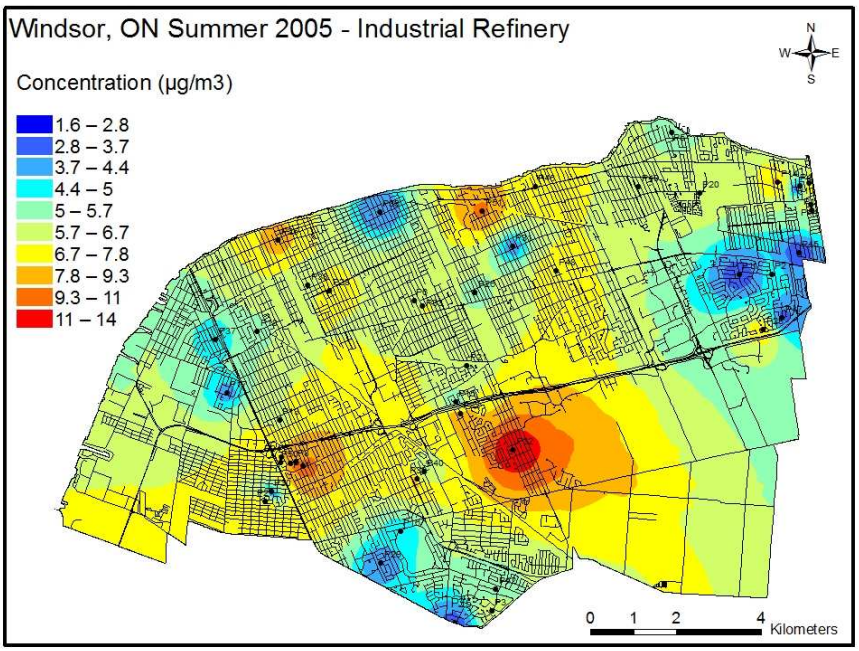
Figure 4.1 Source contribution spatial maps in winter 2005

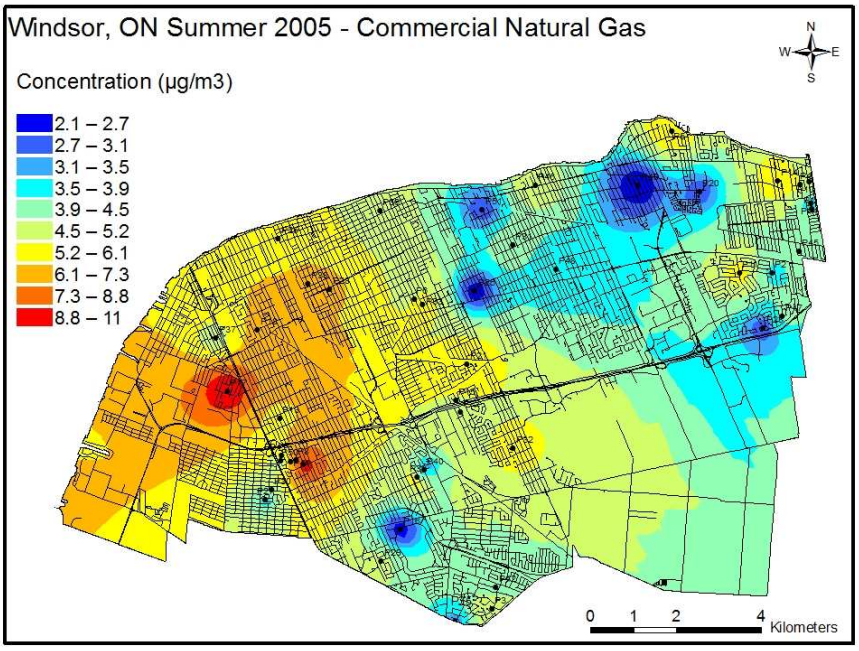
The maps of winter 2005 reveal spatial distribution of source contribution of sources. They are:

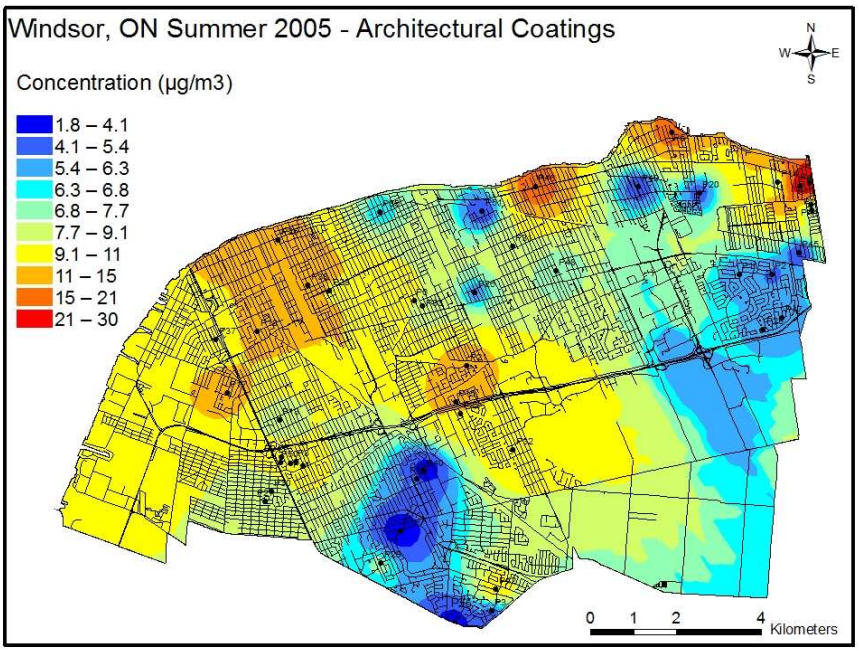
- The spatial trend of the total measured ambient VOC concentrations was similar with that of All vehicle. The high concentration was observed near the northern part of Huron Church Road.
- The concentration of VOC emitted from All vehicles, Industrial Refinery, and the Commercial Natural Gas was high near the northern part of Huron Church Road. This could be caused by heavy traffic on the Huron Church Road.
- The concentration of Commercial Natural Gas was high in the western Windsor regions and along Riverside Drive. This could be caused by the VOC emission from the industries in Detroit.
- The concentration in the southern part of Windsor was low with the exceptions of Site 27 near the southern Huron Church Road, and Site 22 near the middle section of E.C. Expressway of Commercial Natural Gas, Site 27 near the southern Huron Church Road, and Site 29 near the middle of the 401 Highway of Architectural Coatings.
- The correlation results showed that total measured VOCs was correlated with all the other 11 sources with the exception of Liquid Gasoline ($r= 0.112$; $p= 0.454$). All vehicle was correlated with Diesel Exhaust ($r= 0.599$; $p= 0$), Gasoline Exhaust ($r= 0.926$), and Gasoline Vapour ($r= 0.900$; $p= 0$), and all other 6 sources ($r=0.478$ to 0.804; $p=0.001$) other than vehicle-related sources. Among the 15 pairs of the six sources other than vehicle-related sources, 14 pairs were correlated. Architectural Coatings and Biogenic Emission were not related, with the coefficient of 0.243 and p value of 0.1.


Windsor, ON Summer 2005 - Total measured VOC concentrations
N
W
E
S
Concentration (µg/m3)
27 – 31
31 – 35
35 – 37
37 – 41
41 – 45
45 – 52
52 – 60
60 – 70
70 – 85
85 – 100
0 1 2 4
Kilometers


Windsor, ON Summer 2005 - All Vehicles
N
W
E
S
Concentration (µg/m3)
14 – 19
19 – 22
22 – 24
24 – 25
25 – 27
27 – 30
30 – 35
35 – 42
42 – 54
54 – 72
0 1 2 4
Kilometers


Windsor, ON Summer 2005 - Industrial Refinery
Concentration (µg/m3)
1.6 – 2.8
2.8 – 3.7
3.7 – 4.4
4.4 – 5
5 – 5.7
5.7 – 6.7
6.7 – 7.8
7.8 – 9.3
9.3 – 11
11 – 14
N
W
E
S
0 1 2 4
Kilometers


Windsor, ON Summer 2005 - Commercial Natural Gas
Concentration (µg/m3)
2.1 – 2.7
2.7 – 3.1
3.1 – 3.5
3.5 – 3.9
3.9 – 4.5
4.5 – 5.2
5.2 – 6.1
6.1 – 7.3
7.3 – 8.8
8.8 – 11
N
W
E
S
0 1 2 4
Kilometers



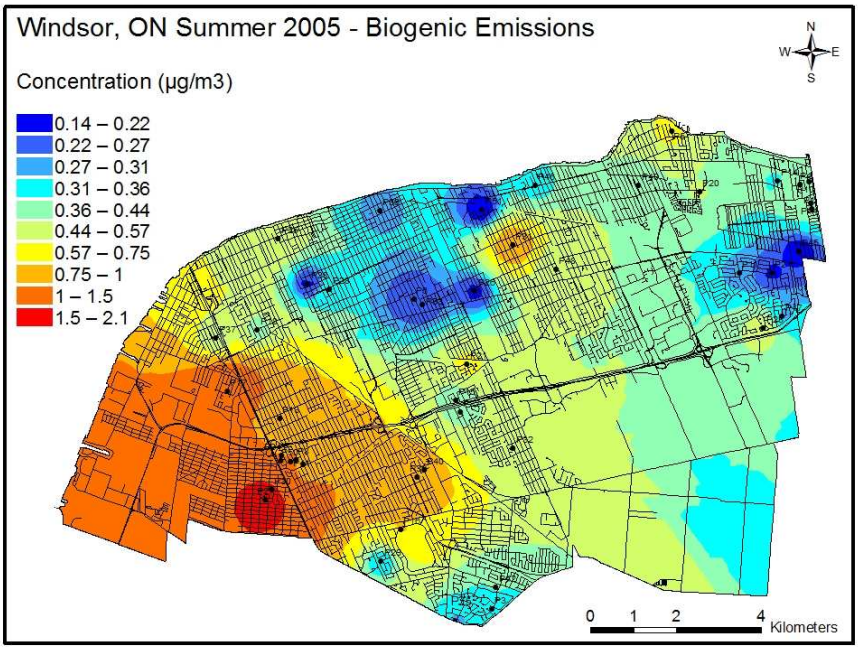
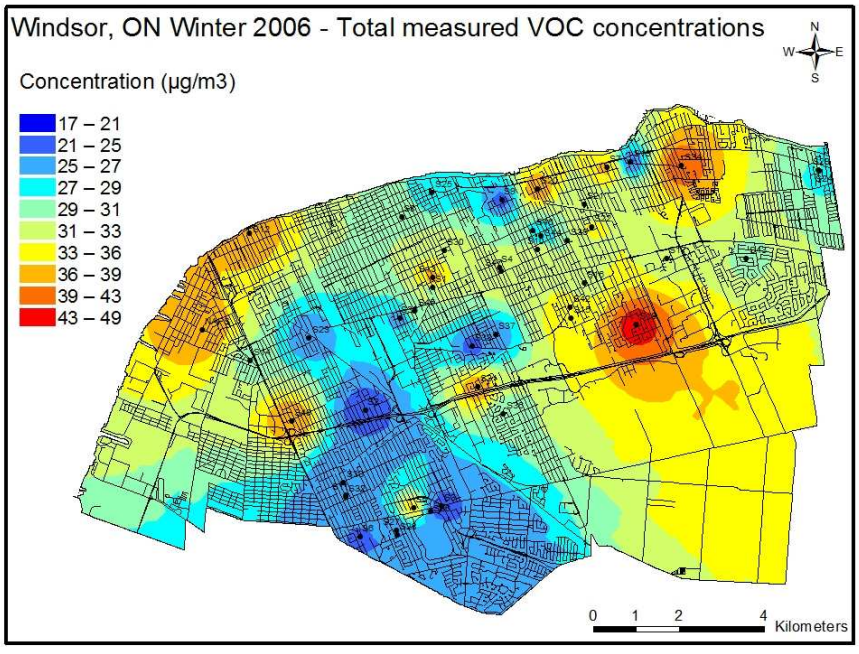


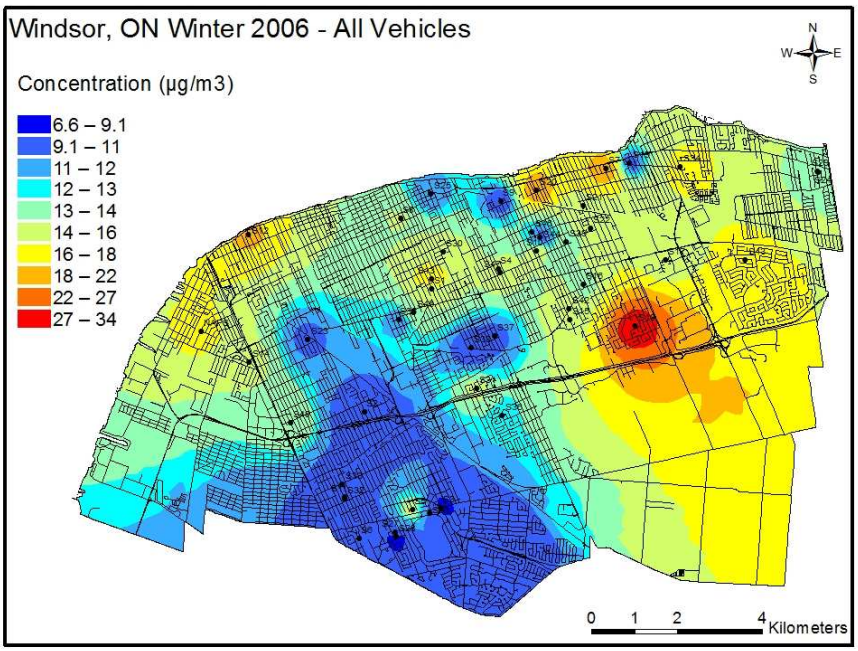
Figure 4.2 Source contribution maps in summer 2005

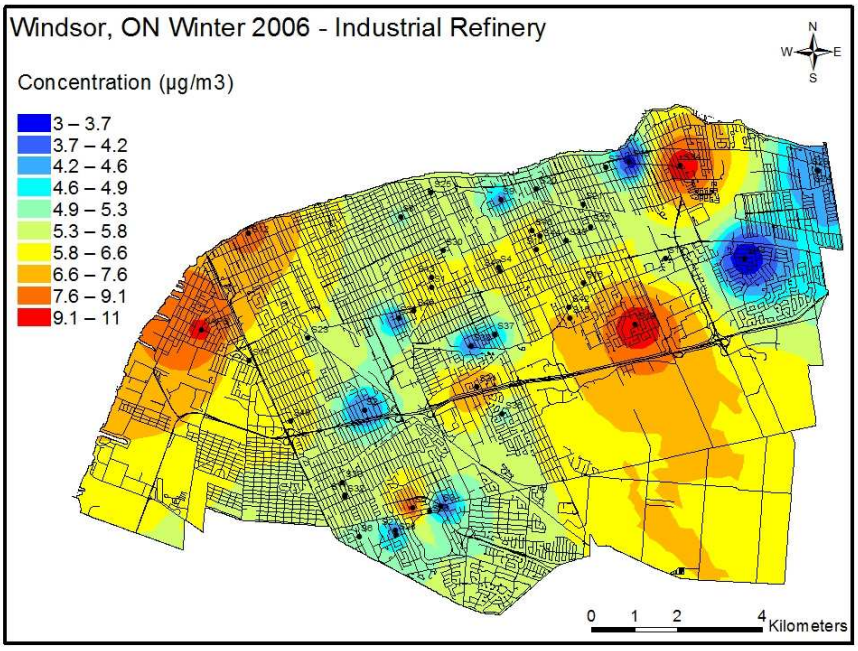
The maps of summer 2005 reveal spatial distribution of source contribution of sources. They are:

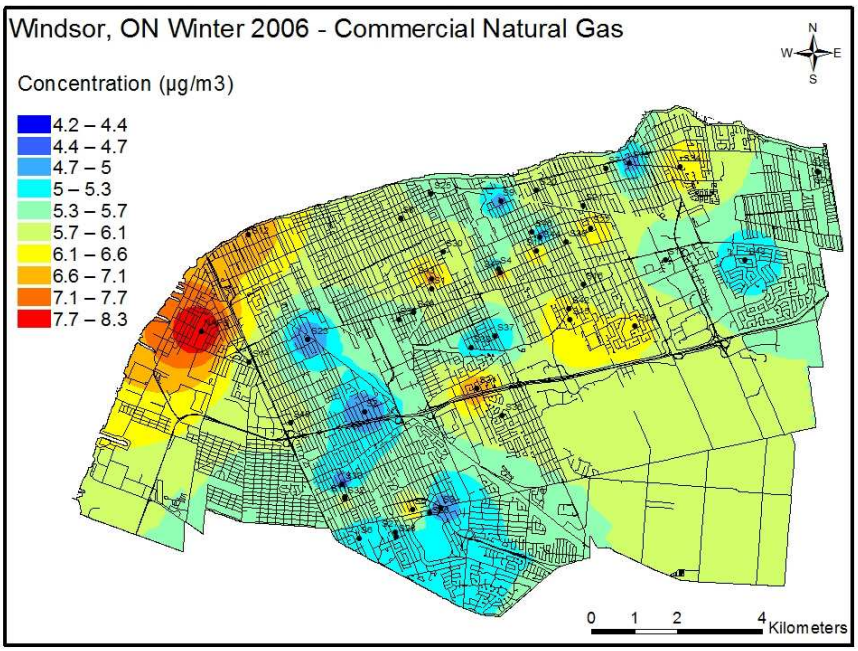
- The spatial trend of the total measured ambient VOC concentrations was similar with that of All vehicle. The high concentration was observed near the northern part of Huron Church Road. There were slight differences between the trend of total VOC concentrations and the vehicle in summer 2005. The high total VOC concentration at site 40 near E.C. Row Expressway was not reflected in the one of model calculated vehicle-related. This may due to the model only explained 37.1% of the concentration at this site. Model overestimated the concentration at site 10 and site 14, leading the hot spots at northeastern corner of Windsor.
- High concentration was observed near the northern part of Huron Church Road for All vehicles, Industrial Refinery, and the Commercial Natural Gas.
- The high concentration at site 14 and site 10 in the northeastern area of Windsor were caused by the model overestimate.
- The concentration in the southern part of Windsor was low with the exceptions of Site 12 and Site 32 near the E.C. Expressway of Industrial refinery; and Site 12 near the intersection of Huron Church Road and E.C. Expressway of Commercial Natural Gas. The low concentration was due to that there is much less residents, commercial activities or industries. The airport is also located in this area.
- The correlation results showed that total measured VOCs was correlated with All vehicle ($r= 0.736$; $p=0$), Gasoline Vapour ($r= 0.607$; $p=0$), and Architectural Coatings ($r= 0.551$; $p=0$) with moderate correlation coefficients. The correlations of total measured VOCs with Gasoline Exhaust ($r= 0.481$; $p=0.001$) and Commercial Natural

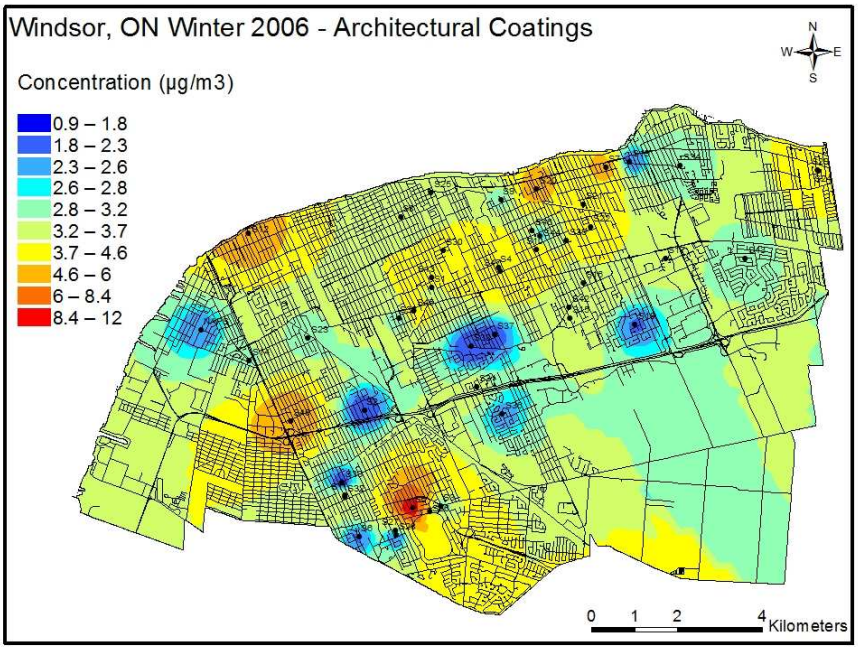
Gas (r= 0.334; p=0.023) were weak. . Diesel Exhaust, Liquid Gasoline, Liquid Petroleum Gas, Industrial Refinery, Coke Oven, and Biogenic Emission were not correlated with total measured VOCs. All vehicle was strongly correlated with Gasoline Vapour (0.874), moderately correlated with Gasoline Exhaust (0.575) and Architectural Coatings (r= 0.781; p= 0), Liquid Petroleum Gas (r= 0.324; P= 0.028); weakly with Commercial Natural Gas (r=0.429; p=0.003). ,. Among the six sources other than the vehicle-related sources, Industrial Refinery was correlated with Liquid Petroleum Gas (r= 0.366; p= 0.012), and Coke Oven (r= 0.298; p= 0.044). Commercial Natural Gas was correlated with Coke Oven (r= 0.369; p= 0.012), and Architectural Coatings (r= 0.378; p= 0.01). Architectural Coatings was correlated with Liquid Petroleum Gas (r= 0.335; p= 0.023). However, all of them were weak.




Windsor, ON Winter 2006 - All Vehicles
Concentration (µg/m3)
6.6 – 9.1
9.1 – 11
11 – 12
12 – 13
13 – 14
14 – 16
16 – 18
18 – 22
22 – 27
27 – 34
N
W
E
S
0 1 2 4 Kilometers


Windsor, ON Winter 2006 - Industrial Refinery
Concentration (µg/m3)
3 – 3.7
3.7 – 4.2
4.2 – 4.6
4.6 – 4.9
4.9 – 5.3
5.3 – 5.8
5.8 – 6.6
6.6 – 7.6
7.6 – 9.1
9.1 – 11
N
W
E
S
0 1 2 4 Kilometers


Windsor, ON Winter 2006 - Commercial Natural Gas
N
W
E
S
Concentration (µg/m3)
4.2 – 4.4
4.4 – 4.7
4.7 – 5
5 – 5.3
5.3 – 5.7
5.7 – 6.1
6.1 – 6.6
6.6 – 7.1
7.1 – 7.7
7.7 – 8.3
0 1 2 4 Kilometers


Windsor, ON Winter 2006 - Architectural Coatings
N
W
E
S
Concentration (µg/m3)
0.9 – 1.8
1.8 – 2.3
2.3 – 2.6
2.6 – 2.8
2.8 – 3.2
3.2 – 3.7
3.7 – 4.6
4.6 – 6
6 – 8.4
8.4 – 12
0 1 2 4 Kilometers

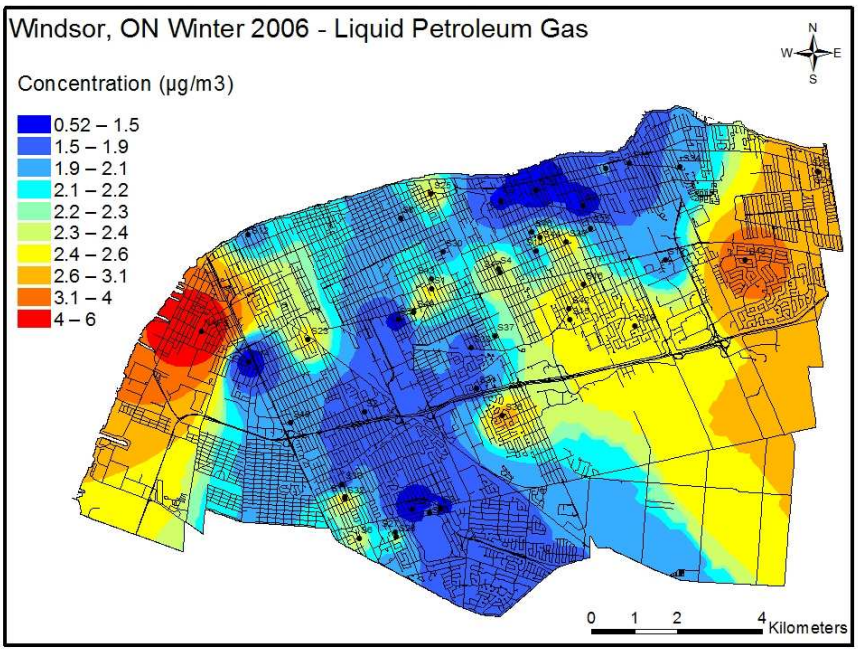


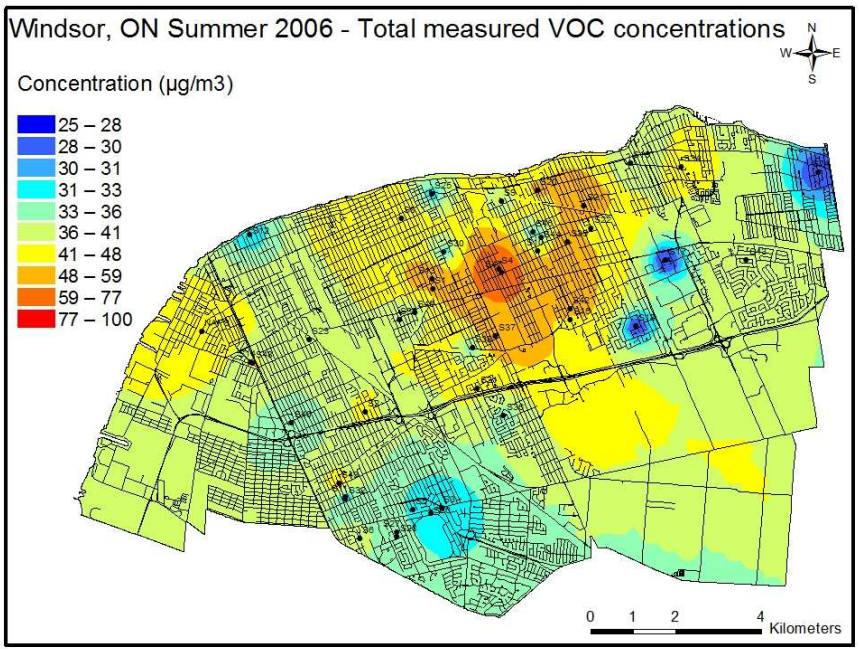
Figure 4.3 Source contribution maps in winter 2006

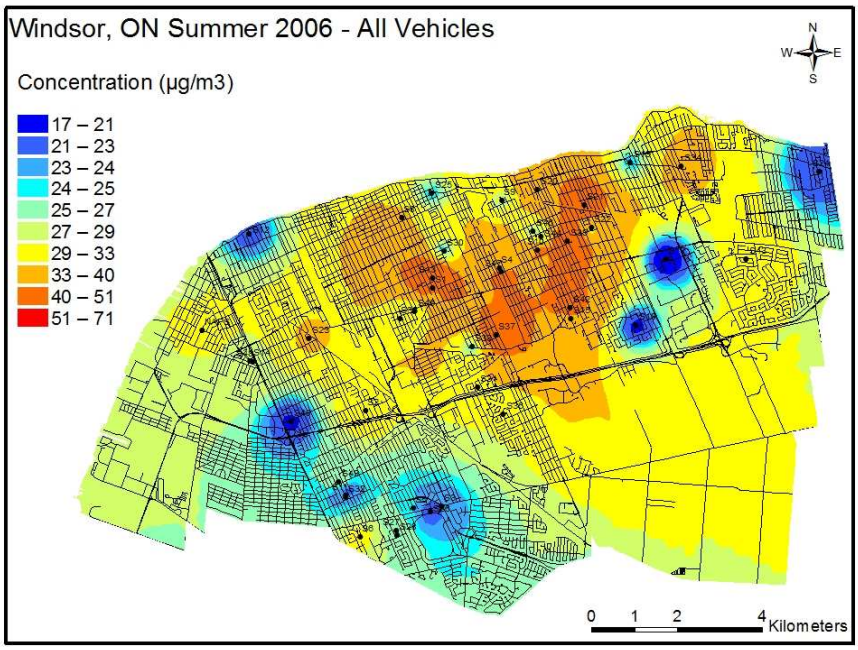
The maps of winter 2006 reveal spatial distribution of source contribution of sources. They are:

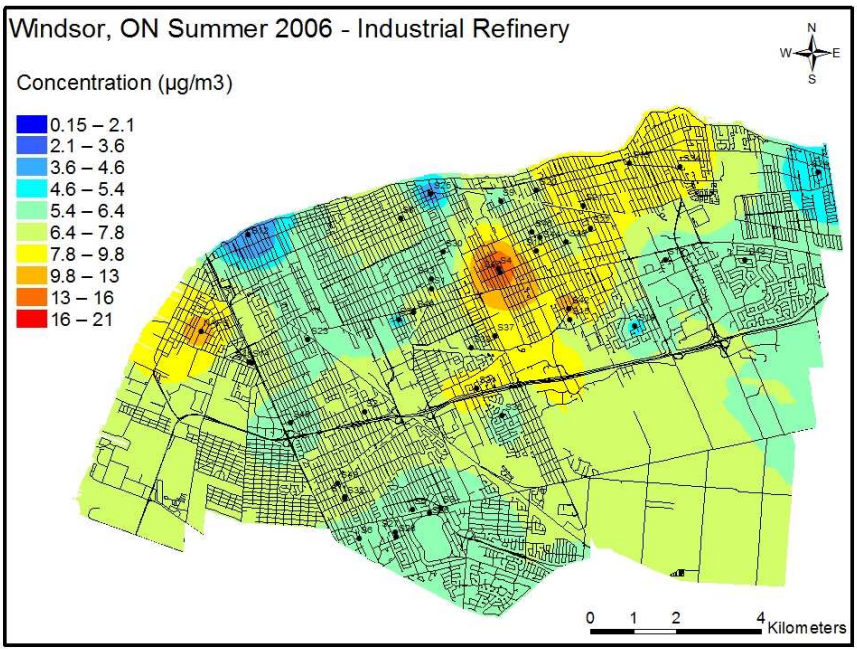
- ient VOC concentrations was similar with that of All vehicle. The high concentration was observed near the northern part of Huron Church Road.
- The concentration of VOC emitted from All vehicle, Industrial Refinery, and the Commercial Natural Gas was high near the northern part of Huron Church Road. This could be caused by heavy traffic on the Huron Church Road. The concentration of Commercial Natural Gas was also high.
- There was hot spot at site 18 near the east section of E.C. Expressway of All Vehicle. This could be caused by the traffic associated with transportation of goods and

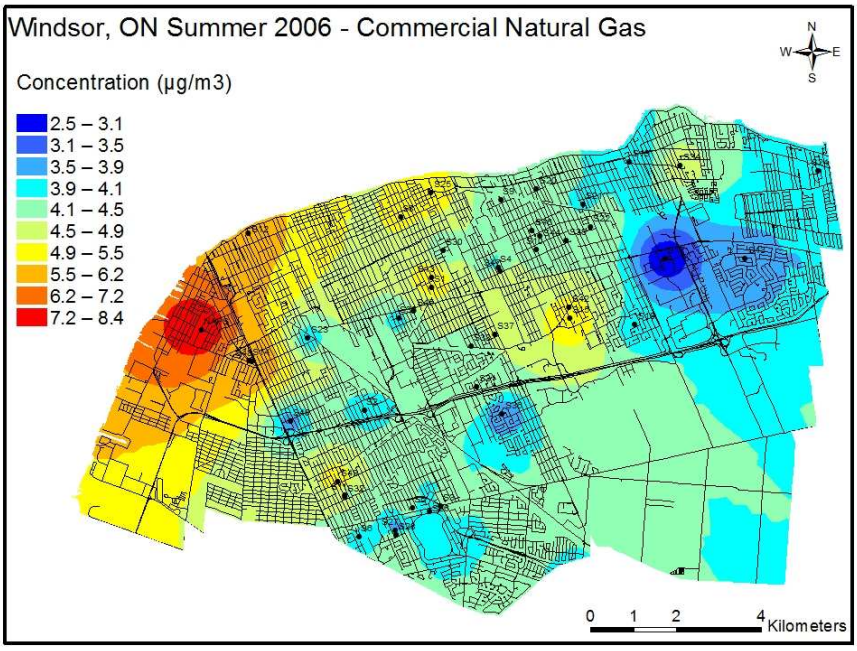
employees of Ford Essex Engine Plant. The high concentration was shown in the southeastern part of Windsor (at the airport), although no measurement was taken at the airport. This was because by using Inverse Distance Weighted Interpolation method, the software predicts the concentration with the measurements at the neighbors of the predicted site. The high concentration measured at site 18 gave the great influence on the prediction of the southeastern area.

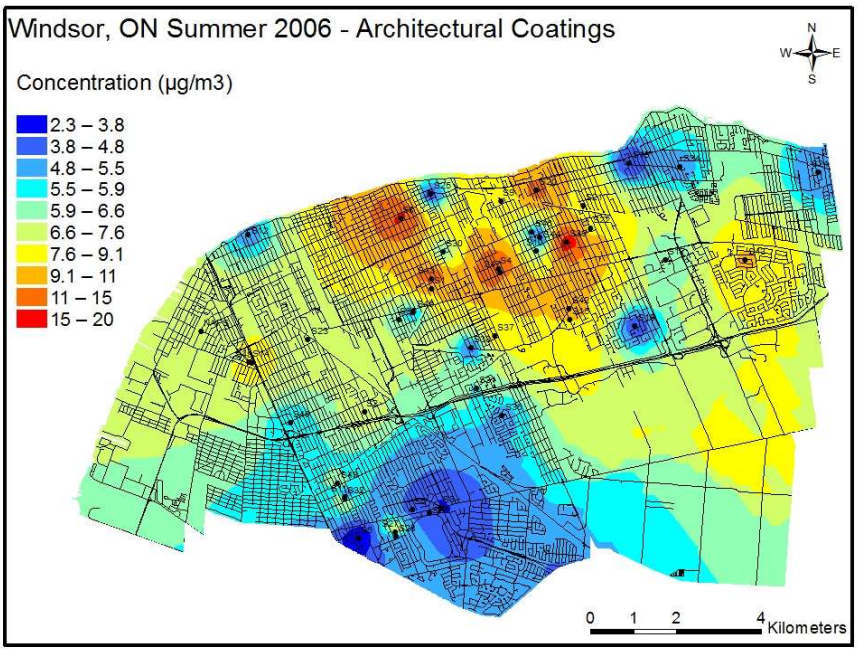
- The concentration in the southern part of Windsor was low with the exceptions of Site 5 near the E.C. Expressway of Industrial refinery and Architectural Coatings. The low concentration was due to that there is much less residents, commercial activities or industries. The airport is also located in this area. The high concentration of those sites was caused by model overestimation.
- The correlation results showed that total measured concentration were correlated with all sources with the exception of Liquid Petroleum Gas ($r= 0.217$; $p= 0.139$). All vehicle was related with all four vehicle-related sources and all the other 6 sources with the exception of Liquid Petroleum Gas ($r= 0.128$; $p= 0.386$). Among the 15 pairs of the six other than vehicle-related sources, 10 pairs were related. The relation observed between Industrial Refinery and Coke Oven ($r= 0.285$; $p= 0.049$) was weak. There was no relations between Commercial Natural Gas and Liquid Petroleum Gas ($r= 0.21$; $p= 0.15$), Liquid Petroleum Gas and Industrial Refinery (0.218; $p= 0.137$), Liquid Petroleum Gas and Coke ($r= 0.204$; $p= 0.164$), Liquid Petroleum Gas and Architectural Coatings ($r= -0.212$; $p= 0.148$), or Liquid Petroleum Gas and Biogenic Emission ($r= -0.066$; $p= 0.655$).


Windsor, ON Summer 2006 - Total measured VOC concentrations
N
W
E
S
Concentration (µg/m3)
25 – 28
28 – 30
30 – 31
31 – 33
33 – 36
36 – 41
41 – 48
48 – 59
59 – 77
77 – 100
0 1 2 4
Kilometers


Windsor, ON Summer 2006 - All Vehicles
N
W
E
S
Concentration (µg/m3)
17 – 21
21 – 23
23 – 24
24 – 25
25 – 27
27 – 29
29 – 33
33 – 40
40 – 51
51 – 71
0 1 2 4
Kilometers


Windsor, ON Summer 2006 - Industrial Refinery
Concentration (µg/m3)
0.15 – 2.1
2.1 – 3.6
3.6 – 4.6
4.6 – 5.4
5.4 – 6.4
6.4 – 7.8
7.8 – 9.8
9.8 – 13
13 – 16
16 – 21
N
W
E
S
0 1 2 4 Kilometers


Windsor, ON Summer 2006 - Commercial Natural Gas
Concentration (µg/m3)
2.5 – 3.1
3.1 – 3.5
3.5 – 3.9
3.9 – 4.1
4.1 – 4.5
4.5 – 4.9
4.9 – 5.5
5.5 – 6.2
6.2 – 7.2
7.2 – 8.4
N
W
E
S
0 1 2 4 Kilometers



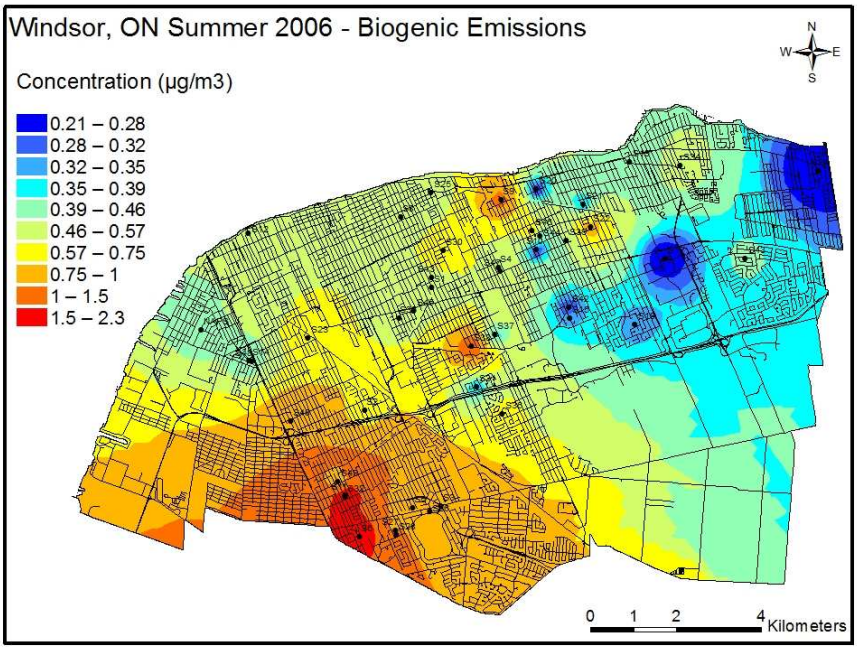


Figure 4.4 Source contribution maps in summer 2006

The maps of summer 2006 reveal spatial distribution of source contribution of sources. They are:

- The spatial trend of the total measured ambient VOC concentrations was similar with All Vehicle. The high concentration was observed in the surrounding areas of Windsor Engine Plant, and the Chrysler Canada-Windsor Assembly Plant for both All vehicle and Architectural Coatings. The reason of the all vehicle could be the result of the traffic associated with the transportations of goods and employees. The similar high concentration patterns of Architectural Coatings could be due to the automotive paintings.
- The concentration in the southern part of Windsor was low as there is much less residents, commercial activities or industries. The airport is also located in this area.
- The correlation results showed that total measured concentration was related with all the other 11 sources with the exception of Commercial Natural Gas ($r= 0.209$; $p= 0.164$) and Coke Oven ($r= -0.081$; $p= 0.593$). All vehicle was related with all four vehicle-related sources, and Architectural Coatings ($r= -0.651$; $p= 0$), although the correlation was weak. Liquid Petroleum Gas was moderately correlated with Industrial Refinery ($r= 0.675$; $p= 0$), and weakly with Arch ($r= 0.464$; $p= 0.001$). Industrial Refinery was weakly correlated with Architectural Coatings ($r= 0.429$; $p= 0.003$).

The spatial trend of the total measured ambient VOC concentrations was similar with All Vehicle for winter and summer 2005 and 2006. For winter and summer 2005 and winter 2006, the high concentration was observed near the northern part of Huron Church Road. For summer 2006, the high concentration was observed in the surrounding areas of Windsor Engine Plant, and the Chrysler Canada-Windsor Assembly Plant. Total measured

VOCs concentration was correlated with All vehicle for all four seasons.

High concentration was observed near the northern part of Huron Church Road for All vehicles, Industrial Refinery, and the Commercial Natural Gas for winter and summer 2005, and winter 2006. This could be caused by heavy traffic on the Huron Church Road. The high concentration of Industry Refinery may due to the Industrial sources on the other side of Detroit River. The All Vehicle was related with Commercial Natural Gas and Industrial Refinery in winter and summer 2005 and winter 2006 with the exception of Industrial Refinery in summer 2005. In summer 2006, the high concentration was observed in the surrounding areas of Windsor Engine Plant, and the Chrysler Canada-Windsor Assembly Plant for both All Vehicle and Architectural Coatings. The high vehicle concentration could be caused by the traffic associated with the transportations of goods and employees. The similar high concentration patterns of Architectural Coatings could be due to the automotive paintings in the Windsor Engine Plant and Chrysler Canada-Windsor Assembly Plant.

The overall concentration in the southern part of Windsor was low. The low concentration was due to that there is much less residents, commercial activities or industries. The airport is also located in this area.

For the Biogenic Emission in summer 2005 and 2006, high concentration was observed in southwestern area of Windsor. Region of Windsor, Ontario on the Google Map and Goolge Earth indicates that the trees were the most concentrated in this area compared to the others. Also, the Ojibway Prairie Provincial Nature Reserve is located in the southwestern Windsor. The deciduous trees density is higher compared with

elsewhere of Windsor. The concentration of middle area of Windsor was observed high with the exception of the north middle in summer 2005. The concentration was not as high as that of in southwestern area. The reason why the concentration was not high in this area for year 2005 was still unclear.

The low concentration was observed on in southeastern along with the eastern part of Windsor. It is because there was much less trees than anywhere else. The concentration along the west end of the city was high, however, the density of trees was very low, this may due to that there were limited amount of measurement sites nearby. The Inverse Distance Squared Weighted Interpolation was applied in this study. The prediction was influenced by the measurements of the surroundings. Thus, the concentration in the west end of the city would be similar as that of the nearest area, northwestern and southwestern areas.The concentration of liquid Petroleum Gas was high near the northern part of Huron Church Road for winter of both 2005 and 2006. In winter 2005, the concentration decreased from western area to eastern area. The total measured VOCs concentration and All Vehicle were both correlated with Liquid Petroleum Gas. In winter 2005, the high concentration was observed in eastern area. The area with the lowest concentration was middle part of Windsor. Neither the total measured VOCs concentration nor All Vehicle were correlated with Liquid Petroleum Gas.

4.3 PMF Source Apportionment Results

4.3.1 Performance measures

The scaled residuals of all species in both winter and summer 2006 were in the range of -3 and 3, indicating that the model reproduced the measurements of every species in each sample well. The range of the Q (robust) among all 20 runs for winter was 84.2 to 85.5 with the difference of 1.6%. In summer, the range was 226.5 to 226.7 with a change of 0.08%, indicating a stable performance. The best runs of PMF model outputs for both winter and summer 2006 are listed in Appendix G.

4.3.2 PMF factor profiles interpretations

The 56 species were classified into six groups. The species classification is listed in Table 3.9 in Chapter 3. The sum percentage of each group in winter 2006 is listed in Table 4.7, followed by the source identification results.

Table 4.7 Sum percentage of six classes in each PMF factor for winter 2006

Factor	aromatics	isoalkanes	|isoalkanes-aromatics| (larger one)*100%	alkene	alkane	isoprene	cycloalkane
Factor 1 Liquid Gasoline	24.9	30.4	18.1	7.1	35.2	0.1	0.9
Factor 2 Gasoline Exhaust	17.1	13.1	-23.4	12.5	55.3	0.2	1.8
Factor 3 Architectural Coatings	49.9	9.9	-80.2	3.4	35.7	0	1.1
Factor 4 Gasoline Exhaust	40	21.5	-46.3	6.2	21.1	0.2	1.8
Factor 5 Gasoline Vapour	16.7	21.6	22.7	2.7	58.3	0.1	0.6
Factor 6 Adhesive & Sealant Coatings	32.9	5	-84.8	9.9	45.5	0.2	0.8
Factor 7 Industrial Refinery	4.9	23.3	79.0	9.9	56.9	0.1	0.7
Factor 8 Liquid Petroleum Gas	20.7	9.4	-54.6	10.4	54.2	0.1	1.2
Factor 9 Diesel Exhaust	7.7	20.6	62.6	2.3	67.8	0	1.5
Factor 10 Coke Oven	27.5	8.8	-68.0	11.2	43.5	0.1	0.6
Factor 11 Undetermined	18.4	25	26.4	1.6	49.4	0	4.5
Factor 12 Gasoline Exhaust	16.4	18.1	9.4	15.6	38	0.1	6
Factor 13 Commercial Natural Gas	6.9	9.8	29.6	10.8	63.7	0	0.7

The source identification was done from Gasoline-related sources to the other sources. Thus, the source with percentage of isoalkanes and aromatics being top one and two or two and three were identified. The most abundant compound class was alkanes in all 13 factors with the exception of Factor 3 and Factor 4. In Factor 3, aromatics accounted for 49.9% of the total concentration, followed by alkanes (35.7%) and isoalkanes (9.9%). However, the percentage of aromatics outweighed that of isoalkanes 80%. Thus, Gasoline Exhaust was ruled out for Factor 3.

Factor 4 was identified as Gasoline Exhaust as toluene and acetylene accounted for 16.8% and 9.3% of total concentration, respectively, according to the studies of Harley and Kean (2004), Wang et al. (2013), Yuan et al. (2009), Song et al. (2008), and Templer (2007). Although the differences between isoalkanes and aromatics were nearly 50%, Factor 4 was still identified as Gasoline Exhaust. This is because Factor 4 was not Architectural Coatings. N&iso-pentane (12.1% and 9.8%) were the dominant species other than aromatics. N&iso-pentane are species markers for Gasoline Exhaust (Harley and Kean, 2004; Song et al., 2008; Yuan et al., 2009; Templer, 2007; Wang et al., 2013), Gasoline Vapour (Harley and Kean, 2004; Morino et al., 2011; Templer, 2007), and Liquid Gasoline (Song et al., 2008; Yuan et al., 2009; Templer, 2007). However, Factor 4 was not Gasoline Vapour or Liquid Gasoline as the percentage of aromatics (40%) outweighs the isoalkanes (21.5%). Factor 4 was not Industrial Refinery, as there is large proportion of butane and n&iso-pentane account for higher portion than toluene in Industrial Refinery, according to the studies of Cai et al. (2010) and Templer (2007). Thus, Factor 4 was identified as Gasoline Exhaust.

Among all 13 factors, the percentage differences between aromatics and isopentane of Factor 1, 2, 5, 11, 12, and 13 were less than 30%. According to Harley and Kean (2004), they could be Gasoline Exhaust, Diesel Exhaust, or Liquid Gasoline.

There were more aromatics than isopentane in Factor 2 (17.1% aromatics; 13.1% isopentane). Gasoline Exhaust species markers ethylene, and xylene accounted for 7% and 4.9% of total concentration, respectively. According to studies of Harley and Kean (2004), Wang et al. (2013); Yuan et al. (2009); Song et al. (2008) and Templer (2007), ethylene and xylene are species markers for Gasoline Exhaust. Thus, Factor 2 was identified as Gasoline Exhaust, although Factor 4 was identified as Gasoline Exhaust. Factor 4 is not Commercial Natural Gas although ethane accounted for 22.1% of the profile. This is because Factor 4 is not the profile consists of most ethane among all profiles. Factor 4 is not Industry Refinery although the percentage of butane was high (19.2%). This is because another species marker n&iso-pentane (Cai et al., 2010; Chan et al., 2011; Templer, 2007) for Industry Refinery do not have high percentage in Factor 4. Thus, Factor 4 was identified as Industry Refinery.

The differences between the percentage of isoalkanes and aromatics were less than 30% in Factor 11 (26.4%) and Factor 12 (9.4%). Factor 11 consisted of 23.5% hexane. There was 87.6% of the hexane apportioned to Factor 11. Therefore, there could be large uncertainty of Factor 11. Therefore, Factor 11 was undetermined. Factor 12 included 15.6% alkene; and species markers ethylene (12.6%), ethane (18%), and acetylene (5.7%). Thus, Factor 12 was identified as Gasoline Exhaust. Although Factor 2 was identified as Gasoline Exhaust, Factor 12 was identified as another Gasoline Exhaust. It was not Industrial Refinery as it was not rich on n&iso-butane or n&iso-pentane.

Species n&iso-butane and n&iso-pentane are species markers for Industrial Refinery (Cai et al., 2010; Chan et al., 2011; Templer, 2007). Factor 12 was not Commercial Natural Gas either, although it contains 18% ethane, species markers for Commercial Natural Gas. This is because ethane accounts for 35% or more in Commercial Natural Gas profile (Song et al., 2008; Templer, 2007). Thus, Factor 12 was considered as Gasoline Exhaust in spite of the amount of aromatics (16.4%) was slightly lower than that of isopentane (18.1%).

Isoalkanes are the most abundant species classes in Gasoline Vapour and Liquid Gasoline (Harley and Kean, 2004). None of factors among 1, 5 or 13 consisted of isoalkanes as the top one species class. Factor 1 and Factor 5 consisted of the highest amount of isopentane (11.2%; 11.6%) among the 13 Factors. According to studies of Morino et al. (2011); Templer (2007) and Harley and Kean (2004), Gasoline Vapour consists of less aromatics than Liquid Gasoline. Compared with Factor 1, Factor 5 contained less aromatics, thus, Factor 5 was identified as Gasoline Vapour. Factor 1 contained 30.4% and 24.9% isoalkanes and aromatics, respectively. It was identified as Liquid Gasoline.

Species markers for Diesel Exhaust, decane and undecane accounted for the highest amount of total concentration in Factor 9 (2.0%; 1.6%) among all factors. The proportion of alkanes (67.8%) was the highest among all the profiles; and the percentage of aromatics (7.7%) was the second lowest among all the profiles. There was also significant amount of ethane (15.9%) and n&iso-pentane (18.2%) in Factor 9. According to the studies of Lam et al. (2013); Yuan et al. (2009) and Song et al. (2008), Factor 9 was Diesel Exhaust.

Factor 3 consisted of 46.1% toluene. According to studies of Cai et al. (2010) and Lam et al. (2013), Factor 3 was identified as Architectural Coatings dominated aromatics. Factor 13 was considered to be Commercial Natural Gas as it consisted of 27.2% ethane, followed by lower amount of propane (26.7%), acetylene (7.9%), and ethylene (7.9%). Factor 6 consisted of 17.7% m and p-xylene, followed by 14.1% hexane. According to studies of Lam et al. (2013), Factor 6 was Adhesive Sealant Coating.

Factor 8 was identified as Liquid Petroleum Gas (Song et al., 2008; Morino et al., 2011; Yuan et al., 2009; Templer, 2007) as propane accounted for 18.7% of total concentration, followed by 12.1% butane. Factor 7 was Industrial Refinery becuase butane and n&isopentane accounted for large amount with 21.6% and 17.9%, respectively. There was also lower amount of benzene (3.5%) in Factor 7. Thus, Factor 7 was identified as Industrial Refinery. Factor 10 was considered as Coke Oven because it consisted of 23.1% ethane, 18.5% toluene, 12.4% butane, 8.6% ethylene and 8.4% acetylene, which are the species markers of Coke Oven.

For summer 2006, the species were also classified into six groups. The sum percentage of each group of winter 2006 is listed in Table 4.8, followed by the source identification results.

Table 4.8 Sum percentage of six classes in each PMF factor for summer 2006

Factor	aromatics	isoalkanes	|isoalkanes-aromatics|/(larger one)*100%	alkene	alkane	isoprene	cycloalkane
Factor 1 Liquid Gasoline	19.1	29.9	36.1	7.9	30.9	0	2.2
Factor 2 Coke Oven	36.2	14.6	-59.7	7.6	25.6	0	2
Factor 3 Commercial Natural Gas	22	7.9	-64.1	17.2	35.8	5.5	1.8
Factor 4 Liquid Petroleum Gas	8.7	9.1	4.4	6.3	63.3	0	2.9
Factor 5 Gasoline Exhaust	28.2	17.9	-36.5	5.6	38.6	0	1
Factor 6 Biogenic Emission	27.3	17.1	-37.4	3	23.9	13.3	2.2
Factor 7 Industrial Refinery	28	20.5	-26.8	2.8	43.1	0.9	0.5
Factor 8 Gasoline Vapour	20.5	34.6	40.8	2.2	34.2	0	2.9
Factor 9 Diesel Exhaust	34.6	19.5	-43.6	2.2	36.2	0	1
Factor 10 Gasoline Exhaust	32.6	28.7	-12.0	4.1	26.6	0.1	3
Factor 11 Architectural Coatings	66.3	17.7	-73.3	1.7	7.2	0	2.9
Factor 12 Gasoline Vapour	10.8	32.9	67.2	4	32.8	2.8	2.8
Factor 13 Adhesive and Sealant Coatings	41.3	25.8	-37.5	5.8	22.4	0	3.7

Among the profiles of summer 2006, Factor 10, 11, and 13 consisted of aromatics and isopentane as the most abundant species. The differences between the per cent of aromatics and isopentane in Factor 11 and 13 exceeded 30%. The amount of aromatics in Factor 10 was 32.6%, slightly higher than isopentane (28.7%). According to Harley and Kean (2004), Gasoline Exhaust consists of higher proportion of aromatics compared to isoalkanes. Thus, Factor 10 could be Gasoline Exhaust. There were 11.1% isopentane, 8.4% m and p-xylene, and 5.2% toluene in Factor 10. According to Song et al. (2008), Yuan et al., (2009), and Templer (2007), isopentane, m and p-xylene, and toluene are species markers of Gasoline Exhaust profile. Thus, Factor 10 was identified as Gasoline Exhaust.

Toluene and m and p-xylene accounted for significant amount of total concentration of Factor 11 with 35.1% and 14.3%, respectively. The aromatics species accounted for 66.3% of total concentration of Factor 11. According to studies of Cai et al., (2010), Lam et al. (2013), aromatics are the leading species in Architectural Coatings profile. Thus, Factor 11 was considered as Architectural Coatings. Factor 13 consisted of significant amount of aromatics including 12.9% toluene, 9.1% xylene, and also 10.6% hexane, which are typical compounds emitted from Adhesive and Sealant Coatings (Lam et al., 2013). Thus, Factor 13 was identified as Adhesive and Sealant Coatings.

Factor 8 and 12 were both dominated by isoalkanes with percentage of 34.6% and 32.9%, respectively. Isopentane in both Factor 8 and Factor 12 took 22.2% and 16.3% of total concentration, indicating that Factor 8 and 12 could both being Gasoline Vapour. Factor 12 consisted of low amount of aromatics (10.8%), indicating that Factor 12 was Gasoline Vapour. Factor 8 was identified as Gasoline Vapour although Factor 12 was

Gasoline Vapour. Factor 8 was not Gasoline Exhaust as species markers including ethylene or acetylene was not rich in this profile. Factor 8 was not liquid Gasoline because the difference between the aromatics and isoalkanes (40.8%) was much higher than 30%. Thus, Factor 8 was identified as Gasoline Vapour.

Decane and undecane were most abundant in Factor 9 with 4% and 3.8%, respectively among all factors. The amount of aromatics (34.6%) was higher than that of isoalkanes (19.5%). According to studies of Lam et al. (2013); Yuan et al. (2009); Song et al. (2008), decane and undecane are species markers of Diesel Exhaust profile. Thus, Factor 9 was Diesel Exhaust. Ethane was most abundant species in Factor 3 with 28.5% of total concentration, followed by lower amount of other species with less than 10% including m, p-xylene (8.5%), and acetylene (5.4%). Thus, Factor 3 was Commercial Natural Gas.

Factor 4 was dominated by propane with 44.2% of total concentration, indicating that Factor 4 being Liquid Petroleum Gas. Factor 6 consists of significant amount of isoprene (13.3%). Hence, it was Biogenic Emission. Factor 1 consisted of 29.9% isoalkanes, followed by 19.1% aromatics. Thus, Factor 1 was Liquid Gasoline. There were 17.9% isopentane, followed by 13.6% toluene in Factor 1. Thus, Factor 1 was identified as Liquid Gasoline.

Factor 7 was considered as Industrial Refinery as it contained arge proportion of isobutene (11.9%) and isopentane (7.2%), followed by lower amount of toluene (11.9%), and m and p-xylene (8.9%). According to studies of Cai et al. (2010), Song et al. (2008), Chan et al. (2011), and Templer (2007), n&iso-butene and isopentane are the leading

spicies in Industrial Refinery. Factor 2 was rich on 1,2,4-trimethylbenzene (11.1%), followed by ethane (9.7%), isopentane (8.0%), and butane (4.4%). Both ethane and 1,2,4-trimethylbenzene were considered as species markers for Coke Oven emission (US EPA, 2013; U.S. Government, 2011). Thus, Factor 2 was identified as Coke Oven.

Factor 5 was Gasoline Exhaust (Harley and Kean, 2004) as aromatics (28.2%) accounted for higher proportion compared with isopentane (17.9%). Also, toluene (20.2%) and isopentane (9.9%), species markers of Gasoline Exhaust were rich in Factor 5. Although Factor 10 was identified as Gasoline Exhaust, Factor 5 was interpreted as Gasoline Exhaust as well. Factor 5 was not Architectural Coatings as Coating profile contain mostly aromatics species. The percentage of xylene, another species maker for Coatings, was not high either in Factor 5. Factor 5 was not Industrial Refinery, although species markers including toluene, butane, and n&iso-pentane were rich. This is because the proportion of butane (8.4%), and n&iso-pentane (17.2%), respectively were lower than aromatics toluene (20.2%). Thus, Factor 5 was identified as Gasoline Exhaust. There could be large uncertainties of the identification results because the identification procedure has not been tested.

The sources in both winter and summer and the source contributions are shown in Table 4.9. There were ten sources in both seasons: Gasoline Exhaust, Gasoline Vapour, Liquid Gasoline, Diesel Exhaust, Commercial Natural Gas, Liquid Petroleum Gas, Industrial Refinery, Coke Oven, Architectural Coatings, and Adhesive & Sealant Coatings. Biogenic Emission (2.8 $\mu g/m^3$; 6.3%) with small contribution was identified in summer but not in winter. In winter, there were three source profiles identified as

Gasoline Exhaust; in summer, two were Gasoline Exhaust, and two were Gasoline Vapour.

Table 4.9 List of sources and source contributions in winter and summer 2006 from PMF

Winter	**Concentration ($\mu g/m^3$)**	**Per cent (%)**	**Summer**	**Concentration ($\mu g/m^3$)**	**Per cent (%)**
Gasoline Exhaust (F 2)	2.2	6.8	Gasoline Exhaust (F5)	5.6	12.7
Gasoline Exhaust (F4)	2.5	7.8	Gasoline Exhaust (F10)	2.8	6.3
Gasoline Exhaust (F12)	1.9	5.9			
Gasoline Vapour (F5)	3.1	9.6	Gasoline Vapour (F8)	3.9	8.8
			Gasoline Vapour (F12)	3.4	7.7
Diesel Exhaust (F 9)	1.4	4.3	Diesel Exhaust (F9)	3.4	7.7
Liquid Gasoline (F1)	2.5	7.8	Liquid Gasoline (F1)	3.4	7.7
Industrial Refinery (F7)	3.8	11.8	Industrial Refinery (F7)	4.3	9.8
Liquid Petroleum Gas (F8)	2.4	7.5	Liquid Petroleum Gas (F4)	3.2	7.3
Commercial Natural Gas (F13)	3.1	9.6	Commercial Natural Gas (F3)	2.6	5.9
Coke Oven (F10)	3.7	11.5	Coke Oven (F2)	2.3	5.2
Architectural Coatings (F3)	2.5	7.8	Architectural Coatings (F11)	3.6	8.2
Adhesive and Sealant Coatings (F 6)	1.4	4.3	Adhesive and Sealant Coatings (F13)	2.8	6.3
Undetermined (Factor 11)	1.7	5.3			
			Biogenic Emission (Factor 6)	2.8	6.3
Total	32.2	100		44.1	100

There were three profiles identified as Gasoline Exhaust with total contribution of 20.5% in winter 2006. There two profiles identified as Gasoline Exhaust with total contribution of 19%, and another two identified as Gasoline Vapour with total contribution of 16.5% in summer 2006. The contributions from all sources increased from winter to summer with the exception of Commercial Natural Gas (9.6% vs. 5.9%) and Coke Oven (11.5% vs. 5.2%). The surge decrease of Coke Oven contribution from winter to summer may due to the uncertainty of the Coke Oven contribution to the VOC concentrations. Two vehicle-related sources Gasoline Exhaust and Gasoline vapour were the largest contributors in both winter and summer 2006. Gasoline Exhaust contributed 20.5% and 19%, in winter and summer, respectively. Gasoline Vapour contributed 3.1μg/m^3 (9.6%) in winter, 7.3μg/m^3 (16.6%) in summer. Industrial Refinery was also the dominant source in both seasons (winter: 11.8%; summer: 9.8%). In winter, Commercial Natural Gas and Coke Oven were also observed to be the major contributors with the contribution mass percentage 9.6% and 11.5%, respectively. In summer, Architectural Coatings was another major contributor with mass percentage of 8.2%.

The sources identified in both seasons with species accounting for 6% or more of source profiles are listed in Table 4.10. The same source profiles in different seasons were similar with slight differences.

Table 4.10 Sources and the species accounted for 6% or more in profiles in winter and summer 2006 (pink shade indicates the same species in the same profiles of winter and summer)

Winter factor	Species	Per cent (%)	Summer factor	Species	Per cent (%)
Factor 1 Liquid Gasoline	butane	13.8	**Factor 1 Liquid Gasoline**	isopentane	17.9
	toluene	12.4		toluene	13.6
	isopentane	11.2		ethane	9.4
	ethane	6.7		pentane	9.1
	isobutane	6.3		other	8.2
				butane	7.4
Factor 2 Gasoline Exhaust	ethane	22.1	**Factor 5 Gasoline Exhaust**	toluene	20.2
	butane	19.2		propane	12.8
	ethylene	7		isopentane	9.9
	propane	6.4		butane	8.4
	others	6		other	8.1
Factor 3 Architectural Coatings	toluene	46.1	**Factor 11 Architectural Coatings**	toluene	35.1
	propane	12.9		m and p-xylene	14.3
	ethane	11		isobutane	7.5
	butane	7.3			
Factor 4 Gasoline Exhaust	toluene	16.8	**Factor 10 Gasoline Exhaust**	isopentane	11.1
	isopentane	12.1		butane	10.0
	m and p-xylene	10.2		m and p-xylene	8.4
	pentane	9.8		2-methylpentane	7.2
	acetylene	9.3		ethane	6.2

Table 4.10-continued 1

Factor 5 Gasoline Vapour	propane	19	**Factor 8 Gasoline Vapour**	isopentane	22.2
	butane	18.3		pentane	19.9
	isopentane	11.6		butane	7.7
	pentane	9.3		toluene	7.3
	m and p-xylene	9			
	ethane	7.1			
Factor 6 Adhesive and Sealant Coatings	ethane	19.2	**Factor 13 Adhesive and Sealant Coatings**	toluene	12.9
	m and p-xylene	17.7		hexane	10.6
	hexane	14.1		m and p-xylene	9.1
	ethylene	6.4		isobutane	6.5
				3-methylpentane	6.0
Factor 7 Industrial Refinery	butane	21.6	**Factor 7 Industrial Refinery**	propane	28.2
	propane	12.9		isobutane	11.9
	ethane	12.5		toluene	11.9
	isopentane	11.1		m and p-xylene	8.9
	ethylene	7.1		isopentane	7.2
	pentane	6.8			
	isobutane	6.6			
Factor 8 Liquid Petroleum Gas	propane	18.7	**Factor 4 Liquid Petroleum Gas**	propane	44.2
	ethane	13.3		ethane	12.9
	butane	12.1		other	7.7
	ethylene	7.6			

Table 4.10 - continued 2

Factor 9 Diesel Exhaust	propane	16.5	**Factor 9 Diesel Exhaust**	toluene	18.7
	ethane	15.9		isopentane	14.1
	butane	14.5		pentane	10.3
	isopentane	10.8		ethane	9.2
	others	7.8		butane	6.9
	pentane	7.4		other	6.1
Factor 10 Coke Oven	ethane	23.1	**Factor 2 Coke Oven**	other	11.7
	toluene	18.5		1,2,4-trimethylbenzene	11.1
	butane	12.4		ethane	9.7
	ethylene	8.6		isopentane	8.0
	acetylene	8.4		3-ethyltoluene	6.0
Factor 11 Undetermined	hexane	23.5			
	toluene	11			
	3-methylpentane	9.2			
	butane	7.7			
	2-methylpentane	6.7			
	ethane	6.4			
	propane	6.1			
Factor 12 Gasoline Exhaust	ethane	18			
	ethylene	12.6			
	others	7.8			
Factor 13 Commercial Natural Gas	ethane	27.2	**Factor 3 Commercial Natural Gas**	ethane	28.7
	propane	26.7		ethylene	12.9
	acetylene	7.9		m and p-xylene	8.5
	ethylene	7.9			

Table 4.10 - continued 3

			Factor 6 Biogenic Emission	isoprene	13.3
				toluene	12.6
				other	12.3
				isopentane	9.0
			Factor 12 Gasoline Vapour	isopentane	16.3
				other	12.8
				pentane	11.5
				butane	9.4
				ethane	7.3

The Liquid Gasoline profiles in two seasons included butane, toluene, isopentane, and ethane. In winter profile, butane (13.8%) was the top one abundant species, while in summer profile; isopentane (17.9%) was the dominant species. Toluene accounted for the similar proportion with 12.4% and 13.6% in winter and summer profiles, respectively. The three Gasoline Exhausts profiles in winter were rich on ethane (Factor 2: 22.1%; Factor 12: 18%), butane (Factor 2: 19.2%), ethylene (Factor 2: 7%; Factor 12: 12.6%), propane (Factor 2: 6.4%), toluene (Factor 4: 16.8%), isopentane (Factor 4: 12.1%), m and p-xylene (Factor 4: 10.2%), and acetylene (Factor 4: 9.3%). Butane (Factor 10: 10%; Factor 5: 8.4%), m and p-xylene (Factor 10: 8.4%), ethane (Factor 10: 6.2%), toluene (Factor 5: 20.2%), propane (Factor 5: 12.8%), and isopentane (Factor 10: 11.1%; Factor 5: 9.9%) were also found with high percentage in Gasoline Exhaust profiles in summer. The Gasoline Vapour profiles in both seasons were dominated by butane, isopentane, pentane, and ethane. Species m and p-xylene was rich in Gasoline Vapour profiles of winter but not in that of summer; toluene was abundant in summer but not in winter.

The Architectural Coatings profiles were dominated by toluene with 46.1% and 35.1% in winter and summer profiles, respectively. In the profiles of Adhesive and Sealant Coatings, hexane accounted for 14.1% and 10.6% in winter and summer, respectively. M and p-xylene accounted for 17.7% and 9.1% in Adhesive and Sealant Coatings in winter and summer, respectively. Propane, isopentane, and isobutane accounted for large proportion of the profiles of Industrial Refinery in both winter and summer. In winter, ethane, ethylene, and pentane were also abundant; while in summer, toluene, and m and p-xylene were rich in Industrial Refinery profile. Profiles of Liquid Petroleum Gas in both seasons were rich on propane (winter: 18.7%; summer: 44.2%), and ethane (winter: 13.3%; summer: 12.9%). Diesel Exhaust profiles were with large percentage of ethane (winter: 15.9%; summer: 9.2%), butane (winter: 14.5%; summer: 6.9%), isopentane (winter: 10.8%; summer: 14.1%), and pentane (winter: 7.4%; summer: 10.3%) in both winter and summer.

The profiles of Coke Oven in different seasons were different. In winter profile, it was rich on ethane, toluene, butane, ethylene, and acetylene; while in summer it was rich on 1,2,4-trimethylbenzene, ethane, isopentane, and 3-ethyltoluene. Species including ethane, toluene, butane, ethylene, and acetylene were species markers of Coke Oven emission. However, none of the species toluene, butane, ethylene, and acetylene was abundant in summer compared to winter. This could be due to the different vapour pressure of the species markers of Coke Oven, leading to different source composition from winter to summer. Commercial Natural Gas source profiles in both seasons were dominated by ethane (winter: 27.2%; summer: 28.7%), followed by ethylene (winter: 7.9%; summer: 12.9%).

Overall, the profiles with the same titles identified from two seasons had a great agreement in terms of species with large proportion, with slight differences. This was expected as the properties of the sources remained unchanged. The slight variations of species might be due to the weaker atmospheric mixing and slower chemical reactions caused by lower temperature in winter.

4.4 PCA Source Apportionment Results

4.4.1 Principal Components Results

Species 1,3-diethylbenzene, 1,4-diethylbenzene, iso-propylbenzene, and others were excluded from winter 2006 dataset. Species 1,3-diethylbenzene, 1,4-diethylbenzene, 1-butene, iso-propylbenzene, trans-2-butene were excluded from summer 2006 dataset. The species with factor loadings equal or greater than 0.26 in one component or more for both winter and summer 2006 are shown in Table 4.11.

Table 4.11 Components and species with absolute loadings equal or greater than 0.26 or greater in any of the nine components

(The species with absolute loadings equal or greater than 0.26 were highlighted in pink)

(a) Winter 2006

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
BZ123M	-0.01	0.01	0.00	-0.26	-0.02	0.02	-0.01	0.04	0.02
BZ124M	-0.02	0.02	-0.04	-0.35	0.02	0.00	-0.05	-0.02	-0.02
BZ135M	0.01	0.01	-0.02	-0.31	0.03	0.02	-0.02	0.00	-0.02
LBUT1E	-0.01	0.04	0.03	-0.06	-0.26	0.16	0.01	-0.05	-0.01
P1E2ME	-0.04	-0.01	0.02	-0.03	-0.43	-0.04	-0.13	-0.21	0.09
PENTE1	-0.09	0.00	0.02	-0.04	-0.50	-0.11	-0.12	-0.14	-0.01
PA224M	0.38	0.03	-0.01	0.06	0.04	-0.02	-0.06	0.00	-0.05
PA234M	0.32	0.13	-0.04	0.02	0.07	-0.02	-0.04	0.06	-0.09
PEN24M	0.09	0.11	-0.01	0.05	-0.03	0.01	0.03	-0.07	0.41
O_ETOL	-0.01	0.01	-0.02	-0.32	0.01	0.01	0.01	0.01	-0.01
PENA2M	0.07	0.41	-0.08	-0.03	-0.03	0.01	0.01	0.00	-0.02
M_ETOL	0.04	0.01	0.00	-0.28	0.00	0.04	0.00	-0.04	-0.02
HEP3ME	0.26	-0.05	0.03	-0.11	0.02	-0.01	0.02	-0.02	0.00
PENA3M	-0.06	0.52	-0.08	-0.04	0.01	-0.01	0.00	0.04	-0.04
P_ETOL	0.04	0.00	-0.01	-0.29	-0.01	0.04	0.01	-0.05	-0.02
ACETYL	0.00	0.02	-0.04	-0.18	0.05	0.34	0.45	-0.02	-0.01
BENZE	0.07	-0.04	0.01	0.05	-0.07	0.35	-0.12	-0.04	0.07
N_BUTA	0.03	0.04	-0.04	0.02	-0.08	0.01	-0.02	0.35	-0.02
C2BUTE	0.07	0.00	-0.01	0.08	-0.27	0.06	0.04	0.20	-0.05
C2PENE	0.05	0.00	-0.04	0.02	-0.30	0.03	0.07	0.12	0.01
CYHEXA	0.07	0.12	0.01	0.01	0.03	0.14	-0.17	-0.30	0.30
N_DEC	-0.11	0.00	0.09	-0.24	-0.14	-0.25	0.08	0.11	0.08
ETHANE	-0.17	-0.05	0.04	-0.10	0.07	0.04	0.09	0.38	0.20
ETBZ	0.04	-0.03	0.55	0.03	0.02	0.01	0.00	-0.01	-0.01
ETHENE	-0.08	0.04	-0.04	-0.12	0.10	0.49	0.09	0.10	-0.01
N_HEPT	0.27	-0.03	0.02	-0.06	-0.02	0.00	0.02	-0.01	0.02
N_HEX	-0.09	0.46	0.27	0.03	0.05	-0.06	-0.03	-0.02	-0.04
I_BUTA	0.05	0.04	-0.04	0.06	0.03	0.01	-0.19	0.34	0.07
MP_XYL	0.05	-0.02	0.54	0.03	0.03	0.03	-0.01	-0.02	-0.01

(a) - continued

MECYHX	0.07	-0.04	-0.05	-0.16	0.06	0.00	-0.43	-0.05	0.05
MCYPNA	-0.10	0.44	0.02	0.01	0.00	-0.02	0.01	-0.03	0.20
N_PRBZ	0.04	0.00	0.02	-0.28	-0.01	-0.01	0.05	0.00	-0.02
N_OCT	0.13	-0.05	-0.02	-0.25	0.04	-0.15	-0.17	-0.05	0.02
O_XYL	0.01	-0.02	0.49	-0.01	-0.01	0.04	0.01	-0.01	0.00
N_PROP	-0.03	0.05	0.01	0.05	0.17	0.12	-0.45	0.29	-0.16
PROPE	-0.01	-0.01	0.06	-0.07	-0.08	0.35	-0.03	-0.01	0.00
STYR	-0.19	0.01	0.04	-0.08	-0.13	0.29	-0.42	0.02	-0.06
T2BUTE	0.06	0.02	-0.01	0.07	-0.28	0.02	0.04	0.21	-0.06
T2PENE	0.04	0.01	-0.03	0.01	-0.31	0.03	0.08	0.10	0.00
TOLUE	-0.11	-0.14	-0.05	0.04	0.04	0.00	-0.08	0.14	0.68
N_UNDE	-0.13	0.02	0.11	-0.20	-0.02	-0.22	0.09	0.29	0.05
Eigenvalue	31.1	3.9	3.2	2.7	2.3	1.6	1.4	1.3	1.0
Variance Explained (%)	59.7	7.5	6.2	5.2	4.4	3.0	2.8	2.4	2.0

(b) Summer 2006

	PC1	**PC2**	**PC3**	**PC4**	**PC5**	**PC6**	**PC7**	**PC8**	**PC9**
BZ123M	-0.04	-0.3	-0.01	0.04	0.05	-0.01	0.03	-0.07	-0.04
BZ124M	-0.03	-0.32	0	0.01	0.03	0.01	-0.03	-0.04	-0.01
BZ135M	-0.05	-0.32	0	0.03	0	-0.01	-0.02	-0.04	-0.01
P1E2ME	-0.03	0.01	0	-0.03	-0.01	0	0.46	-0.09	-0.11
PENTE1	-0.04	0.03	0.04	0.03	-0.04	-0.03	0.44	0.05	-0.19
PA224M	0.15	0.1	0	-0.05	-0.31	0.11	0.17	-0.04	0.13
BU22DM	0.31	0.05	-0.01	-0.07	0.08	0.04	0.08	-0.08	0
PA234M	0.03	0.03	0	0.03	-0.38	0.01	0.14	-0.01	0
BU23DM	0.16	0	0	0.02	0.01	0.08	0.01	-0.21	-0.04
PEN23M	0.26	0.02	-0.03	0	-0.12	0.01	0.02	-0.01	-0.02
PEN24M	0.15	0.04	-0.02	0	-0.06	0.14	0.11	-0.13	-0.03
O_ETOL	-0.03	-0.31	0	0.02	0.01	-0.01	-0.01	-0.05	0
IPENTA	0.24	0.05	0.03	0.15	-0.03	-0.07	-0.06	-0.01	-0.11
HEP2ME	0.12	-0.23	0.04	-0.06	-0.01	-0.01	0.06	0.12	-0.01
HEXA2M	0.28	-0.02	-0.01	-0.01	-0.02	-0.01	-0.06	0.02	-0.1
PENA2M	0.15	-0.04	0	0.02	0.02	0.05	0.01	-0.22	-0.03

(b)-continued

M_ETOL	-0.02	-0.31	0.01	0.02	0.01	0	-0.02	-0.05	0
HEP3ME	0.16	-0.19	-0.03	0	0	-0.02	0	0.09	-0.08
HEXA3M	0.33	-0.01	0	-0.03	0	0.02	-0.05	0	0.01
PENA3M	0.03	-0.09	0	0.01	-0.05	0.01	0	-0.28	-0.09
P_ETOL	-0.01	-0.3	0.02	0.01	0.02	0.01	-0.01	-0.06	0.03
ACETYL	0.06	-0.05	0	-0.12	0.14	0.51	-0.04	-0.06	0.03
BENZE	0.05	0.03	0.02	0.14	-0.1	0.19	-0.02	0.26	-0.25
N_BUTA	0.13	0.09	0.13	0.08	-0.07	-0.06	-0.02	-0.02	-0.23
C2BUTE	-0.03	-0.02	0	0	-0.09	-0.06	0.06	-0.02	-0.42
C2PENE	0.02	0.01	-0.03	-0.05	0.12	0.04	0.05	-0.18	-0.38
CYHEXA	0.16	-0.04	-0.08	-0.19	-0.34	-0.21	-0.11	0.07	-0.15
CPENTA	0.31	0.03	0.05	0.1	0.09	0.04	0.02	-0.1	0.18
N_DEC	-0.02	-0.02	0	0.53	0.02	0.04	0	-0.06	0.05
ETHANE	-0.07	0.08	-0.06	0.27	-0.03	0.45	0	0.07	-0.09
ETBZ	0	-0.02	0.43	-0.01	0.02	0.02	-0.02	-0.01	0.01
ETHENE	-0.06	-0.01	0.03	-0.13	-0.18	0.5	-0.11	-0.21	0.17
N_HEPT	0.37	-0.05	0.01	-0.08	0	-0.04	0.03	0.05	0.14
N_HEX	-0.04	-0.11	0.01	0	-0.09	0.04	0.05	-0.31	-0.04
I_BUTA	-0.06	0.01	0.46	-0.06	-0.03	-0.05	0	-0.03	0.01
I_PREN	0.08	-0.04	0.01	-0.11	0.54	0.1	0.11	0.28	-0.18
MP_XYL	0.01	-0.03	0.41	0	0.03	0	-0.02	-0.01	0
MECYHX	0.03	-0.3	0	-0.1	-0.11	0.01	0.01	0.11	0.07
MCYPNA	0.02	-0.05	0.04	-0.06	0.02	0.12	0.07	-0.24	-0.12
N_NON	0	-0.1	-0.03	0.42	-0.08	-0.04	-0.02	0.03	-0.05
N_PRBZ	0	-0.28	0.01	0.04	0.01	0	0.01	-0.04	0.02
N_OCT	0.09	-0.26	-0.01	-0.02	-0.07	0	0.01	0.15	0.02
O_XYL	0.05	-0.05	0.38	0	0.07	0	-0.01	-0.02	0
N_PENT	0.27	0.05	0.03	0.19	0	-0.06	-0.06	-0.02	-0.01
N_PROP	-0.12	0.06	0.41	0.02	-0.04	0.03	0.06	-0.03	-0.02
PROPE	-0.15	-0.09	0.02	-0.02	-0.38	0.09	-0.1	0.12	-0.23
STYR	0.07	-0.07	0.01	-0.04	-0.07	0.3	0.13	0.49	-0.05
T2PENE	0.01	0.01	-0.03	-0.05	0.12	0.02	0.04	-0.17	-0.41
TOLUE	0.12	-0.01	0.29	0.04	-0.08	-0.01	0.01	0.16	-0.01
N_UNDE	0.02	-0.04	0.00	0.49	0.06	-0.03	0.04	0.02	0.05
OTHERS	-0.02	-0.06	-0.04	0.02	-0.02	-0.06	0.64	-0.01	0.25
Eigenvalue	27.2	5.4	3.8	3.0	2.0	1.6	1.3	1.2	0.9
Variance Explained (%)	53.4	10.6	7.4	5.9	4.0	3.2	2.6	2.3	1.7

There were nine components with eigenvalue greater than one for winter 2006. In summer, the first eight components had eigenvalues greater than one. The ninth with a margin eigenvalue of 0.88 was kept as well in order to keep the number of components consistent with winter 2006. These nine factors in winter and summer were rotated, respectively. By using the species with factor loadings equal or greater than 0.26, four or more species were used to identify sources. The full names of the abbreviation of species name are listed in Appendix G. Full PCA outputs are listed in Appendix H.

PCA was run with all 56 species, using Z score and varimax rotation for winter and summer 2006. There were nine components retained for both winter and summer 2006. The results of winter and summer were very similar with that of with species exclusion. However, in summer, component 8 and 9 was dominated by only styrene and others, respectively. With exclusion of the five species in summer 2006, the loadings of styrene, 3-methylpentane, benzene, hexane, and isoprene were high in component 8. The loadings of others, cis-2-butene, cis-2-pentene, trans-2-pentene were high in component 9. However, the different number of species used as model inputs could bring uncertainties to the components identifications. The results before species exclusion are listed in Appendix I. PCA was also run without using Z score, the results are listed in Appendix J.

4.4.2 Winter Factor Interpretation

The nine principal components in winter 2006 were identified. Table 4.12 shows the results and the species with loadings of 0.26 or greater in any component.

Table 4.12 Principal components of winter 2006 and loadings 0.26 or greater

PC1 (Diesel Exhaust)	**Loadings**	**PC 2 (Adhesive and Sealants Coatings)**	**Loadings**
2,2,4-trimethylpentane	0.38	2-methylpentane	0.41
2,3,4-trimethylpentane	0.32	3-methylpentane	0.52
3-methylheptane	0.26	hexane	0.46
heptane	0.27	methylcyclopentane	0.44
PC 3 (Architectural Coatings)	**Loadings**	**PC4 (Auto Painting)**	**Loadings**
ethylbenzene	0.55	1,2,3-trimethylbenzene	-0.26
hexane	0.27	1,2,4-trimethylbenzene	-0.35
m and p-xylene	0.54	1,3,5-trimethylbenzene	-0.31
o-xylene	0.49	2-ethyltoluene	-0.32
		3-ethyltoluene	-0.28
		4-ethyltoluene	-0.29
		n-propylbenzene	-0.28
PC5 (Industrial Refinery)	**Loadings**	**PC6 (Gasoline Exhaust)**	**Loadings**
1-hexene/2-methyl-1-pentene	-0.43	acetylene	0.34
1-pentene	-0.5	benzene	0.35
cis-2-butene	-0.27	propylene	0.49
cis-2-pentene	-0.3	styrene	0.35
trans-2-butene	-0.28	decane	0.29
trans-2-pentene	-0.31		
1-butene	-0.26		
PC7 (Undetermined)	**Loadings**	**PC8 (Commercial Natural Gas)**	**Loadings**
acetylene	0.45	butane	0.35
methylcyclohexane	-0.43	cyclohexane	-0.30
propane	-0.45	ethane	0.38
styrene	-0.42	isobutane	0.34
		propane	0.29
		undecane	0.29
PC9 (Liquid Gasoline)	**Loadings**		
2,4-dimethylpentane	0.41		
cyclohexane	0.3		
toluene	0.68		

Component 1 was likely to be the Diesel Exhaust. It contained abundant C_8 alkanes including 2,2,4-trimethylpentane (0.38), 2,3,4-trimethylpentane (0.32), and 3-methylheptane (0.26); and C_7 alkanes heptane (0.27) (Lai et al., 2013). According to the studies of Huang et al. (2012); Duan et al. (2008); Guo et al. (2007); Lam et al. (2013), Component 2 was Adhesive Sealant Coatings identified by heavy loadings of 3-methylpentane (0.52), hexane (0.46), methylcyclopentane (0.44), and 2-methylpentane (0.41). Species 3-methylpentane was found in glue used in shoe manufacturing (U.S. National Library of Medicine, 2014). Hexane was used as an aliphatic solvent in Adhesive and Sealant Coatings (Wypych, 2000). Species 2-methylpentane and methylcyclopentane were also considered as main ingredient of glues (U.S. National Library of Medicine, 2014).

Component 3 was considered as Architectural Coatings as it was influenced strongly by ethylbenzene (0.55), and m and p-xylenes (0.54), o-xylene (0.49). According to Huang et al. (2012); Duan et al. (2008); and Guo et al. (2007), those species are abundant in Architectural Coatings. Component 4 was identified as Auto Paintings. It had high loadings of 1,2,4-trimethylbenzene (-0.35), 2-ethyltoluene (-0.31), and 1,3,5-trimethylbenzene (-0.31). According to the Substance Reporting by Toyota Motor Manufacturing Canada (Woodstock) (2009), 1,2,4-trimethylbenzene is a component of auto paint. According to a report from New York Department of Environmental Conservation (2014), 1,3,5-trimethylbenzene is used as a paint thinner. Species n-ethyltoluene, n-propylbenzene are species markers, according to Huang et al. (2012).

Component 5 was considered to be Industrial Refinery because it was rich on alkenes including 1-pentene (-0.5), cis-2-butene (-0.27), cis-2-pentene (-0.3), trans-2-butene (-0.28), and trans-2-pentene (-0.31). Studies Chang et al. (2009), Guo et al. (2007), Huang et al. (2012), and Guo et al. (2006) indicated that Industrial Refinery consisted of abundant alkenes. The high loadings of Component 5 consisted of propylene (0.49), benzene (0.35), acetylene (0.34), styrene (0.35), and undecane (0.29). According to Lai et al. (2013), Wang et al. (2013), and Song et al. (2008), propylene, benzene, and acetylene were the species markers of Gasoline Exhaust. According to the Technical Factsheet on styrene by U.S. EPA (2013), styrene is emitted in automobile exhaust. The loading of decane is moderate, indicating that decane is not significant factor on Component 5.

In component 7, the species with high positive loading is acetylene (0.45); and species with high negative loadings are propane (-0.45), methylcyclohexane (-0.43), and styrene (-0.42). Component 7 is the source that could reveal the differences between acetylene with propane, methylcyclohexane, and styrene in terms of the contribution to the source. No profile was found to match the three species with positive loadings. Acetylene points towards Gasoline Exhaust; however, source could not be determined by one species. Therefore, Component 7 was undetermined.

Component 8 was Commercial Natural Gas because there were high positive loadings of ethane (0.38), iso&n-butane (0.34 and 0.35), and propane (0.29). The negative sign of cyclohexane (-0.30) reflects the difference between the species ethane, iso&n-butane, and propane with cyclohexane in terms of the mass fraction in Commercial Natural Gas. There is no study in the review showing high percentage of cyclohexane and low of ethane, iso&n-butane, and propane. According to Guo et al.

(2007) and Wang et al. (2006), toluene and 2,4-dimethylpentane have high loadings in Gasoline Evaporations. Thus, the high loading of toluene (0.68), and 2,4-dimethylpentane (0.41) indicated that Component 9 was Gasoline Evaporations.

4.4.3 Summer Factor Interpretation

The nine Principal Components in summer 2006 were identified. Table 4.13 shows the results and the species with loadings of 0.26 or greater in each component.

Table 4.13 Principal components of summer 2006 and loadings 0.26 or greater

PC 1 (Gasoline Exhaust)	**Loadings**	**PC 2 (Auto Paintings)**	**Loadings**
2,2-dimethylbutane	0.31	1,2,3-trimethylbenzene	-0.30
2,3-dimethylpentane	0.26	1,2,4-trimethylbenzene	-0.32
2-methylhexane	0.28	1,3,5-trimethylbenzene	-0.32
3-methylhexane	0.33	2-ethyltoluene	-0.31
cyclopentane	0.31	3-ethyltoluene	-0.31
heptane	0.37	4-ethyltoluene	-0.30
pentane	0.27	methylcyclohexane	-0.30
		n-propylbenzene	-0.28
		octane	-0.26
PC 3(Architectural Coatings/Solvents)	**Loadings**	**PC 4 (Diesel Exhaust)**	**Loadings**
ethylbenzene	0.43	decane	0.53
Iso-butane	0.46	ethane	0.27
m and p-xylene	0.41	nonane	0.42
o-xylene	0.38	undecane	0.49
propane	0.41		
toluene	0.29		
PC 5 (Biogenic)	**Loadings**	**PC 6 (Gasoline Exhaust)**	**Loadings**
2,2,4-trimethylpentane	-0.31	acetylene	0.51
2,3,4-trimethylpentane	-0.38	ethane	0.45
cyclohexane	-0.34	ethylene	0.50
isoprene	0.54	styrene	0.30
PC7 (Industrial Refinery)	**Loadings**	**PC8 (Undetermined)**	**Loadings**
1-hexene/2-methyl-1-pentene	0.46	3-methylpentane	-0.28
1-pentene	0.44	benzene	0.26
others	0.64	hexane	-0.31
		isoprene	0.28
		styrene	0.49
PC9 (Industrial Refinery)	**Loadings**		
cis-2-butene	-0.42		
cis-2-pentene	-0.38		
trans-2-pentene	-0.41		

In summer 2006, there were 9 principal components. Heptane (0.37), 3-methylhexane (0.33), 2,2-dimethylbutane (0.31), and cyclopentane (0.31) were rich in Component 1. According to Lai et al. (2013), heptane and 2,2-dimethylbutane have high loadings in Gasoline Exhaust. According to the report of U.S. National Library of Medicine (2014), traffic emission is a major source of 3-methylhexane. Species cyclopentane is emitted from Gasoline Exhaust (U.S. National Library of Medicine, 2014). The loadings of 2,3-dimethylpentane (0.26), 2-methylhexane (0.28), and pentane (0.27) are moderate, indicating that weak relationships between the species and the source. Thus, Component 1 was identified as Gasoline Exhaust.

Component 2 was identified as Auto-painting because it was loading high on aromatics species including 2-ethyltoluene (-0.31), 3-ethyltoluene (-0.31), 1,3,5-trimethylbenzene (-0.32), 1,2,3-trimethylbenzene (-0.30), and n-propylbenzene (-0.28). Component 3 was identified to be Architectural Coatings as it was loading high on ethylbenzene (0.43), m and p-xylene (0.41), o-xylene (0.38), and toluene (0.29) with lower loadings of iso-butane (0.46) and propane (0.41). According to Huang et al. (2012), Duan et al. (2008), and Guo et al. (2007), those species had high loadings in Architectural Coatings.

Component 4 was considered to be Diesel Exhaust. It was rich on decane (0.53), undecane (0.49), nonane (0.42), and ethane (0.27) (Lai et al., 2013), indicating that it is Diesel Exhaust. Component 5 was Biogenic Emission because the loading of isoprene (0.54) was much higher than the other loadings (2,2,4-trimethylpentane: -0.31; 2,3,4-trimethylpentane: -0.38; cyclohexane: -0.34). The loading of isoprene is higher than any other negative loadings in this component. Thus, it played dominant role in explaining

the component.

Component 6 was identified as Gasoline Exhaust. Component 6 was rich on ethylene (0.50), acetylene (0.51), ethane (0.45), and less related with aromatics styrene (0.30). According to Wang et al. (2013), Yuan et al. (2009), Song et al. (2008), and Templer (2007), ethylene and acetylene were species markers for Gasoline Exhaust. Although Component 1 has been identified as Gasoline Exhaust, component 6 was not any other source. It was not Industrial Refinery as alkenes including 1-butene (Guo et al., 2007; Huang et al., 2012), cis/trans-butene (Huang et al., 2012), propene (Chang et al., 2009; Guo et al., 2007) were not rich in component 6. It was not Gasoline Vapour or Liquid Gasoline as the species marker n&iso-pentane (Guo et al., 2007; Wang et al., 2006) was not with high loadings. Thus, component 6 was identified as Gasoline Exhaust.

Component 7 was considered to be Industrial Refinery, because the loadings of species others (0.64), 1-hexene (0.46) and 1-pentene (0.44) are high. According to Templer (2007), others is the top 1 species in Industry Refinery emission. Species 1-hexene and 1-pentene are also significant species in Industry Refinery (Cai et al., 2010; Huang et al., 2012).

Component 8 consisted of species with high positive loadings including styrene (0.49), isoprene (0.28), and benzene (0.26); and species with high negative loadings including hexane (-0.31) and 3-methylpentane (-0.28). Component 8 is a source that could show the percentage difference between hexane and 3-methylpentane with styrene, isoprene, and benzene. No profile is found to match the three species with positive loadings. 3-methylpentane and hexane could point towards Diesel Exhaust; however,

either decane or undecane having high loadings in Component 8, and Component 4 was identified as Diesel Exhaust. Therefore, Component 8 was undetermined.

Component 9 was identified as Industrial Refinery as cis-2-butene (-0.42), trans-2-pentene (-0.41), and cis-2-pentene (-0.38). Industrial Refinery consisted of abundant alkenes including cis-2-butene, trans-2-pentene, and cis-2-pentene, according to Chang et al. (2009), Guo et al. (2007), Huang et al. (2012), and Guo et al. (2006). Although Component 7 has been identified as Industrial Refinery; component 9 was not any other source. Component 9 was Gasoline Exhaust as alkenes are part of species markers for Gasoline Exhaust. However, component 9 was not Gasoline Exhaust as the loadings of species markers including 2,2,4-trimethylpentane, iso-butane, and n-pentane, n-pentane, n-heptane, 2,3-dimethylbutane, benzene, propene, or 2-methylpentane were not high.

There were similarities and differences of the sources identified from PCA profiles in winter and summer 2006. Table 4.14 lists all the sources in both seasons and the species with loadings 0.26 or greater.

Table 4.14 Sources from PCA in winter and summer 2006 (Pink shade indicates the same species with high loadings in the same profiles of winter and summer)

PC6 (Gasoline Exhaust)	**Loadings**	**PC1 (Gasoline Exhaust)**	**Loadings**
acetylene	0.34	2,2-dimethylbutane	0.31
benzene	0.35	2,3-dimethylpentane	0.26
propylene	0.49	2-methylhexane	0.28
styrene	0.35	3-methylhexane	0.33
decane	0.29	cyclopentane	0.31
		heptane	0.37
		pentane	0.27
		PC 6 (Gasoline Exhaust)	**Loadings**
		acetylene	0.51
		ethane	0.45
		ethylene	0.5
		styrene	0.3
PC9 (Liquid Gasoline)	**Loadings**		
2,4-dimethylpentane	0.41		
cyclohexane	0.3		
toluene	0.68		
PC1 (Diesel Exhaust)	**Loadings**	**PC 4 (Diesel Exhaust)**	**Loadings**
2,2,4-trimethylpentane	0.38	decane	0.53
2,3,4-trimethylpentane	0.32	ethane	0.27
3-methylheptane	0.26	nonane	0.42
heptane	0.27	undecane	0.49
PC8 (Commercial Natural Gas)	**Loadings**		
butane	0.35		
cyclohexane	-0.3		
ethane	0.38		
isobutane	0.34		
propane	0.29		
Undecane	0.29		

Table 4.14 – continued 1

PC5 (Industrial Refinery)	**Loadings**	**PC9 (Industrial Refinery)**	**Loadings**
1-hexene/2-methyl-1-pentene	-0.43	cis-2-butene	-0.42
1-pentene	-0.5	cis-2-pentene	-0.38
cis-2-butene	-0.27	trans-2-pentene	-0.41
cis-2-pentene	-0.3	others	0.25
trans-2-butene	-0.28		
trans-2-pentene	-0.31		
1-butene	-0.26		
		PC7 (Industrial Refinery)	**Loadings**
		1-hexene/2-methyl-1-pentene	0.46
		1-pentene	0.44
		others	0.64
PC 3 (Architectural Coatings/Solvents)	**Loadings**	**PC 3(Architectural Coatings/Solvents)**	**Loadings**
ethylbenzene	0.55	ethylbenzene	0.43
hexane	0.27	isobutane	0.46
m and p-xylene	0.54	m and p-xylene	0.41
o-xylene	0.49	o-xylene	0.38
		propane	0.41
		toluene	0.29
PC 2 (Adhesive and Sealants Coatings)	**Loadings**		
2-methylpentane	0.41		
3-methylpentane	0.52		
hexane	0.46		
methylcyclopentane	0.44		

Table 4.14 – continued 2

PC4 (Auto Painting)	Loadings	PC 2 (Auto Paintings)	Loadings
1,2,3-trimethylbenzene	-0.26	1,2,3-trimethylbenzene	-0.3
1,2,4-trimethylbenzene	-0.35	1,2,4-trimethylbenzene	-0.32
1,3,5-trimethylbenzene	-0.31	1,3,5-trimethylbenzene	-0.32
2-ethyltoluene	-0.32	2-ethyltoluene	-0.31
3-ethyltoluene	-0.28	3-ethyltoluene	-0.31
4-ethyltoluene	-0.29	4-ethyltoluene	-0.3
n-propylbenzene	-0.28	methylcyclohexane	-0.3
		n-propylbenzene	-0.28
		octane	-0.26
PC7 (Undetermined)	**Loadings**	**PC8 (Undetermined)**	**Loadings**
acetylene	0.45	3-methylpentane	-0.28
methylcyclohexane	-0.43	benzene	0.26
propane	-0.45	hexane	-0.31
styrene	-0.42	isoprene	0.28
		PC 5 (Biogenic)	**Loadings**
		2,2,4-trimethylpentane	-0.31
		2,3,4-trimethylpentane	-0.38
		cyclohexane	-0.34
		isoprene	0.54
		propylene	-0.38

Overall, the sources profiles identified in both seasons were very similar. However, there were differences among the species with high loadings in the same profile of winter and summer. The relationships between the species vary from winter to summer because some species may evaporate or react more than others in summer when temperature is higher. Thus, the components provided by PCA were affected by the variation of species relationships from season to season. Also, it takes the variance of the

measurements into consideration when solving the Principal Components. PCA could be more sensitive to the changes of ratios among the concentrations of different species. There could be variations to the interpretation results due to some species could react more than others in summer.

There were six source profiles identified in both seasons: Gasoline Exhaust, Diesel Exhaust, Industrial Refinery, Architectural Coatings, Adhesive and Sealant Coatings, and Auto Paints. In summer 2006, there were two profiles identified as Gasoline Exhaust, and another two were interpreted as Industrial Refinery. Sources like Liquid Gasoline and Commercial Natural Gas were only in winter but not in summer; whereas Biogenic Emission was only in summer.

The compositions of Gasoline Exhaust identified from Component 6 in summer and the one in winter were similar. Both of them were loading high on acetylene (winter: 0.33; summer: 0.51), ethylene (winter: 0.49, summer: 0.5), and styrene (winter: 0.31, summer: 0.3). For Diesel Exhaust, the high loading species were different in two seasons. The component in winter had high loadings of 2,2,4-trimethylpentane (-0.4), 2,3,4-trimethylpentane (-0.3), 3-methylheptane (-0.3), and heptane (-0.3). In summer, decane (0.53), nonane (0.42), and undecane (0.49) had high loadings. This could due to that the heavier alkanes including decane, nonane, and undecane have higher boiling point (151 - 196 °C) and lower vapour pressure (0.4-10 mmHg) than trimethylpentane, methylheptane, and heptane (average boiling point: 98°C; average vapour pressure: 41mmHg) (ALS Environmental, 2014). Under lower temperature condition, species like trimethylpentane, methylheptane, and heptane more likely to evaporate than decane, nonane, and undecane. The differences of Diesel Exhaust from PCA indicate that different source profiles may

be needed in different seasons. However, this may need more study to support.

The Industrial Refinery profiles in both seasons had high loadings on alkenes including 1-pentene, cis-2-butene, cis-2-pentene, trans-2-butene, and 1-hexene/2-methyl-1-pentene. Architectural Coatings profiles in both seasons had high loadings on ethylbenzene (winter: 0.55; summer: 0.43), m and p-xylene (winter: 0.54; summer: 0.41), and o-xylene (winter: 0.49; summer: 0.38). In the Architectural Coatings profiles of winter, it was also rich on hexane (0.27), while in summer, it was rich on toluene (0.29). Both hexane and toluene are species markers of Architectural Coatings. The boiling point of hexane is 69°C, and vapour pressure is 132 mmHg. The boiling point of toluene is 110.6°C, and vapour pressure is 22 mmHg (ALS Environmental, 2014). In winter when the temperature is relatively low, hexane is more likely evaporate compared with toluene. Therefore, the impact of hexane on Architectural Coatings was greater than that of toluene. The loading of hexane was higher than that of toluene.

Adhesive and Sealant Coatings profiles in both seasons had high loadings on hexane (winter: 0.46; summer: -0.31), and 3-methylpentane (winter: 0.52; summer: -0.28). The auto-painting in both seasons were both rich on trimethylbenzenes, and ethyltoluenes.

4.5 Comparison of results from CMB, PMF, and PCA

The sources of all three models in winter and summer are listed in Table 4.15. They were compared to see the similarities and differences.

Table 4.15 Source comparison of CMB, PMF, and PCA in winter 2006

CMB	**Conc ($\mu g/m^3$)**	**Per cent (%)**	**PMF**	**Conc ($\mu g/m^3$)**	**Per cent (%)**	**PCA**
Gasoline Exhaust	5.1	16.7	**Gasoline Exhaust** (F2, 6.8%; F4, 7.8%; F12, 5.9%)	2.2	6.8	**Gasoline Exhaust** (PC6, Variance Explained: 3.0%)
Gasoline Vapour	5.0	16.4	**Gasoline Vapour** (F5)	3.1	9.6	
Diesel Exhaust	2.1	6.9	**Diesel Exhaust** (F9)	1.4	4.3	**Diesel Exhaust** (PC1, 59.7%)
Liquid Gasoline	0.5	1.6	**Liquid Gasoline** (F1)	2.5	7.8	**Liquid Gasoline** (PC9, 2.0%)
Industrial Refinery	5.4	17.7	**Industrial Refinery** (F7)	3.8	11.8	**Industrial Refinery** (PC5, 4.4%)
Liquefied Petroleum Gas	2.0	6.6	**Liquid Petroleum Gas** (F8)	2.4	7.5	
Commercial Natural Gas	5.4	17.7	**Commercial Natural Gas** (F13)	3.1	9.6	**Commercial Natural Gas** (PC8, 2.4%)
Coke Oven	1.7	5.6	**Coke Oven** (F10)	3.7	11.5	
Architectural Coatings	3.3	10.8	**Architectural Coatings** (F3)	2.5	7.8	**Architectural Coatings** (PC3, 6.2%)
Biogenic Emissions	0	0.0				
			Adhesive and Sealant Coatings (F6)	1.4	4.3	**Adhesive and Sealant Coatings** (PC2, 7.5%)
			Undetermined (F11)	1.7	5.3	
						Auto Paintings (PC4, 5.2%)
						Undetermined (PC7, 2.8%)
Total	30.5	100		32.2	100	

For winter 2006, there were six common sources of all three models. They were Gasoline Exhaust, Diesel Exhaust, Liquid Gasoline, Industrial Refinery, Commercial Natural Gas, and Architectural Coatings.

The 13 sources from PMF in winter 2006 included all the ten sources prepared for CMB model with the exception of Biogenic Emission. The lack of Biogenic Emission source profile may be due to that there are few deciduous trees in Windsor, the source of isoprene in winter. The total calculated source contributions by CMB (30.5 $\mu g/m^3$), and PMF (32.2 $\mu g/m^3$) were very similar. Among the 13 sources from PMF, Gasoline Exhaust (20.5%), Gasoline Vapour (9.6%), Industrial Refinery (11.8%), Commercial Natural Gas (9.6%), and Coke Oven (11.5%) were the major contributors in winter 2006. This was similar with the dominant sources of CMB results with the exception of Coke Oven as the contribution was only 5.6% of the total concentration. The reasons were unclear. “Adhesive and Sealant Coatings” was an additional source with low contributions (4.3%) provided by PMF.

Upon cross-checking sources of PCA and CMB, Gasoline Vapour, Liquid Petroleum Gas, Coke Oven, and Biogenic Emissions were only in CMB but not in PCA. This may be due to the eigenvalues of those factors were less than one in PCA winter 2006 results, indicating that not enough variance explained by these four factors. In PCA winter 2006 results, component 15 (eigenvalue: 0.22) has isoprene with loading of -0.31, the highest among all 20 components. Thus, component 15 is Biogenic Emission. “Adhesive and Sealant Coatings”, Auto Paintings were two additional sources extracted

from PCA compared to that of CMB.

There were less sources of PCA (six) overlapped with CMB sources compared with the sources of PMF (nine). This was expected because there were 13 factors from PMF; whereas only nine with eigenvalue greater than one from PCA. Both PMF and PCA provided profiles of “Adhesive and Sealant Coatings”. PCA provided additional source, Auto Paintings. The results from all three models for summer 2006 are listed in Table 4.16.

Table 4.16 Source comparison of CMB, PMF, and PCA in summer 2006

CMB	**(μg/m^3)**	**Per cent (%)**	**PMF**	**(μg/m^3)**	**Per cent (%)**	**PCA**
Gasoline Exhaust	6.6	16.0	**Gasoline Exhaust** (F5, 12.7%; F10, 6.3%)	5.6	12.7	**Gasoline Exhaust** (PC1, Variance explained: 53.4%; PC6, 3.2%)
Gasoline Vapour	8.3	20.1	**Gasoline Vapour** (F8, 8.8%; F12, 7.7%)	3.9	8.8	
Diesel Exhaust	6.1	14.8	**Diesel Exhaust** (F9)	3.4	7.7	**Diesel Exhaust** (PC4, 5.9%)
Liquid Gasoline	2.5	6.1	**Liquid Gasoline** (F4)	3.4	7.7	
Industrial Refinery	5.5	13.3	**Industrial Refinery** (F7)	4.3	9.8	**Industrial Refinery** (PC7, 2.6%; PC9, 1.7%)
Liquid Petroleum Gas	2	4.9	**Liquid Petroleum Gas** (F4)	3.2	7.3	
Commercial Natural Gas	3.4	8.3	**Commercial Natural Gas** (F3)	2.6	5.9	
Coke Oven	0.8	1.9	**Coke Oven** (F2)	2.3	5.2	
Architectural Coatings	5.5	13.3	**Architectural Coatings** (F11)	3.6	8.2	**Architectural Coatings** (PC3, 7.4%)
Biogenic Emission	0.5	1.2	**Biogenic Emission** (F 6)	2.8	6.3	**Biogenic Emissions** (PC5, 4.0%)
			Adhesive and Sealant Coatings (F13)	2.8	6.3	**Auto Paintings** (PC2, 10.6%)
						Undetermined (PC8, 2.3%)
Total	41.2	100		44.1	100	**Undetermined** (PC8, 2.3%)

For summer 2006, there were five common sources among all three models. They were Gasoline Exhaust, Diesel Exhaust, Industrial Refinery, Architectural Coatings, and Biogenic Emission.

All the ten source profiles prepared for CMB model were provided by PMF model. The total calculated source contribution from PMF was 44.1 μg/m^3, very close to 41.2μg/m^3 derived from CMB model. Gasoline Exhaust (19%), Gasoline Vapour (16.5%), Industrial Refinery (9.8%), and Architectural Coatings (8.2%) were the major sources according to PMF results. They were also the big contributors based on the results of CMB model. “Adhesive and Sealant Coatings” was additional source from PMF other than the ten sources for CMB.

There were five sources of CMB not included in PCA sources. They were Gasoline Vapour, Liquid Gasoline, Liquid Petroleum Gas, Commercial Natural Gas, and Coke Oven. Auto Paintings was an additional sources provided from PCA compared to that of CMB.

In both seasons, Gasoline Exhaust, Diesel Exhaust, Industrial Refinery, and Architectural Coatings were the common sources of PMF and CMB. All sources of CMB were included in identified sources of PMF in both seasons with the exception of Biogenic because it was not in winter PMF source profiles. The total calculated source contribution from PMF and the seasonal major contributors were very similar with that of CMB in both seasons. “Adhesive and Sealant Coatings” was the additional source of PMF compared with the ten sources for CMB for both winter and summer 2006. Gasoline Vapour, Liquid Petroleum Gas, and Coke Oven were the common sources of

PCA and CMB regardless of season. Auto Paintings was the additional sources other than the ten for CMB in both seasons. In winter, Adhesive and Sealant Coatings was also identified by PCA as an additional source other than the ten sources prepared for CMB.

Gasoline Exhaust, Diesel Exhaust, Industrial Refinery, and Architectural Coatings were common sources of all three models regardless of season. Adhesive and Sealant Coatings was identified from both PMF and PCA. There were more sources from PMF overlapped with ten sources for CMB than the sources from PCA regardless of season.

CHAPTER 5

CONCLUSIONS AND RECOMMNDATIONS

5.1 Conclusions

The concentration of 49 out of 55 and 52 out of 55 PAMS species increased from winter to summer in years 2005 and 2006, respectively. The concentration of 50 out of 55 PAMS species were observed to decrease from 2005 to 2006. The total NMHC concentrations decreased from 2005 to 2006.

Based on the CMB model estimation of ambient VOCs source contribution in winter and summer 2006, vehicle-related sources were the dominant VOC contributors in 2006 regardless of season. The major sources in winter 2006 were Gasoline Exhaust (16.2%), Gasoline Vapour (16.2%), Commercial Natural Gas (18%), and Industrial Refinery (17.8%). The major VOCs contributors in summer 2006 were Gasoline Exhaust (16.6%), Gasoline Vapour (20.1%), and Architectural Coatings (12.7%). The major sources were similar in year 2005 (Templer, 2007). This was expected because there was no major road facilities or industries were built or torn down, and no major industries started or out of operations in year 2006 compared to year 2005. Therefore, there were no dramatic VOC emission changes caused by surge increase or decrease of traffic or industries in certain areas. The contribution from Diesel was expected to be high. However, the moderate contribution from Diesel Exhaust according to CMB results could be due to the lack of measurements and the composition of important species markers including PAHs and SO_2.

The spatial trends of All Vehicle, Industrial Refinery, and Commercial Natural Gas were similar in winter 2005. The high concentration was observed near the northern

part of Huron Church Road. This could be caused by heavy traffic on the Huron Church Road. All vehicle source contributions were statistically correlated with that of all the other six sources. For Commercial Natural Gas, the concentration was also high along the riverside. This could be caused by the VOC emission from the industries in Detroit. In summer 2005, high concentration was observed near the northern part of Huron Church Road for both All Vehicle and Commercial Natural Gas. This could be caused by heavy traffic on the Huron Church Road. All vehicle concentrations were statistically correlated with all the other six sources with the exceptions of Industrial Refinery and the Biogenic Emission. In winter 2006, high concentrations near the northern part of Huron Church Road were observed for All Vehicles, Industrial Refinery, and Commercial Natural Gas.

All Vehicles was correlated with all the other six sources with the exception of Liquid Petroleum Gas. For summer 2006, high concentrations were observed in the surrounding areas of the Ford Windsor Engine Plant, and the Chrysler Canada-Windsor Assembly Plant, instead of Huron Church Road for All Vehicles and Architectural Coatings. The high concentration of All Vehicle could be the result of the traffic associated with the transportations of goods and employees, and the high concentration of Architectural Coatings could be due to the Automotive Paintings. All vehicles were only statistically related with Architectural Coatings and Coke Oven. The overall concentration in the southern part of Windsor was low regardless of season. This was because there are much less residents, commercial activities or industries located in those areas. The airport is also located in this area.

There were 10 and 11 sources identified from factors provided by PMF in winter and summer 2006, respectively. The ten common sources in winter and summer 2006

identified from PMF factors were Gasoline Exhaust, Gasoline Vapour, Liquid Gasoline, Diesel Exhaust, Commercial Natural Gas, Liquid Petroleum Gas, Industrial Refinery, Coke Oven, Architectural Coatings, and Adhesive & Sealant Coatings. Among the ten sources, Adhesive & Sealant Coatings is not in the profiles for CMB. The ten sources for CMB were observed in the sources provided by PMF with the exception of Biogenic Emission in winter 2006. For summer 2006, the total calculated source contributions by PMF (44.1μg/m^3) and CMB (summer: 41.2μg/m^3) were similar. Gasoline Exhaust (winter: 20.5%; summer: 19%), Gasoline vapour (winter: 9.6%; summer: 16.6%), and Industrial Refinery (winter: 11.8%; summer: 9.8%) were the biggest contributors in both seasons by PMF, similar with CMB results. Commercial Natural Gas (9.6%) and Coke Oven (11.5%) were also observed to be the major contributors in winter 2006. In summer, Architectural Coatings was another major contributor with mass percentage of 8.2%, similar pattern with that of CMB results. PMF provided "Adhesive and Sealant Coatings" as an additional source with low contribution other than the ten prepared for CMB in summer 2006.

There were eight and six sources identified by PCA in winter and summer 2006, respectively. Gasoline Exhaust, Diesel Exhaust, Industrial Refinery, Architectural Coatings, Adhesive and Sealant Coatings, and Auto Paintings were the six common sources in both seasons. There were five sources including Gasoline Exhaust, Diesel Exhaust, Industrial Refinery, Architectural Coatings, and Biogenic Emission from PCA which overlapped with those of CMB. However, PCA provided sources other than the ten for CMB. They were Auto Paintings in both seasons, and "Adhesive & Sealant Coatings" in winter, although these had low source contributions.

5.2 Recommendations

Future study:

- Investigating the meaning of negative source contribution provided by PMF.
- Further studying on how other people identify the source profiles from PMF and PCA.
- Testing the sensitivity of the PMF and PCA models with additional species markers to see if the model has a stable performance.
- Using the PMF source profiles results as input data to the CMB, and running CMB. Comparing results of CMB with PMF to see if the source contributions are similar or not.
- Requesting ten factors from PMF and running the PMF model again. Comparing the sources with the ten sources prepared by Templer (2007) to see if they are similar.
- Including source profiles of VOC emitters from Detroit.
- Including other species markers including PAHs and MEK to identify the sources.
- Running three models for 2005 data.

APPENDICES

Appendix A: Ten Source Profiles (Templer, 2007)

Table A.1

Species	Diesel Exhaust	Species	Gasoline Exhaust	Species	Liquid Gasoline	Species	Gasoline Vapour
m and p-xylene	10	other	24.6	toluene	14.9	isopentane	28.5
other	9.2	toluene	7.7	m and p-xylene	9.8	butane	23.8
ethylene	8.9	isopentane	6.9	isopentane	9.4	pentane	12.2
1,2,4-trimethylbenzene	6.8	ethylene	6.5	pentane	6.3	toluene	4.4
undecane	4.8	m and p-xylene	4.1	other	4.6	2-methylpentane	3.6
toluene	4.1	acetylene	3.7	2-methylpentane	4.3	isobutane	2.7
3-ethyltoluene	3.8	2,2,4-trimethylpentane	3.5	1,2,4-trimethylbenzene	3.9	m and p-xylene	2.4
propylene	3.6	benzene	3.3	o-xylene	3.7	other	2.4
o-xylene	3.4	propylene	3	hexane	3.6	hexane	2.2
benzene	2.9	2-methylpentane	2.8	2,2,4-trimethylpentane	3.6	3-methylpentane	2
1-butene	2.7	pentane	2.6	benzene	3	benzene	1.4
ethylbenzene	2.6	butane	2.2	butane	2.8	2,3-dimethylbutane	1.2
2,2-dimethylbutane	2.4	1,2,4-trimethylbenzene	2	3-methylpentane	2.6	trans-2-pentene	1
decane	2.4	3-methylpentane	1.8	ethylbenzene	2.6	2,2,4-trimethylpentane	0.9

Table A.1-continued 1

Species	**Diesel Exhaust**	**Species**	**Gasoline Exhaust**	**Species**	**Liquid Gasoline**	**Species**	**Gasoline Vapour**
acetylene	2.3	ethane	1.7	3-ethyltoluene	2.4	o-xylene	0.9
3-methylhexane	2.1	hexane	1.7	2,3-dimethylpentane	2.3	cyclopentane	0.8
propane	2	o-xylene	1.5	2,3-dimethylbutane	2	2,3-dimethylpentane	0.8
1,3,5-trimethylbenzene	1.9	2-methylhexane	1.3	3-methylhexane	1.8	1-pentene	0.7
2-methylpentane	1.8	3-ethyltoluene	1.3	2-methylhexane	1.6	ethylbenzene	0.7
2-ethyltoluene	1.8	methylcyclopentane	1.2	2,3,4-trimethylpentane	1.6	3-methylhexane	0.6
styrene	1.7	3-methylhexane	1.2	heptane	1.5	1,2,4-trimethylbenzene	0.6
1,2,3-trimethylbenzene	1.5	2,3,4-trimethylpentane	1.2	2,4-dimethylpentane	1.2	cis-2-butene	0.5
pentane	1.4	ethylbenzene	1.1	1,3,5-trimethylbenzene	1.2	cis-2-pentene	0.5
2,2,4-trimethylpentane	1.3	2,3-dimethylbutane	0.9	4-ethyltoluene	1	2,4-dimethylpentane	0.5
4-ethyltoluene	1.3	2,3-dimethylpentane	0.9	1,2,3-trimethylbenzene	0.9	2-methylhexane	0.5
isopentane	1.2	heptane	0.8	n-propylbenzene	0.8	heptane	0.5
ethane	1.1	trans-2-pentene	0.7	2-ethyltoluene	0.8	trans-2-butene	0.4
nonane	1	2,2-dimethylbutane	0.7	3-methylheptane	0.7	2,2-dimethylbutane	0.4

Table A.1- continued 2

Species	Diesel Exhaust	Species	Gasoline Exhaust	Species	Liquid Gasoline	Species	Gasoline Vapour
n-propylbenzene	1	2,4-dimethylpentane	0.7	2-methylheptane	0.6	3-ethyltoluene	0.4
hexane	0.9	1,3,5-trimethylbenzene	0.7	octane	0.6	cyclohexane	0.3
1-pentene	0.8	methylcyclohexane	0.6	trans-2-pentene	0.5	2,3,4-trimethylpentane	0.3
3-methylpentane	0.8	4-ethyltoluene	0.6	cyclohexane	0.5	3-methylheptane	0.2
2,3-dimethylpentane	0.8	isobutane	0.5	isobutane	0.3	4-ethyltoluene	0.2
butane	0.6	trans-2-butene	0.5	1-pentene	0.3	1,3,5-trimethylbenzene	0.2
methylcyclopentane	0.6	2-methylheptane	0.5	cis-2-pentene	0.3	2-ethyltoluene	0.2
heptane	0.5	3-methylheptane	0.5	2,2-dimethylbutane	0.3	1-hexene/2-methyl-1-pentene	0.1
methylcyclohexane	0.4	1,2,3-trimethylbenzene	0.5	methylcyclohexane	0.3	methylcyclohexane	0.1
3-methylheptane	0.4	1-butene	0.4	nonane	0.3	2-methylheptane	0.1
cis-2-butene	0.3	cis-2-butene	0.4	1,3-diethylbenzene	0.3	octane	0.1
trans-2-pentene	0.3	cis-2-pentene	0.4	1-hexene/2-methyl-1-pentene	0.2	n-propylbenzene	0.1
cis-2-pentene	0.3	octane	0.4	iso-propylbenzene	0.2	1,2,3-trimethylbenzene	0.1
cyclopentane	0.3	2-ethyltoluene	0.4	trans-2-butene	0.1	ethane	0

Table A.1-continued 3

Species	**Diesel Exhaust**	**Species**	**Gasoline Exhaust**	**Species**	**Liquid Gasoline**	**Species**	**Gasoline Vapour**
2,3-dimethylbutane	0.3	1,4-diethylbenzene	0.4	cis-2-butene	0.1	ethylene	0
2,4-dimethylpentane	0.3	1-pentene	0.3	undecane	0.1	acetylene	0
2,3,4-trimethylpentane	0.3	cyclopentane	0.3	ethane	0	1-butene	0
octane	0.3	n-propylbenzene	0.3	ethylene	0	propylene	0
iso-propylbenzene	0.3	1-hexene/2-methyl-1-pentene	0.2	acetylene	0	propane	0
isobutane	0.2	cyclohexane	0.2	1-butene	0	isoprene	0
trans-2-butene	0.2	styrene	0.1	propylene	0	methylcyclopentane	0
1-hexene/2-methyl-1-pentene	0.2	nonane	0.1	propane	0	styrene	0
cyclohexane	0.2	decane	0.1	isoprene	0	nonane	0
isoprene	0	1,3-diethylbenzene	0.1	cyclopentane	0	iso-propylbenzene	0
2-methylhexane	0	propane	0	methylcyclopentane	0	decane	0
2-methylheptane	0	isoprene	0	styrene	0	1,3-diethylbenzene	0
1,3-diethylbenzene	0	iso-propylbenzene	0	decane	0	1,4-diethylbenzene	0
1,4-diethylbenzene	0	undecane	0	1,4-diethylbenzene	0	undecane	0

Table A.1-continued 4

Species	Commercial Natural Gas	Species	Liquid Petroleum Gas	Species	Industrial Refinery	Species	Coke Oven
ethane	68.9	propane	90.6	other	36.3	other	59.3
propane	21.1	propylene	5.1	butane	22.9	benzene	10.5
butane	3.1	ethane	4.1	isobutane	9.6	1,2,3-trimethylbenzene	4.1
isobutane	2.1	isobutane	0.2	pentane	6.6	2,3-dimethylpentane	3.5
methylcyclopentane	1	ethylene	0	propane	3.7	nonane	3.1
isopentane	0.7	acetylene	0	hexane	2.9	butane	2
pentane	0.7	1-butene	0	toluene	1.9	toluene	2
other	0.5	butane	0	3-methylpentane	1.6	o-xylene	1.4
hexane	0.4	trans-2-butene	0	benzene	1.6	2,2,4-trimethylpentane	1.3
2-methylheptane	0.4	cis-2-butene	0	propylene	1.3	decane	1.3
2-methylpentane	0.3	isopentane	0	isopentane	1.3	m and p-xylene	1.2
2,2,4-trimethylpentane	0.3	1-pentene	0	methylcyclopentane	1.3	heptane	1
3-methylhexane	0.2	pentane	0	trans-2-pentene	0.9	3-methylhexane	0.9
heptane	0.2	isoprene	0	trans-2-butene	0.8	ethylbenzene	0.9
3-methylpentane	0.1	trans-2-pentene	0	2,2-dimethylbutane	0.7	iso-propylbenzene	0.9

Table A.1-continued 5

Species	**Commercial Natural Gas**	**Species**	**Liquid Petroleum Gas**	**Species**	**Industrial Refinery**	**Species**	**Coke Oven**
methylcyclohexane	0.1	cis-2-pentene	0	heptane	0.7	isopentane	0.7
ethylene	0	2,2-dimethylbutane	0	cis-2-butene	0.6	methylcyclohexane	0.7
acetylene	0	cyclopentane	0	1-pentene	0.6	n-propylbenzene	0.7
1-butene	0	2,3-dimethylbutane	0	ethane	0.5	3-ethyltoluene	0.6
propylene	0	2-methylpentane	0	cyclopentane	0.5	pentane	0.5
trans-2-butene	0	3-methylpentane	0	3-methylhexane	0.5	hexane	0.5
cis-2-butene	0	1-hexene/2-methyl-1-pentene	0	cis-2-pentene	0.4	2-methylpentane	0.4
1-pentene	0	hexane	0	2,4-dimethylpentane	0.4	3-methylpentane	0.4
isoprene	0	methylcyclopentane	0	cyclohexane	0.3	4-ethyltoluene	0.4
trans-2-pentene	0	2,4-dimethylpentane	0	o-xylene	0.3	1,3,5-trimethylbenzene	0.4
cis-2-pentene	0	benzene	0	1,2,4-trimethylbenzene	0.3	isobutane	0.3
2,2-dimethylbutane	0	cyclohexane	0	2-methylpentane	0.2	2-ethyltoluene	0.3
cyclopentane	0	2-methylhexane	0	2,2,4-trimethylpentane	0.2	2,2-dimethylbutane	0.2

Table A.1-continued 6

methylcyclohexane	0.1	cis-2-pentene	0	heptane	0.7	isopentane	0.7
ethylene	0	2,2-dimethylbutane	0	cis-2-butene	0.6	methylcyclohexane	0.7
acetylene	0	cyclopentane	0	1-pentene	0.6	n-propylbenzene	0.7
1-butene	0	2,3-dimethylbutane	0	ethane	0.5	3-ethyltoluene	0.6
propylene	0	2-methylpentane	0	cyclopentane	0.5	pentane	0.5
trans-2-butene	0	3-methylpentane	0	3-methylhexane	0.5	hexane	0.5
cis-2-butene	0	1-hexene/2-methyl-1-pentene	0	cis-2-pentene	0.4	2-methylpentane	0.4
1-pentene	0	hexane	0	2,4-dimethylpentane	0.4	3-methylpentane	0.4
isoprene	0	methylcyclopentane	0	cyclohexane	0.3	4-ethyltoluene	0.4
trans-2-pentene	0	2,4-dimethylpentane	0	o-xylene	0.3	1,3,5-trimethylbenzene	0.4
cis-2-pentene	0	benzene	0	1,2,4-trimethylbenzene	0.3	isobutane	0.3
2,2-dimethylbutane	0	cyclohexane	0	2-methylpentane	0.2	2-ethyltoluene	0.3
cyclopentane	0	2-methylhexane	0	2,2,4-trimethylpentane	0.2	2,2-dimethylbutane	0.2

Table A.1-continued 7

2,3-dimethylbutane	0	2,3-dimethylpentane	0	methylcyclohexane	0.2	2,4-dimethylpentane	0.2
1-hexene/2-methyl-1-pentene	0	3-methylhexane	0	ethylbenzene	0.2	octane	0.2
2,4-dimethylpentane	0	2,2,4-trimethylpentane	0	2-methylhexane	0.1	2,3,4-trimethylpentane	0.1
benzene	0	heptane	0	2,3,4-trimethylpentane	0.1	3-methylheptane	0.1
cyclohexane	0	methylcyclohexane	0	3-methylheptane	0.1	1,2,4-trimethylbenzene	0.1
2-methylhexane	0	2,3,4-trimethylpentane	0	octane	0.1	ethane	0
2,3-dimethylpentane	0	toluene	0	iso-propylbenzene	0.1	ethylene	0
2,3,4-trimethylpentane	0	2-methylheptane	0	ethylene	0	acetylene	0
toluene	0	3-methylheptane	0	acetylene	0	1-butene	0
3-methylheptane	0	octane	0	1-butene	0	propylene	0
octane	0	ethylbenzene	0	isoprene	0	propane	0
ethylbenzene	0	m and p-xylene	0	2,3-dimethylbutane	0	trans-2-butene	0
m and p-xylene	0	styrene	0	1-hexene/2-methyl-1-pentene	0	cis-2-butene	0

Table A.1-continued 8

styrene	0	o-xylene	0	2,3-dimethylpentane	0	1-pentene	0
o-xylene	0	nonane	0	2-methylheptane	0	isoprene	0
nonane	0	iso-propylbenzene	0	m and p-xylene	0	trans-2-pentene	0
iso-propylbenzene	0	n-propylbenzene	0	styrene	0	cis-2-pentene	0
n-propylbenzene	0	3-ethyltoluene	0	nonane	0	cyclopentane	0
3-ethyltoluene	0	4-ethyltoluene	0	n-propylbenzene	0	2,3-dimethylbutane	0
4-ethyltoluene	0	1,3,5-trimethylbenzene	0	3-ethyltoluene	0	1-hexene/2-methyl-1-pentene	0
1,3,5-trimethylbenzene	0	2-ethyltoluene	0	4-ethyltoluene	0	methylcyclopentane	0
2-ethyltoluene	0	1,2,4-trimethylbenzene	0	1,3,5-trimethylbenzene	0	cyclohexane	0
1,2,4-trimethylbenzene	0	decane	0	2-ethyltoluene	0	2-methylhexane	0
decane	0	1,2,3-trimethylbenzene	0	decane	0	2-methylheptane	0
1,2,3-trimethylbenzene	0	1,3-diethylbenzene	0	1,2,3-trimethylbenzene	0	styrene	0
1,3-diethylbenzene	0	1,4-diethylbenzene	0	1,3-diethylbenzene	0	1,3-diethylbenzene	0
1,4-diethylbenzene	0	undecane	0	1,4-diethylbenzene	0	1,4-diethylbenzene	0
undecane	0	other	0	undecane	0	undecane	0

Table A.1-continued 9

Species	**Architectural Coatings**	**Species**	**Biogenic Emission**
other	66.9	isoprene	100
toluene	25.9	ethane	0
o-xylene	2.9	ethylene	0
m and p-xylene	2.7	acetylene	0
2,4-dimethylpentane	1.1	1-butene	0
ethylbenzene	0.5	propylene	0
benzene	0.1	propane	0
ethane	0	isobutane	0
ethylene	0	butane	0
acetylene	0	trans-2-butene	0
1-butene	0	cis-2-butene	0
propylene	0	isopentane	0
propane	0	1-pentene	0
isobutane	0	pentane	0
butane	0	trans-2-pentene	0
trans-2-butene	0	cis-2-pentene	0

Table A.1-continued 10

cis-2-butene	0	2,2-dimethylbutane	0
isopentane	0	cyclopentane	0
1-pentene	0	2,3-dimethylbutane	0
pentane	0	2-methylpentane	0
isoprene	0	3-methylpentane	0
trans-2-pentene	0	1-hexene/2-methyl-1-pentene	0
cis-2-pentene	0	hexane	0
2,2-dimethylbutane	0	methylcyclopentane	0
cyclopentane	0	2,4-dimethylpentane	0
2,3-dimethylbutane	0	benzene	0
2-methylpentane	0	cyclohexane	0
3-methylpentane	0	2-methylhexane	0
1-hexene/2-methyl-1-pentene	0	2,3-dimethylpentane	0
hexane	0	3-methylhexane	0
methylcyclopentane	0	2,2,4-trimethylpentane	0
cyclohexane	0	heptane	0
2-methylhexane	0	methylcyclohexane	0
2,3-dimethylpentane	0	2,3,4-trimethylpentane	0
3-methylhexane	0	toluene	0
2,2,4-trimethylpentane	0	2-methylheptane	0
heptane	0	3-methylheptane	0
methylcyclohexane	0	octane	0
2,3,4-trimethylpentane	0	ethylbenzene	0
2-methylheptane	0	m and p-xylene	0
3-methylheptane	0	styrene	0
octane	0	o-xylene	0
styrene	0	nonane	0

Table A.1-continued 11

nonane	0	iso-propylbenzene	0
iso-propylbenzene	0	n-propylbenzene	0
n-propylbenzene	0	3-ethyltoluene	0
3-ethyltoluene	0	4-ethyltoluene	0
4-ethyltoluene	0	1,3,5-trimethylbenzene	0
1,3,5-trimethylbenzene	0	2-ethyltoluene	0
2-ethyltoluene	0	1,2,4-trimethylbenzene	0
1,2,4-trimethylbenzene	0	decane	0
decane	0	1,2,3-trimethylbenzene	0
1,2,3-trimethylbenzene	0	1,3-diethylbenzene	0
1,3-diethylbenzene	0	1,4-diethylbenzene	0
1,4-diethylbenzene	0	undecane	0
undecane	0	other	0

Appendix B: PMF Source Profiles Literature Review

Table B.1 Gasoline Exhaust

Song et al. (2008)		Yuan et al. (2009) (location 1)		Yuan et al. (2009) (Location 2)		Templer (2007)	
Species	Per Cent (%)	Species	Per Cent (%)	Species	Per Cent (%)	Species	Per Cent (%)
acetylene	16.8	toluene	18.3	benzene	30.5	other	24.6
propane	12.0	isopentane	15.2	toluene	27.3	toluene	7.7
isopentane	11.9	benzene	9.1	isopentane	10.5	isopentane	6.9
ethane	11.7	pentane	8.7	2-methylhexane	7.7	ethylene	6.5
ethylene	9.9	hexane	7.7	pentane	4.1	m and p-xylene	4.1
butane	8.4	2-methylpentane	5.6	butane	4.0	acetylene	3.7
toluene	6.6	3-methylpentane	4.7	3-methylpentane	3.2	2,2,4-trimethylpentane	3.5
isobutane	6.2	3-methylhexane	4.1	hexane	3.0	benzene	3.3
benzene	5.2	butane	3.7	iso-butene	2.8	propylene	3
pentane	4.7	2-methylhexane	3.7	isobutane	2.5	2-methylpentane	2.8
MTBE	1.9	isobutane	3.5	1-butene	2.4	pentane	2.6
hexane	1.3	propane	3.2	octane	0.6	butane	2.2
ethylbenzene	0.9	heptane	2.9	m and p-xylene	0.5	1,2,4-trimethylbenzene	2
propylene	0.9	m and p-xylene	2.6	ethylbenzene	0.4	3-methylpentane	1.8
o-xylene	0.5	ethylbenzene	1.6	isoprene	0.3	ethane	1.7
1-butene	0.4	o-xylene	1.4	o-xylene	0.1	hexane	1.7
2m-propylene	0.3	octane	1.3	propane	0.1	o-xylene	1.5

Table B.1- continued 1

isoprene	0.1	1,2,4-trimethylbenzene	1.2	1,2,3-trimethylbenzene	0	2-methylhexane	1.3
2m-1-butene	0.1	isoprene	0.8	1,2,4-trimethylbenzene	0	3-ethyltoluene	1.3
2m-2-butene	0.1	nonane	0.5	1,3,5-trimethylbenzene	0	methylcyclopentane	1.2
1,2,4-trimethylbenzene	0	decane	0.3	1,3-diethylbenzene	0	3-methylhexane	1.2
1-pentene	0	1,2,3-trimethylbenzene	0	1,4-diethylbenzene	0	2,3,4-trimethylpentane	1.2
2-methylhexane	0	1,3,5-trimethylbenzene	0	1-hexene/2-methyl-1-pent	0	ethylbenzene	1.1
2-methylpentane	0	1,3-diethylbenzene	0	1-pentene	0	2,3-dimethylbutane	0.9
3-methylhexane	0	1,4-diethylbenzene	0	2,2,4-trimethylpentane	0	2,3-dimethylpentane	0.9
3-methylpentane	0	1-butene	0	2,2-dimethylbutane	0	heptane	0.8
cis-2-butene	0	1-hexene/2-methyl-1-pent	0	2,3,4-trimethylpentane	0	trans-2-pentene	0.7
cis-2-pentene	0	1-pentene	0	2,3-dimethylbutane	0	2,2-dimethylbutane	0.7
decane	0	2,2,4-trimethylpentane	0	2,3-dimethylpentane	0	2,4-dimethylpentane	0.7
heptane	0	2,2-dimethylbutane	0	2,4-dimethylpentane	0	1,3,5-trimethylbenzene	0.7

Table B.1- continued 2

m and p-xylene	0	2,3,4-trimethylpentane	0	2-ethyltoluene	0	methylcyclohexane	0.6
nonane	0	2,3-dimethylbutane	0	2-methylheptane	0	4-ethyltoluene	0.6
octane	0	2,3-dimethylpentane	0	2-methylpentane	0	isobutane	0.5
trans-2-butene	0	2,4-dimethylpentane	0	3-ethyltoluene	0	trans-2-butene	0.5
trans-2-pentene	0	2-ethyltoluene	0	3-methylheptane	0	2-methylheptane	0.5
3m-1-butene	0	2-methylheptane	0	3-methylhexane	0	3-methylheptane	0.5
a-pinene	0	3-ethyltoluene	0	4-ethyltoluene	0	1,2,3-trimethylbenzene	0.5
b-pinene	0	3-methylheptane	0	acetylene	0	1-butene	0.4
limonene	0	4-ethyltoluene	0	cis-2-butene	0	cis-2-butene	0.4
1,2,3-trimethylbenzene	0	acetylene	0	cis-2-pentene	0	cis-2-pentene	0.4
1,3,5-trimethylbenzene	0	cis-2-butene	0	cyclohexane	0	octane	0.4
1,3-diethylbenzene	0	cis-2-pentene	0	cyclopentane	0	2-ethyltoluene	0.4
1,4-diethylbenzene	0	cyclohexane	0	decane	0	1,4-diethylbenzene	0.4
1-hexene/2-methyl-1-pent	0	cyclopentane	0	ethane	0	1-pentene	0.3
2,2,4-trimethylpentane	0	ethane	0	ethylene	0	cyclopentane	0.3
2,2-dimethylbutane	0	ethylene	0	heptane	0	n-propylbenzene	0.3
2,3,4-trimethylpentane	0	iso-propylbenzene	0	iso-propylbenzene	0	1-hexene/2-methyl-1-pentene	0.2
2,3-dimethylbutane	0	methylcyclohexane	0	methylcyclohexane	0	cyclohexane	0.2
2,3-dimethylpentane	0	methylcyclopentane	0	methylcyclopentane	0	styrene	0.1
2,4-dimethylpentane	0	propylbenzene	0	nonane	0	nonane	0.1
2-ethyltoluene	0	propylene	0	propylbenzene	0	decane	0.1
2-methylheptane	0	styrene	0	propylene	0	1,3-diethylbenzene	0.1
Total	99.9		100		100		

Table B.2 Liquid Gasoline

Song et al., (2008)		Yuan et al. (2009)		Templer (2007)	
Liquid/evaporated/exhaust gasoline		Evaporated and Liquid Gasoline		Liquid Gasoline	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
isopentane	21.8	butane	21.1	toluene	14.9
acetylene	18.5	isopentane	19.5	m and p-xylene	9.8
ethylene	11.6	isobutane	14.6	isopentane	9.4
pentane	6.3	propane	8.7	pentane	6.3
toluene	5.8	benzene	8.1	other	4.6
MTBE	4.6	pentane	7.2	2-methylpentane	4.3
2m-2-butene	4.0	toluene	4.5	1,2,4-trimethylbenzene	3.9
benzene	3.8	hexane	4.1	o-xylene	3.7
2m-propylene	3.3	m and p-xylene	3.0	hexane	3.6
2m-1-butene	2.7	ethylbenzene	2.6	2,2,4-trimethylpentane	3.6
butane	2.5	3-methylhexane	1.5	benzene	3
propylene	2.1	2-methylpentane	1.1	butane	2.8
trans-2-butene	2.1	3-methylpentane	1.1	3-methylpentane	2.6
cis-2-butene	1.9	o-xylene	1.0	ethylbenzene	2.6
ethane	1.7	heptane	0.7	3-ethyltoluene	2.4
trans-2-pentene	1.7	2-methylhexane	0.5	2,3-dimethylpentane	2.3
hexane	1.3	1,2,4-trimethylbenzene	0.2	2,3-dimethylbutane	2

Table B.2- continued 1

isobutane	1.3	octane	0.2	3-methylhexane	1.8
cis-2-pentene	1.0	decane	0.1	2-methylhexane	1.6
o-xylene	0.7	isoprene	0.0	2,3,4-trimethylpentane	1.6
1-butene	0.5	nonane	0.0	heptane	1.5
1-pentene	0.5	1,2,3-trimethylbenzene	0	2,4-dimethylpentane	1.2
isoprene	0.4	1,3,5-trimethylbenzene	0	1,3,5-trimethylbenzene	1.2
3m-1-butene	0.1	1,3-diethylbenzene	0	4-ethyltoluene	1
a-pinene	0.1	1,4-diethylbenzene	0	1,2,3-trimethylbenzene	0.9
1,2,4-trimethylbenzene	0	1-butene	0	n-propylbenzene	0.8
2-methylhexane	0	1-hexene/2-methyl-1-pent	0	2-ethyltoluene	0.8
2-methylpentane	0	1-pentene	0	3-methylheptane	0.7
3-methylhexane	0	2,2,4-trimethylpentane	0	2-methylheptane	0.6
3-methylpentane	0	2,2-dimethylbutane	0	octane	0.6
decane	0	2,3,4-trimethylpentane	0	trans-2-pentene	0.5
ethylbenzene	0	2,3-dimethylbutane	0	cyclohexane	0.5
heptane	0	2,3-dimethylpentane	0	isobutane	0.3
m and p-xylene	0	2,4-dimethylpentane	0	1-pentene	0.3
propane	0	2-ethyltoluene	0	cis-2-pentene	0.3
b-pinene	0	2-methylheptane	0	2,2-dimethylbutane	0.3
limonene	0	3-ethyltoluene	0	methylcyclohexane	0.3
1,2,3-trimethylbenzene	0	3-methylheptane	0	nonane	0.3
1,3,5-trimethylbenzene	0	4-ethyltoluene	0	1,3-diethylbenzene	0.3
1,3-diethylbenzene	0	acetylene	0	1-hexene/2-methyl-1-pentene	0.2
1,4-diethylbenzene	0	cis-2-butene	0	iso-propylbenzene	0.2
1-hexene/2-methyl-1-pent	0	cis-2-pentene	0	trans-2-butene	0.1

Table B.3 Diesel Exhaust

Lam et al. (2013)	Per cent (%)	Yuan et al. (2009) (Location 1)	Per cent (%)	Yuan et al. (2009) Location 2	Per cent (%)
toluene	19	toluene	11.9	isopentane	17.1
butane	15.6	isopentane	9.9	isobutane	15.7
hexane	11.5	m and p-xylene	7.8	propane	14.9
propane	10.9	benzene	7.1	pentane	10.1
acetylene	9.2	1,2,4-trimethylbenzene	6	toluene	9.6
isobutane	6.9	decane	5.9	1-butene	8.6
ethylbenzene	6.4	propane	5.2	butane	7.9
ethylene	5.6	hexane	5.2	iso-butene	6.79
ethane	4.2	nonane	5	2-methylhexane	2.4
benzene	3.2	isobutane	4.9	m and p-xylene	1.7
2-methylpentane	2.3	pentane	4.1	ethylbenzene	1.6
heptane	1.2	2-methylpentane	3.6	octane	1.5
CO	1.1	o-xylene	3.6	3-methylpentane	1.4
m and p-xylene	1	3-methylpentane	3.3	o-xylene	0.7
o-xylene	0.6	butane	3	benzene	0
pentane	0.3	3-methylhexane	2.6	isoprene	0
1,3,5-trimethylbenzene	0	heptane	2.6	hexane	0
1,2,3-Trimethylbenzene	0	Octane	2.5	1,2,3-Trimethylbenzene	
Total	99.1	Total	100	Total	100

Table B.3 – continued 1

Song, et al. (2007)	Per cent (%)	Templer (2007)	Per cent (%)
ethane	0.2	m and p-xylene	10
acetylene	0.2	other	9.2
ethylene	0.1	ethylene	8.9
decane	0.1	1,2,4-trimethylbenzene	6.8
isopentane	0.1	undecane	4.8
benzene	0	toluene	4.1
propane	0	3-ethyltoluene	3.8
toluene	0	propylene	3.6
butane	0	o-xylene	3.4
isobutane	0	benzene	2.9
pentane	0	1-butene	2.7
propylene	0	ethylbenzene	2.6
hexane	0	2,2-dimethylbutane	2.4
o-xylene	0	decane	2.4
MTBE	0.01	acetylene	2.3
2m-2-butene	0.005	3-methylhexane	2.1
isoprene	0	propane	2
2m-propene	0.004	1,3,5-trimethylbenzene	1.9
limonene	0.004	2-methylpentane	1.8
1-butene	0	2-ethyltoluene	1.8

Table B.3- continued 2

ethylbenzene	0	styrene	1.7
m and p-xylene	0	1,2,3-trimethylbenzene	1.5
1-pentene	0	pentane	1.4
cis-2-butene	0	2,2,4-trimethylpentane	1.3
cis-2-pentene	0	4-ethyltoluene	1.3
trans-2-butene	0	isopentane	1.2
trans-2-pentene	0	ethane	1.1
2m-1-butene	0	nonane	1
3m-1-butene	0	n-propylbenzene	1
â-pinene	0	hexane	0.9
r-pinene	0	1-pentene	0.8
1,2,3-trimethylbenzene	0	3-methylpentane	0.8
1,2,4-trimethylbenzene	0	2,3-dimethylpentane	0.8
1,3,5-trimethylbenzene	0	butane	0.6
1,3-diethylbenzene	0	methylcyclopentane	0.6
1,4-diethylbenzene	0	heptane	0.5
1-hexene/2-methyl-1-pent	0	methylcyclohexane	0.4
2,2,4-trimethylpentane	0	3-methylheptane	0.4
2,2-dimethylbutane	0	cis-2-butene	0.3
2,3,4-trimethylpentane	0	trans-2-pentene	0.3

Table B.3- continued 3

2,3-dimethylbutane	0	cis-2-pentene	0.3
2,3-dimethylpentane	0	cyclopentane	0.3
2,4-dimethylpentane	0	2,3-dimethylbutane	0.3
2-ethyltoluene	0	2,4-dimethylpentane	0.3
2-methylheptane	0	2,3,4-trimethylpentane	0.3
2-methylhexane	0	octane	0.3
2-methylpentane	0	iso-propylbenzene	0.3
3-ethyltoluene	0	isobutane	0.2
3-methylheptane	0	trans-2-butene	0.2
3-methylhexane	0	1-hexene/2-methyl-1-pentene	0.2
3-methylpentane	0	cyclohexane	0.2

Table B.4 Gasoline Vapour

Morino et al. (2011) (Gasoline Vapour 1)		Morino et al. (2011) (Gasoline Vapour 2)	
Species	Per cent (%)	Species	Per cent (%)
butane	47.6	isopentane	42.8
isobutane	33.3	butane	23.3
propane	9.5	pentane	15.6
toluene	9.5	isobutane	11.7
isopentane	0	benzene	1.9
acetylene	0	hexane	1.9
benzene	0	propane	1.9
ethane	0	toluene	0.8
Total	100	Total	100

Table B.4- continued 1

Lam et al. (2013)		Templer (2007)	
Species	Per cent (%)	Species	Per cent (%)
butane	36.6	isopentane	28.5
propane	20.8	butane	23.8
isobutane	19.6	pentane	12.2
ethylene	11.1	toluene	4.4
propylene	4.2	2-methylpentane	3.6
acetylene	3.8	isobutane	2.7
toluene	2.3	m and p-xylene	2.4
ethane	0.6	other	2.4
2-methylpentane	0.2	hexane	2.2
heptane	0.2	3-methylpentane	2
o-xylene	0.1	benzene	1.4
pentane	0.1	2,3-dimethylbutane	1.2
1,2,4-trimethylbenzene	0.1	trans-2-pentene	1
isopentane	0	2,2,4-trimethylpentane	0.9
benzene	0	o-xylene	0.9
1,3,5-trimethylbenzene	0	cyclopentane	0.8
1,2,3-trimethylbenzene	0	2,3-dimethylpentane	0.8
1,3-diethylbenzene	0	1-pentene	0.7
1,4-diethylbenzene	0	ethylbenzene	0.7
1-butene	0	3-methylhexane	0.6

Table B.4- continued 3

1-hexene/2-methyl-1-pent	0	1,2,4-trimethylbenzene	0.6
1-pentene	0	cis-2-butene	0.5
2,2,4-trimethylpentane	0	cis-2-pentene	0.5
2,2-dimethylbutane	0	2,4-dimethylpentane	0.5
2,3,4-trimethylpentane	0	2-methylhexane	0.5
2,3-dimethylbutane	0	heptane	0.5
2,3-dimethylpentane	0	trans-2-butene	0.4
2,4-dimethylpentane	0	2,2-dimethylbutane	0.4
2-ethyltoluene	0	3-ethyltoluene	0.4
2-methylheptane	0	cyclohexane	0.3
2-methylhexane	0	2,3,4-trimethylpentane	0.3
3-ethyltoluene	0	3-methylheptane	0.2
3-methylheptane	0	4-ethyltoluene	0.2
3-methylhexane	0	1,3,5-trimethylbenzene	0.2
3-methylpentane	0	2-ethyltoluene	0.2
4-ethyltoluene	0	1-hexene/2-methyl-1-pentene	0.1
cis-2-butene	0	methylcyclohexane	0.1
cis-2-pentene	0	2-methylheptane	0.1
cyclohexane	0	octane	0.1
cyclopentane	0	n-propylbenzene	0.1
decane	0	1,2,3-trimethylbenzene	0.1

Table B.5 Paint and Solvent related sources

Cai et al. (2010)			
Paint solvent usage		Industrial sources (solvent based)	
Species	Percent (%)	Species	Percent (%)
toluene	19.4	toluene	36.2
m and p-xylene	17.2	ethylacetate	28.6
ethylbenzene	14.1	propane	4.3
propane	13.9	methylenechloride	3.2
isopentane	5.9	butane	3.2
o-xylene	5	isobutane	2.8
benzene	3.4	m and p-xylene	2.4
butane	3	ethylbenzene	2.4
isobutane	2.1	propylene	1.6
2-methylpentane	1.7	hexane	1.5
methylenechloride	1.7	chloromethane	1.5
1,2-dichloroethane	1.2	benzene	1.3
hexane	1.1	1,2-dichloroethane	1.1
3-methylpentane	1	1-butene	1.1
chloromethane	1	o-xylene	1.1
styrene	0.9	2-methylpentane	1
trans-2-butene	0.8	3-methylhexane	1

Table B. 5 – continued 1

cis-2-butene	0.8	2-methylhexane	0.8
1-butene	0.7	heptane	0.7
methylcyclopentane	0.7	methyltertbutylether	0.7
decane	0.6	cis-2-butene	0.4
heptane	0.6	3-methylpentane	0.4
nonane	0.6	styrene	0.4
2,4-dimethylpentane	0.5	isoprene	0.3
isoprene	0.5	2,4-dimethylpentane	0.2
2-methylhexane	0.4	isopentane	0.2
3-methylhexane	0.4	methylcyclopentane	0.2
1-pentene	0.4	decane	0.2
methyltertbutylether	0.3	1-pentene	0.1
ethylacetate	0.2	nonane	0.1

Table B.5- continued 2

Lam et al. (2013)					
Adhesive & sealants		Solvent		Paint & varnish	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
isopentane	25.2	butane	17.8	acetylene	20.2
isobutane	22.7	acetylene	15.2	ethane	18.6
pentane	14.6	propane	11.4	butane	14.3
propane	12.7	isoprene	10.2	propane	14
butane	11.1	isobutane	10.2	ethylene	9.3
toluene	6	ethylene	9.2	isobutane	6.4
ethylene	1.4	toluene	5.3	benzene	5.4
2-methylpentane	1.3	ethane	5.3	CO	5.2
ethane	1.1	CO	3.6	toluene	2.2
m and p-xylene	0.8	isopentane	2.7	propylene	1.9
propylene	0.7	propylene	2.4	hexane	1
heptane	0.7	benzene	2.1	ethylbenzene	0.5
hexane	0.6	pentane	1.2	m and p-xylene	0.3
benzene	0.4	2-methylpentane	0.8	pentane	0.3
o-xylene	0.2	heptane	0.7	2-methylpentane	0.2
CO	0.1	ethylbenzene	0.6	1,2,4-trimethylbenzene	0.2
acetylene	0.1	m and p-xylene	0.4	isoprene	0.1
isoprene	0.1	hexane	0.3	o-xylene	0.1

Table B.5- continued 3

1,2,4-trimethylbenzene	0	1,2,4-trimethylbenzene	0.2	1,3,5-trimethylbenzene	0.1
1,3,5-trimethylbenzene	0	o-xylene	0.2	1,2,3-trimethylbenzene	0.1
ethylbenzene	0	1,2,3-trimethylbenzene	0.1		
1,2,3-trimethylbenzene		1,3,5-trimethylbenzene	0.1	1,3-diethylbenzene	

Table B.5 – continued 4

Yuan et al. (2009)			
Paint and Industrial Coating (Location 1)		Paint and Industrial Coating (location 2)	
Species	Per cent (%)	Species	Per cent (%)
m and p-xylene	23.6	m and p-xylene	24.3
ethylbenzene	15.3	toluene	20.8
toluene	14.9	benzene	17.2
isobutane	8.6	ethylbenzene	16.8
o-xylene	7.4	o-xylene	9.3
butane	6.1	isopentane	2.4
benzene	5.7	butane	2.1
hexane	3.7	hexane	2.1
1,2,4-trimethylbenzene	3.5	2-methylhexane	2
isopentane	2.1	pentane	1.1

Table B.5 – continued 5

pentane	1.9	1-butene	0.7
3-methylhexane	1.4	propane	0.7
heptane	1	iso-butene	0.5
decane	0.9	isoprene	0.1
propane	0.7	isobutane	0
octane	0.7	3-methylpentane	0
nonane	0.6	octane	0
2-methylpentane	0.6	1,2,3-trimethylbenzene	0
2-methylhexane	0.6	1,2,4-trimethylbenzene	0
3-methylpentane	0.5	1,3,5-trimethylbenzene	0
isoprene	0		
Song et al., (2007)		Templer (2007)	
paint		Architectural Coatings	
Species	Per cent (%)	Species	Per cent (%)
m and p-xylene	0.3	other	66.9
ethylbenzene	0.1	toluene	25.9
o-xylene	0.1	o-xylene	2.9
toluene	0.1	m and p-xylene	2.7
pentane	0.1	2,4-dimethylpentane	1.1
r-pinene	0.1	ethylbenzene	0.5
benzene	0.1	benzene	0.1

Table B.6 Liquid Petroleum Gas

Cai et al. (2010)		Song et al., (2008)	
Fuel evaporation (gasoline,LPG/NG Leakage)		LPG	
Species	Per cent (%)	Species	Per cent (%)
isopentane	21.8	propane	17.9
butane	12.2	isobutane	16
isobutane	10.3	butane	14.2
propane	7.1	1-butene	12.2
methylenechloride	4.6	ethylene	7.1
propylene	4.2	propylene	7.1
2-methylpentane	3.9	trans-2-butene	4.6
ethylbenzene	3.9	cis-2-butene	3.3
methyltertbutylether	3.9	isopentane	3.1
ethylacetate	2.6	2m-propylene	2.9
benzene	2.3	toluene	2.7
chloromethane	1.9	ethane	2.3
m and p-xylene	1.9	m and p-xylene	1.8
3-methylpentane	1.7	acetylene	0.9
trans-2-butene	1.6	o-xylene	0.9
toluene	1.6	hexane	0.6
1-butene	1.5	trans-2-pentene	0.6
heptane	1.5	pentane	0.4
cis-2-butene	1.5	benzene	0.3
3-methylhexane	1.3	cis-2-pentene	0.3

Table B.6 - continued 1

isoprene	1.2	2m-1-butene	0.3
1-pentene	1.1	MTBE	0.3
o-xylene	1.1	1-pentene	0.2
methylcyclopentane	1	isoprene	0.1
2-methylhexane	0.9	decane	0
2,4-dimethylpentane	0.8	ethylbenzene	0
hexane	0.8	3m-1-butene	0
1,2-dichloroethane	0.6	2m-2-butene	0
decane	0.6	limonene	0
nonane	0.4	a-pinene	0
styrene	0.3	b-pinene	0

Table B.6 – continued 2

Morino et al. (2011)		Lam et al. (2013)	
liquefied petroleum gas (LPG)		LPG usage & consumer product propellant	
Species	Per cent (%)	Species	Per cent (%)
ethane	69.1	toluene	38.1
propane	10.6	ethane	16
butane	5.3	acetylene	12.5
toluene	5.3	benzene	6.2
acetylene	4.3	propane	6
benzene	2.7	ethylene	3.8
isobutane	2.7	ethylbenzene	3.7
isopentane	0	co	3.7
hexane	0	2-methylpentane	2.5
pentane	0	heptane	2.1
1,2,3-trimethylbenzene	0	m and p-xylene	1.9
1,2,4-trimethylbenzene	0	isobutane	1.4
1,3,5-trimethylbenzene	0	o-xylene	1
1,3-diethylbenzene	0	pentane	0.5
1,4-diethylbenzene	0	butane	0.5
1-butene	0	isopentane	0.1
1-hexene/2-methyl-1-pent	0	propylene	0
Total	100	Total	100

Table B.6 – continued 3

Yuan et al. (2009) (location 1)		Yuan et al. (2009) (location 2)	
LPG		LPG	
Species	Per cent (%)	Species	Per cent (%)
propane	23.9	propane	38.4
isobutane	22.4	butane	21.2
butane	15.8	isobutane	17.2
toluene	9.6	isopentane	7.5
isopentane	6.3	pentane	5.9
hexane	3.5	benzene	5.4
pentane	3	toluene	2.6
2-methylpentane	2.8	hexane	0.7
3-methylpentane	2.4	1-butene	0.4
benzene	1.8	3-methylpentane	0.3
3-methylhexane	1.6	octane	0.3
1,2,4-trimethylbenzene	1.6	isobutene	0.1
2-methylhexane	1.5	m and p-xylene	0
o-xylene	1	ethylbenzene	0
m and p-xylene	1	isoprene	0
heptane	0.9	o-xylene	0
isoprene	0.6	2-methylhexane	0
octane	0.5	1,2,3-trimethylbenzene	0
nonane	0.1	1,2,4-trimethylbenzene	0
ethylbenzene	0.1	1,3,5-trimethylbenzene	0
Total	100	Total	100

Table B.6 – continued 4

Song et al., (2007)		Templer (2007)	
LPG		LPG	
Species	Per cent (%)	Species	Per cent (%)
propane	0.2	propane	90.6
isobutane	0.2	propylene	5.1
butane	0.1	ethane	4.1
1-butene	0.1	isobutane	0.2
ethylene	0.1	ethylene	0
propylene	0.1	acetylene	0

Table B.7 Petrochemical sources

Cai et al. (2010)				Song et al. (2008)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
propylene	12.5	2,4-dimethylpentane	12	m and p-xylene	20.9
isobutane	9	3-methylpentane	8.5	ethylene	17.4
butane	8	1-hexene	8	toluene	12.8
benzene	7.8	butane	7	ethylbenzene	9.1
3-methylpentane	7.5	pentane	7	o-xylene	8.7
isopentane	6	isopentane	6.5	acetylene	6
toluene	6	benzene	4.8	propylene	4.9
1-butene	4	2,3-dimethylbutane	4.5	benzene	2.8
2,4-dimethylpentane	3	2-methylpentane	4	1-butene	2.7

Table B.7 – continued 1

2-methylpentane	3	heptane	3	pentane	2.6
hexane	3	hexane	3	hexane	2.4
2,3-dimethylbutane	3	2,2,4-trimethylpentane	3	MTBE	2.4
2,2,4-trimethylpentane	2.3	isobutane	2.5	isobutane	1.6
2,3-dimethylpentane	1.7	propylene	2	2m-propylene	1.4
m and p-xylene	1.7	o-xylene	1.8	isopentane	1.3
ethylbenzene	1.6	3-mehtylheptane	1.8	butane	1
cyclohexane	1.5	cyclohexane	1.2	decane	1
trans-2-butene	1.5	2,3-dimethylpentane	1	2m-1-butene	0.4
cis-2-butene	1	cis-2-pentene	1	isoprene	0.3
heptane	1	ethylbenzene	1	1-pentene	0.2
isopropylbenzene	1	trans-2-butene	1	cis-2-butene	0.2
2-methylhexane	0.8	2,2-dimethylbutane	1	cis-2-pentene	0.1
o-xylene	0.8	cyclopentane	0.8	trans-2-pentene	0.1
2,2-dimethylbutane	0.8	1-butene	0.5	ethane	0
1-hexene	0.8	2-methylhexane	0.5	propane	0
1-pentene	0.5	isoprene	0.5	trans-2-butene	0
cyclopentane	0.5	nonane	0.5	3m-1-butene	0
propylbenzene	0.5	toluene	0.5	2m-2-butene	0
pentane	0.5	2,3,4-trimethylpentane	0.5	limonene	0
styrene	0.5	methylcyclopentane	0.4	a-pinene	0

Table B.7 – continued 2

1,2,4-trimethylbenzene	0.2	octane	0.4	b-pinene	0
1,2,3-trimethylbenzene	0.1	2-methylheptane	0.3	1,2,3-trimethylbenzene	0
2-methylheptane	0.1	styrene	0.3	1,2,4-trimethylbenzene	0
cis-2-pentene	0.1	cis-2-butene	0.2	1,3,5-trimethylbenzene	0
decane	0.1	decane	0.2	1,3-diethylbenzene	0
methylcyclopentane	0.1	trans-2-pentene	0.2	1,4-diethylbenzene	0
nonane	0.1	1-pentene	0.1	1-hexene/2-methyl-1-pent	0
octane	0.1	propylbenzene	0.1	2,2,4-trimethylpentane	0
2,3,4-trimethylpentane	0.1	o-ethyltoluene	0.1	2,2-dimethylbutane	0
p-ethyltoluene	0.1	1,2,3-trimethylbenzene	0.1	2,3,4-trimethylpentane	0
m-diethylbenzene	0.1	1,2,4-trimethylbenzene	0.1	2,3-dimethylbutane	0
p-diethylbenzene	0.1	m-ethyltoluene	0.05	2,3-dimethylpentane	0
methylcyclohexane	0.05	p-ethyltoluene	0.05	2,4-dimethylpentane	0
trans-2-pentene	0.05	1,3,5-trimetylbenzene	0.05	2-ethyltoluene	0
undecane	0.05	m-diethylbenzene	0.05		
3-mehtylheptane	0.05	p-diethylbenzene	0.05	2-methylheptane	0
m-ethyltoluene	0.05	3-methylhexane	0	2-methylhexane	0
1,3,5-trimetylbenzene	0.05	acetylene	0	2-methylpentane	0
o-ethyltoluene	0.05	ethane	0	3-ethyltoluene	0

Table B.7 - continued 3

Chan et al. (2011)				Templer (2007)	
Petroleum Refining		petroleum product wholesaling		Industrial Refinery	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
pentane	10	hexane	10	other	36.3
2,3-dimethylbutane	10	pentane	10	butane	22.9
m and p-xylene	5	2,3-dimethylbutane	10	isobutane	9.6
toluene	5	3-methylhexane	8	pentane	6.6
NO_2	5	styrene	8	propane	3.7
coarse particles	5	toluene	8	hexane	2.9
benzene	1	2-methylhexane	5	toluene	1.9
nonane	1	m and p-xylene	5	3-methylpentane	1.6
o-xylene	1	NO_2	5	benzene	1.6
o3	1	benzene	1	propylene	1.3
coarse ec	1	heptane	1	isopentane	1.3
isoprene	0.7	nonane	1	methylcyclopentane	1.3

Table B.7 - continued 4

decane	0.5	octane	1	trans-2-pentene	0.9
ethylbenzene	0.5	NO	1	trans-2-butene	0.8
heptane	0.5	SO2	1	2,2-dimethylbutane	0.7
octane	0.5	1,2,4-trimethylbenzene	0	heptane	0.7
acetaldehyde	0.5	1,3,5-trimethylbenzene	0	cis-2-butene	0.6
SO2	0.5	2-methylpentane	0	1-pentene	0.6
1,2,4-trimethylbenzene	0	cyclohexane	0	ethane	0.5
1,3,5-trimethylbenzene	0	decane	0	cyclopentane	0.5
2-methylhexane	0	ethylbenzene	0	3-methylhexane	0.5
2-methylpentane	0	isoprene	0	cis-2-pentene	0.4
3-methylhexane	0	methylcyclohexane	0	2,4-dimethylpentane	0.4
cyclohexane	0	methylcyclopentane	0	cyclohexane	0.3
hexane	0	propylbenzene	0	o-xylene	0.3
methylcyclohexane	0	o-xylene	0	1,2,4-trimethylbenzene	0.3
methylcyclopentane	0	1,2,3-trimethylbenzene	0	2-methylpentane	0.2
propylbenzene	0	1,3-diethylbenzene	0	2,2,4-trimethylpentane	0.2
styrene	0	1,4-diethylbenzene	0	methylcyclohexane	0.2
1,2,3-trimethylbenzene	0	1-butene	0	ethylbenzene	0.2
1,3-diethylbenzene	0	1-hexene/2-methyl-1-pent	0	2-methylhexane	0.1
1,4-diethylbenzene	0	1-pentene	0	2,3,4-trimethylpentane	0.1
1-butene	0	2,2,4-trimethylpentane	0	3-methylheptane	0.1
1-hexene/2-methyl-1-pent	0			octane	0.1
				iso-propylbenzene	0.1

Table B.8 Commercial Natural Gas (1)

Song et al. (2008) (Using source profiles of Song et al. (2007)		Song et al. (2007)		Templer (2007)	
Species	Per cent (%)	Species	Per cent (%)	Species	Per cent (%)
ethane	38.5	ethane	38.5	ethane	68.9
acetylene	9.5	acetylene	9.5	propane	21.1
toluene	9.4	toluene	9.4	butane	3.1
benzene	5.7	benzene	5.7	isobutane	2.1
m and p-xylene	5.5	m and p-xylene	5.5	methylcyclopentane	1
2m-1-butene	4.3	2m-1-butene	4.3	isopentane	0.7
pentane	3.6	pentane	3.6	pentane	0.7
isopentane	2.9	isopentane	2.9	other	0.5
2m-propylene	2.7	2m-propylene	2.7	hexane	0.4
1-pentene	2.3	1-pentene	2.3	2-methylheptane	0.4
propylene	2.3	propylene	2.3	2-methylpentane	0.3
1-butene	2.2	1-butene	2.2	2,2,4-trimethylpentane	0.3
hexane	1.7	hexane	1.7	3-methylhexane	0.2
propane	1.7	propane	1.7	heptane	0.2
trans-2-pentene	1.6	trans-2-pentene	1.6	3-methylpentane	0.1
3m-1-butene	1.6	3m-1-butene	1.6	methylcyclohexane	0.1
cis-2-pentene	1	cis-2-pentene	1	ethylene	0
cis-2-butene	0.7	cis-2-butene	0.7	acetylene	0
decane	0.7	decane	0.7	1-butene	0

Table B.8- continued

isoprene	0.6	isoprene	0.6	propylene	0
MTBE	0.6	MTBE	0.6	trans-2-butene	0
o-xylene	0.3	o-xylene	0.3	cis-2-butene	0
isobutane	0.2	isobutane	0.2	1-pentene	0
butane	0.1	butane	0.1	isoprene	0
b-pinene	0.1	â-pinene	0.1	trans-2-pentene	0

Table B.9 Commercial Natural Gas (2)

Song et al. (2008)		Templer (2007)	
Species	Per cent (%)	Species	Per cent (%)
ethane	38.5	ethane	68.9
acetylene	9.5	propane	21.1
toluene	9.4	butane	3.1
benzene	5.7	isobutane	2.1
m and p-xylene	5.5	methylcyclopentane	1
2m-1-butene	4.3	isopentane	0.7
pentane	3.6	pentane	0.7
isopentane	2.9	other	0.5
2m-propylene	2.7	hexane	0.4
1-pentene	2.3	2-methylheptane	0.4

Table B.9- continued

propylene	2.3	2-methylpentane	0.3
1-butene	2.2	2,2,4-trimethylpentane	0.3
hexane	1.7	3-methylhexane	0.2
propane	1.7	heptane	0.2
trans-2-pentene	1.6	3-methylpentane	0.1
3m-1-butene	1.6	methylcyclohexane	0.1
cis-2-pentene	1	ethylene	0
cis-2-butene	0.7	acetylene	0
decane	0.7	1-butene	0
isoprene	0.6	propylene	0
MTBE	0.6	trans-2-butene	0
o-xylene	0.3	cis-2-butene	0
isobutane	0.2	1-pentene	0
butane	0.1	isoprene	0
b-pinene	0.1	trans-2-pentene	0

Appendix C: General Statistics of VOC Compounds in Year 2006

Species	Mean	StDev	Coef Var	Minimum	Median	Maximum	IQR	Skewness	Kurtosis
1,2,3-trimethylbenzene	0.07	0.03	39.98	0.04	0.06	0.15	0.04	1.02	0.95
1,2,4-trimethylbenzene	0.32	0.15	47.24	0.13	0.26	0.77	0.18	1.25	1.28
1,3,5-trimethylbenzene	0.09	0.04	44.02	0.04	0.08	0.22	0.05	1.2	1.47
1,3-diethylbenzene	0.04	0	0	0.04	0.04	0.04	0	-	-
1,4-diethylbenzene	0.08	0.01	14.19	0.08	0.08	0.14	0	3.07	10.08
1-butene	0.24	0.05	20.19	0.15	0.24	0.37	0.07	0.65	0.53
1-hexene/2-methyl-1-pent	0.08	0	0	0.08	0.08	0.08	0	-	-
1-pentene	0.06	0	0	0.06	0.06	0.06	0	-	-
2,2,4-trimethylpentane	0.17	0.08	47.96	0.08	0.16	0.63	0.06	4.49	25.94
2,2-dimethylbutane	0.07	0.01	13.21	0.07	0.07	0.13	0	5.74	35.52
2,3,4-trimethylpentane	0.06	0.03	43.64	0.03	0.06	0.21	0.02	3.71	18.97
2,3-dimethylbutane	0.09	0.04	41.16	0.04	0.09	0.24	0.04	1.89	4.84
2,3-dimethylpentane	0.1	0.03	30.78	0.04	0.09	0.23	0.03	1.82	6.16
2,4-dimethylpentane	0.05	0.02	50.43	0.02	0.04	0.16	0.01	3.24	12.98
2-ethyltoluene	0.08	0.03	38.05	0.04	0.07	0.18	0.04	1.13	1.36
isopentane	1.99	0.69	34.65	0.84	1.94	4.4	0.8	0.99	2.11
2-methylheptane	0.06	0.02	36.65	0.03	0.06	0.17	0.02	2.51	9.73
2-methylhexane	0.23	0.08	34.83	0.1	0.22	0.58	0.07	2.33	8.67
2-methylpentane	0.49	0.32	65.6	0.2	0.42	2.03	0.19	3.18	12.43
3-ethyltoluene	0.19	0.08	41.09	0.08	0.17	0.44	0.09	1.38	2.38

Table C.1 - continued 1

3-methylheptane	0.07	0.03	40.5	0.03	0.07	0.19	0.02	2.77	11.04
3-methylhexane	0.24	0.09	36.23	0.11	0.23	0.64	0.08	2.43	9.19
3-methylpentane	0.44	0.39	89.44	0.16	0.37	2.82	0.15	5.18	30.62
4-ethyltoluene	0.09	0.04	41.67	0.04	0.08	0.23	0.05	1.46	2.78
acetylene	1.18	0.29	24.23	0.7	1.15	2.51	0.25	2.22	9.43
benzene	0.85	0.15	17.23	0.57	0.84	1.17	0.17	0.5	-0.15
butane	3.69	0.97	26.34	1.58	3.66	5.8	1.48	0.15	-0.62
cis-2-butene	0.05	0.01	23.22	0.04	0.04	0.09	0.02	1.86	4.92
cis-2-pentene	0.02	0.01	35.08	0.01	0.02	0.04	0.01	1.13	0.8
cyclohexane	0.07	0.03	41.02	0.04	0.06	0.19	0.04	1.71	3.82
cyclopentane	0.09	0.03	38.66	0.04	0.09	0.2	0.03	1.44	3.46
decane	0.11	0.04	35.4	0.05	0.1	0.22	0.06	0.6	-0.29
ethane	4.47	0.52	11.6	3.32	4.44	5.56	0.67	0.09	-0.43
ethylbenzene	0.37	0.19	51.43	0.18	0.34	1.38	0.13	3.48	16.96
ethylene	1.68	0.32	19.15	1.08	1.67	2.9	0.4	1.05	3.27
heptane	0.18	0.06	35.39	0.1	0.17	0.47	0.05	2.62	10.44
hexane	0.64	0.98	154.06	0.19	0.4	5.88	0.18	4.43	20.56
isobutane	1.26	0.33	26.53	0.63	1.24	2.27	0.46	0.66	0.65
isoprene	0.03	0.01	21.95	0.02	0.03	0.05	0.01	1.28	0.87
iso-propylbenzene	0.04	0	0	0.04	0.04	0.04	0	-	-
m and p-xylene	1.08	0.64	58.67	0.41	1.01	4.38	0.5	3.28	15.35
methylcyclohexane	0.07	0.02	31.76	0.04	0.07	0.15	0.02	1.81	4.74
methylcyclopentane	0.18	0.17	91.17	0.07	0.14	1	0.05	4.03	17.07

Table C.1 - continued 2

nonane	0.08	0.02	27.98	0.04	0.08	0.15	0.03	0.77	0.93
n-propylbenzene	0.07	0.02	34.64	0.04	0.06	0.15	0.03	1.32	2.15
octane	0.09	0.03	32.76	0.05	0.08	0.2	0.03	2.03	6.26
o-xylene	0.32	0.15	48.7	0.13	0.3	1.05	0.14	2.66	10.55
pentane	1.31	0.43	32.84	0.54	1.31	2.82	0.52	0.96	2.19
propane	3.29	0.66	19.95	1.96	3.42	4.58	1.08	-0.39	-0.66
propylene	0.46	0.09	19.88	0.27	0.45	0.71	0.12	0.47	0.56
styrene	0.05	0.01	25.03	0.04	0.05	0.09	0.02	1.4	2.2
trans-2-butene	0.33	0	0	0.33	0.33	0.33	0	-	-
trans-2-pentene	0.04	0.02	40.51	0.02	0.04	0.09	0.02	0.92	0.56
toluene	2.67	1.7	63.76	0.92	2.37	11.54	0.91	3.67	16.75
undecane	0.12	0.05	39.53	0.05	0.11	0.23	0.08	0.78	-0.28
other	1.07	0.34	31.32	0.54	0.99	2.11	0.32	0.97	1.27
total	31.3	7.19	23	17.8	31.2	50.9	11.5	0.46	-0.13

Appendix D: MDL of Each VOC Species (Templer, 2007)

Species	MDL ($\mu g/m^3$)	Species	MDL ($\mu g/m^3$)
1,1,1-trichloroethane	0.037	2,5-dimethylhexane	0.009
1,1,2,2-tetrachloroethane	0.039	2-butanol	0.009
1,1,2-trichloroethane	0.049	2-butenal (crotonaldehdye)	0.040
1,1-dichloroethane	0.031	2-ethyl-1-butene	0.048
1,1-dichloroethene	0.034	2-ethyltoluene	0.013
1,2,3-trimethylbenzene	0.016	2-methyl-1-butene	0.006
1,2,4-trichlorobenzene	0.090	2-methyl-2-butene	0.008
1,2,4-trimethylbenzene	0.032	2-methylbutanal	0.009
1,2-dibromoethane (edb)	0.050	2-methylbutane	0.023
1,2-dichlorobenzene	0.044	2-methylfuran	0.009
1,2-dichloroethane	0.034	2-methylheptane	0.016
1,2-dichloropropane	0.024	2-methylhexane	0.012
1,2-diethylbenzene	0.018	2-methylpentane	0.024
1,3,5-trimethylbenzene	0.013	2-methyl-propanal	0.009
1,3-butadiene	0.018	2-pentanone	0.004
1,3-dichlorobenzene	0.036	3,6-dimethyloctane	0.094
1,3-diethylbenzene	0.017	3-ethyltoluene	0.012
1,4-dichlorobenzene	0.017	3-methyl-1-butene	0.009
1,4-dichlorobutane	0.023	3-methyl-1-pentene	0.029
1,4-diethylbenzene	0.051	3-methylheptane	0.007
1-butanol (butyl alcohol)	0.013	3-methylhexane	0.013
1-butene/2-methylpropene	0.038	3-methylpentane	0.033
1-butyne	0.021	4-ethyltoluene	0.027

Table D.1 – continued 1

1-decene	0.017	4-methyl-1-pentene	0.012
1-heptene	0.012	4-methylheptane	0.008
1-hexene/2-methyl-1-pentene	0.038	acetaldehyde	0.009
1-methylcyclohexene	0.022	acetone	0.009
1-methylcyclopentene	0.014	acetonitrile	0.044
1-nonene	0.005	acetylene	0.057
1-octene	0.010	acrolein (2-propenal)	0.027
1-pentene	0.028	acrylonitrile	0.031
1-undecene	0.017	a-pinene	0.030
2,2,3-trimethylbutane	0.007	benzaldehyde	0.004
2,2,4-trimethylpentane	0.027	benzene	0.024
2,2,5-trimethylhexane	0.005	benzyl chloride	0.026
2,2-dimethylbutane	0.025	b-pinene	0.027
2,2-dimethylhexane	0.008	bromodichloromethane	0.056
2,2-dimethylpentane	0.014	bromoform	0.031
2,2-dimethylpropane	0.105	bromomethane	0.051
2,3,4-trimethylpentane	0.012	bromotrichloromethane	0.079
2,3-dimethylbutane	0.009	butane	0.049
2,3-dimethylpentane	0.012	butylacetate	0.018
2,4-dimethylhexane	0.011	butylaldehyde (butanal)	0.022
2,4-dimethylpentane	0.012	c-1,2-dichloroethene	0.024
c-1,2-dimethylcyclohexane	0.019	isobutane (2-methylpropane)	0.022
c-1,3-dichloropropene	0.007	isobutylacetate	0.013
c-1,3-dimethylcyclohexane	0.009	isobutylalcohol	0.022
c-1,4/t-1,3-dimethylcyclohexane	0.004	iso-butylbenzene	0.018
c-2-butene	0.022	isoprene	0.008

Table D.1 – continued 2

c-2-heptene	0.016	isopropyl alcohol	0.009
c-2-hexene	0.020	isopropylacetate	0.004
c-2-pentene	0.005	iso-propylbenzene	0.014
c-3-heptene	0.014	limonene	0.083
c-3-methyl-2-pentene	0.010	m and p-xylene	0.027
c-4-methyl-2-pentene	0.012	mac (2-methyl-2-propenal)	0.009
camphene	0.063	mek	0.009
carbon disulfide	0.004	methanol	0.004
carbontretrachloride	0.028	methyl acetate	0.027
chlorobenzene	0.039	methylcyclohexane	0.007
chloroethane	0.057	methylcyclopentane	0.010
chloroform	0.023	methyl-t-butyl ether (MTBE)	0.025
chloromethane	0.029	mibk	0.009
cyclohexane	0.009	mvk	0.013
cyclohexanone	0.022	naphthalene	0.034
cyclohexene	0.026	n-butylbenzene	0.019
cyclopentane	0.008	nonane	0.010
cyclopentanone	0.000	n-propylbenzene	0.013
cyclopentene	0.017	octane	0.012
decane	0.012	o-xylene	0.013
dibromomethane	0.055	pentanal	0.013
dichloromethane	0.025	pentane	0.086
dodecane	0.029	propane	0.173
ethane	0.057	propene	0.019
ethanol	0.027	propyl alcohol (1-propanol)	0.013
ethylacetate	0.009	propyne	0.010
ethylbenzene	0.015	styrene	0.016

Table D.1 – continued 3

ethylbromide	0.024	t-2-butene	0.027
ethylene	0.067	t-2-heptene	0.012
freon 11	0.026	t-2-hexene	0.014
freon 113	0.028	t-2-octene	0.018
freon 114	0.080	t-2-pentene	0.006
freon 12	0.056	t-3-methyl-2-pentene	0.011
freon 22	0.045	t-4-methyl-2-pentene	0.010
heptane	0.027	tert-butylbenzene	0.012
hexachlorobutadiene	0.083	tetrachloroethene	0.044
hexanal	0.018	toluene	0.025
hexane	0.017	trichloroethene	0.038
hexylbenzene	0.052	undecane	0.014
indan (2,3-dihydroindene)	0.021	vinylchloride (chloroethene)	0.012

Appendix E: The Abbreviation of the Species Names

BZ123M	1,2,3-trimethylbenzene
BZ124M	1,2,4-trimethylbenzene
BZ135M	1,3,5-trimethylbenzene
DETBZ1	1,3-diethylbenzene
DETBZ2	1,4-diethylbenzene
LBUT1E	1-butene
P1E2ME	1-hexene/2-methyl-1-pentene
PENTE1	1-pentene
PA224M	2,2,4-trimethylpentane
BU22DM	2,2-dimethylbutane
PA234M	2,3,4-trimethylpentane
BU23DM	2,3-dimethylbutane
PEN23M	2,3-dimethylpentane
PEN24M	2,4-dimethylpentane
O_ETOL	2-ethyltoluene
IPENTA	isopentane
HEP2ME	2-methylheptane
HEXA2M	2-methylhexane
PENA2M	2-methylpentane
M_ETOL	3-ethyltoluene
HEP3ME	3-methylheptane
HEXA3M	3-methylhexane
PENA3M	3-methylpentane
P_ETOL	4-ethyltoluene
ACETYL	acetylene
BENZE	benzene
N_BUTA	butane
C2BUTE	cis-2-butene
C2PENE	cis-2-pentene
CYHEXA	cyclohexane
CPENTA	cyclopentane
N_DEC	decane
ETHANE	ethane
ETBZ	ethylbenzene
ETHENE	ethylene
N_HEPT	heptane

Table F.1 – continued 1

N_HEX	hexane
I_BUTA	isobutane
I_PREN	isoprene
IPRBZ	iso-propylbenzene
MP_XYL	m and p-xylene
MECYHX	methylcyclohexane
MCYPNA	methylcyclopentane
N_NON	nonane
N_PRBZ	n-propylbenzene
N_OCT	octane
O_XYL	o-xylene
N_PENT	pentane
N_PROP	propane
PROPE	propylene
STYR	styrene
T2BUTE	trans-2-butene
T2PENE	trans-2-pentene
TOLUE	toluene
N_UNDE	undecane

Appendix F: CMB Model Outputs

Table G.1 CMB winter outputs

	R	CHI	%	Tu_MchHD	Exh_Lin1	WA_LIQ	WA_VAP	CNG	LPG	Ind_Ref	Coke_Ovn	Arc_Coat	Biogenic
10250BBPX	0.9	3.5	111.8	1.8	6.8	-0.3	5.5	5.6	2.6	6.3	2.0	2.6	0.0
11377BFDP	0.9	3.9	99.6	2.0	2.7	0.5	2.4	4.7	1.4	4.1	1.2	1.8	0.0
11428BFGZ	0.8	4.1	100.0	1.6	2.7	0.6	3.1	4.6	1.4	3.8	1.3	2.5	0.0
11546BFNQ	0.9	3.8	110.9	1.6	5.4	0.3	5.4	4.1	2.5	6.0	1.2	3.8	0.0
11683BFWD	0.7	7.0	121.8	3.0	9.2	-0.9	3.9	6.8	0.5	9.8	1.6	12.3	0.0
11688BFWK	0.9	3.8	105.2	1.5	5.1	-0.7	3.0	5.0	2.4	5.0	1.6	2.1	0.0
12135BGWR	0.9	2.6	113.3	2.0	9.8	-1.0	10.6	5.8	2.1	5.3	2.4	5.5	0.0
12380BHLJ	0.9	3.6	105.4	2.2	6.2	0.4	5.5	6.2	2.1	5.1	1.9	3.1	0.0
12439BHPD	0.9	3.9	104.1	1.8	2.3	1.4	3.1	4.8	1.3	4.4	1.9	2.7	0.0
12533BHTQ	0.8	3.7	107.2	3.9	3.9	0.8	7.3	6.9	2.0	6.4	1.9	4.6	0.0
12746BJGT	0.8	4.0	101.9	2.1	3.8	0.7	3.9	5.9	2.7	5.9	1.4	3.3	0.0
12889BJPP	0.9	3.5	113.0	2.9	9.3	-0.4	6.8	6.9	2.1	7.9	2.8	5.7	0.0
13601BLFM	0.9	3.4	110.4	3.9	6.0	0.6	9.1	7.2	2.2	6.4	2.2	5.9	0.0
13838BLST	0.9	3.7	109.8	3.5	5.2	0.6	5.7	5.8	1.1	5.8	1.9	3.1	0.0
14015BMDF	0.9	3.7	100.9	2.4	4.9	0.2	6.4	6.9	2.3	7.6	2.2	3.6	0.0
14043BMFN	0.8	4.1	104.3	1.9	5.2	0.4	5.2	5.6	2.4	6.6	1.7	3.3	0.0
14602BNMD	0.9	3.6	99.8	1.8	4.9	0.3	6.6	5.1	2.0	5.0	1.7	3.2	0.0
14880BPCK	0.9	2.5	120.7	2.8	16.6	6.9	8.1	6.2	2.6	11.2	2.2	2.2	0.0
14986BPJL	0.8	3.9	92.3	1.5	2.5	0.3	5.1	4.7	1.2	3.3	1.3	2.1	0.0
15012BPKR	0.8	4.3	106.6	3.0	7.9	4.3	7.9	6.5	0.5	5.0	2.0	5.9	0.0
15906BRLG	0.9	3.6	109.4	3.2	5.0	0.6	6.7	6.0	0.7	5.9	1.7	3.0	0.0
15944BRNB	0.8	3.7	102.6	3.0	3.9	0.6	6.9	6.6	2.1	5.2	1.9	4.8	0.0

Table G.1 – continued 1

16217BSDB	0.9	3.6	109.3	1.1	4.5	0.0	4.1	4.6	2.5	5.8	1.2	2.8	0.0
16911BTSC	0.9	3.2	110.7	1.4	5.5	-0.7	5.5	5.0	3.6	4.4	1.8	3.1	0.0
17847BWVR	0.9	3.9	104.4	1.4	4.6	0.1	4.3	5.1	2.5	5.8	1.3	2.8	0.0
18080BXJT	0.9	3.6	106.7	1.3	4.8	-0.3	4.2	5.1	1.8	4.8	1.5	3.6	0.0
18706BYTP	0.9	3.2	104.1	1.2	4.2	-0.2	6.3	5.5	2.1	3.9	1.6	3.7	0.0
18725BYVM	0.8	4.8	99.2	1.1	2.5	0.6	2.5	4.2	2.4	4.8	1.0	1.3	0.0
19494CBPC	0.9	3.1	106.2	2.5	5.2	-0.5	6.7	6.1	2.3	4.3	1.8	4.9	0.0
19567CBSP	0.9	3.7	107.0	2.0	6.1	0.6	6.2	6.0	2.1	5.7	2.2	3.8	0.0
19796CCGM	0.8	4.5	91.6	3.8	7.1	-1.8	4.3	7.2	1.8	8.6	1.8	3.5	0.0
19831CCJD	0.8	4.4	110.6	1.5	6.1	-0.7	4.1	5.9	2.3	5.7	2.0	3.9	0.0
19833CCJG	0.9	3.4	107.1	1.8	4.1	-0.7	2.6	4.4	1.5	5.2	1.4	1.5	0.0
30003DFKN	0.7	7.7	91.1	2.7	7.7	-0.3	6.3	6.6	2.2	10.5	1.3	2.7	0.0
30182DFVB	0.9	4.0	100.0	1.9	3.4	1.8	3.8	5.5	1.1	3.9	1.7	2.7	0.0
30264DFYY	0.9	3.6	104.0	2.2	4.7	1.2	4.6	5.7	2.8	5.1	1.6	2.4	0.0
31026DHSG	0.8	6.3	102.5	1.8	4.7	0.0	3.0	4.7	2.3	4.5	2.1	1.9	0.0
31027DHSH	0.8	4.1	95.7	2.4	1.7	1.6	2.0	5.0	1.6	4.0	1.6	1.5	0.0
31049DHTJ	0.9	3.5	105.9	3.4	4.3	0.3	5.8	5.8	2.7	4.7	2.1	3.7	0.0
31487DJTF	0.8	4.7	92.5	1.4	7.5	-1.1	6.5	6.0	2.1	6.5	2.2	6.6	0.0
31612DKBD	0.8	5.1	101.7	2.4	2.2	0.0	1.9	4.5	1.0	3.0	1.3	0.9	0.0
32017DKYL	0.9	3.3	106.4	3.3	5.4	0.3	7.0	6.1	2.9	5.6	2.0	3.8	0.0
32331DLRK	0.9	3.2	107.9	2.2	5.8	-0.9	8.6	5.0	3.8	3.2	2.1	2.9	0.0
32769DMRG	0.8	4.6	104.9	1.4	3.6	0.0	3.2	4.4	2.8	5.7	1.4	2.0	0.0
32869DMWZ	0.9	3.7	113.3	1.9	7.0	-0.5	5.4	5.6	2.6	6.7	2.0	4.5	0.0

Table G.1 – continued 2

33003DNFK	0.9	3.8	108.4	2.1	5.6	0.0	5.0	5.5	1.9	6.4	2.0	3.5	0.0
33696DPTK	0.8	3.8	107.2	3.8	5.6	0.2	7.7	7.2	2.2	5.9	2.2	6.0	0.0
NAPS	0.9	3.3	110.4	3.6	7.8	-0.6	5.4	8.3	6.0	9.4	2.1	2.4	0.0

Table G.2 CMB summer outputs

Site name	R	CHI	%	Tu_MchHD	Exh_Lin1	WA_LIQ	WA_VAP	CNG	LPG	Ind_Ref	Coke_Ovn	Arc_Coat	Biogenic
10250BBPX	0.9	2.7	135.4	7.7	14.2	1.4	11.8	5.0	2.4	9.8	2.0	8.4	0.3
11000BDHQ	0.9	2.7	132.3	9.0	9.8	0.9	10.1	7.1	2.4	7.2	1.4	9.1	0.5
11377BFDP	0.9	2.6	137.6	13.1	6.7	8.1	6.9	4.0	2.9	8.6	0.2	7.5	0.6
11428BFGZ	0.9	2.7	134.6	6.7	7.7	1.1	8.2	4.4	1.3	6.2	1.5	3.4	0.8
11546BFNQ	0.8	3.7	97.5	8.0	10.0	0.0	16.1	3.0	21.5	21.4	1.4	19.7	0.6
11683BFWD	0.9	2.2	131.1	7.6	8.0	0.2	9.1	4.4	1.5	6.2	1.3	4.5	0.6
11688BFWK	0.9	3.1	120.6	6.5	11.9	4.7	8.1	4.0	0.9	5.0	-0.1	2.3	2.3
12380BHLJ	0.9	2.0	134.0	7.2	8.1	3.4	14.7	5.0	2.4	8.0	2.1	15.5	0.4
12439BHPD	0.9	2.2	131.1	5.6	10.4	-0.9	10.5	4.1	1.5	5.5	1.8	7.5	1.2
12533BHTQ	0.9	3.4	130.8	12.8	9.0	8.9	11.2	4.5	0.8	9.6	0.4	6.2	0.2
12746BJGT	0.9	1.9	126.5	3.9	7.0	-0.1	6.1	3.8	1.5	4.3	0.6	2.3	2.3
12753BJHC	0.9	3.2	126.3	8.0	8.8	1.7	8.3	5.6	11.8	7.5	1.4	6.3	0.7
12889BJPP	0.9	2.3	124.8	5.5	8.8	0.5	7.3	5.9	0.8	3.6	1.5	5.2	0.5
13601BLFM	0.9	2.0	144.0	32.2	2.9	2.9	33.0	5.6	1.0	0.2	-0.1	15.2	0.6
13838BLST	0.9	2.8	131.2	5.9	10.1	1.4	9.3	4.8	2.0	6.4	1.6	6.7	0.3
14015BMDF	0.9	1.8	132.1	7.7	5.9	3.4	13.3	5.6	2.5	5.6	1.7	9.0	0.3

Table G.2- continued 1

14602BNMD	0.9	1.8	126.1	3.1	4.4	1.1	8.2	2.5	3.6	4.5	1.4	5.5	0.2
14880BPCK	0.9	2.7	126.0	5.2	7.1	0.9	6.3	3.9	1.8	5.0	0.7	4.1	0.3
14986BPJL	0.9	2.9	132.5	6.4	5.1	4.3	8.0	3.7	2.2	9.8	0.3	3.8	0.3
15012BPKR	0.9	2.5	138.9	8.8	6.7	13.1	10.6	4.1	2.9	7.7	1.5	12.7	0.3
15906BRLG	0.9	3.1	131.1	12.6	13.1	6.5	19.7	4.0	3.7	11.9	-0.2	8.5	0.3
15944BRNB	0.9	2.3	136.9	10.2	8.6	3.4	8.6	4.5	1.6	7.7	1.7	8.7	0.9
16217BSDB	0.9	2.4	132.5	5.6	11.9	8.1	8.7	3.9	1.6	5.7	0.6	7.2	0.7
16911BTSC	0.9	2.3	130.6	5.3	6.0	0.3	9.4	4.1	1.5	4.5	1.5	5.1	0.2
17847BWVR	0.9	1.8	127.8	6.1	8.6	-0.5	9.2	5.4	1.3	3.8	1.3	4.1	0.5
18080BXJT	0.9	2.2	132.0	4.9	6.6	1.6	7.8	3.5	1.6	5.6	0.7	4.6	0.5
18706BYTP	0.9	1.8	135.6	10.7	2.3	1.8	11.3	3.3	1.9	7.7	-0.9	8.4	0.9
18725BYVM	0.9	2.9	125.3	6.1	10.9	0.3	9.2	4.7	0.8	4.8	0.7	3.5	1.2
19567CBSP	0.9	1.9	134.6	6.7	6.6	0.1	9.6	4.0	1.5	5.3	0.9	5.6	0.8
19796CCGM	0.9	2.7	132.5	8.6	7.4	7.0	8.5	4.6	1.7	10.0	1.0	5.8	0.3
19831CCJD	0.9	2.3	137.4	4.9	11.3	-0.1	12.4	4.9	2.1	8.7	1.5	9.2	1.3
30003DFKN	0.9	1.7	134.5	8.0	8.4	5.1	14.0	4.7	2.6	8.5	0.9	5.2	0.5
30182DFVB	0.9	2.3	133.8	7.0	8.7	2.7	9.5	3.9	1.8	4.8	0.9	6.0	0.5
30264DFYY	0.9	1.8	135.0	6.2	8.8	0.4	12.8	3.6	2.3	5.4	1.0	5.2	0.6
31026DHSG	0.8	4.6	122.4	11.9	19.4	14.8	5.9	4.5	1.1	9.0	0.4	8.3	0.3
31027DHSH	0.9	2.1	129.2	4.8	9.5	0.3	9.5	4.3	1.9	5.0	0.8	4.4	1.4
31049DHTJ	0.9	2.8	140.3	14.2	9.6	11.9	23.6	4.4	1.9	6.7	-0.4	18.5	0.4
31487DJTF	0.9	3.0	129.8	4.9	7.8	3.9	3.4	3.7	1.6	5.3	0.8	5.3	1.0
31612DKBD	0.9	2.7	121.7	4.6	6.0	1.4	5.5	4.8	0.8	3.8	1.2	2.5	0.3

Table G.2- continued 2

32017DKYL	0.9	2.1	139.3	7.5	13.1	3.3	24.7	4.9	2.7	11.8	1.7	9.7	0.3
32331DLRK	0.9	2.0	136.8	9.3	5.4	1.1	14.5	3.8	2.2	5.4	4.3	9.3	0.4
32769DMRG	0.9	2.7	133.0	7.5	7.5	5.6	5.4	3.4	1.1	7.9	0.7	3.1	0.3
32869DMWZ	0.9	1.8	134.3	5.5	9.1	0.8	12.4	4.4	2.2	7.3	1.5	4.9	0.6
33003DNFK	0.9	2.2	135.8	11.1	4.0	1.7	8.2	4.7	0.8	4.4	0.7	5.5	0.8
33696DPTK	0.9	3.1	129.4	9.5	10.1	10.4	14.6	5.9	0.6	10.7	0.6	7.7	0.4
NAPS-Summer	0.9	2.4	131.0	8.7	10.5	1.1	9.5	8.4	5.9	10.6	1.5	7.2	0.4

Appendix G: PMF Best Run Outputs

Table H.1 Factor Profiles (conc. of species) from Base Run #7 (Convergent Run) PMF of winter 2006

Species	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8	Factor 9	Factor 10	Factor 11	Factor 12	Factor 13
BZ123M	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
BZ124M	0.06	0.00	0.00	0.02	0.01	0.01	0.00	0.09	0.03	0.06	0.02	0.02	0.00
BZ135M	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.01	0.02	0.01	0.01	0.00
LBUT1E	0.03	0.04	0.01	0.02	0.00	0.02	0.03	0.02	0.01	0.03	0.01	0.01	0.03
PA224M	0.05	0.01	0.00	0.01	0.02	0.01	0.03	0.00	0.00	0.00	0.00	0.02	0.02
BU22DM	0.01	0.00	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01
PA234M	0.02	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01
BU23DM	0.02	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.01	0.01
PEN23M	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.01	0.00	0.01	0.01
PEN24M	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.00
O_ETOL	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.01	0.02	0.00	0.00	0.01
IPENTA	0.28	0.09	0.09	0.23	0.35	0.02	0.42	0.09	0.15	0.11	0.06	0.02	0.07
HEP2ME	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.01
HEXA2M	0.02	0.02	0.01	0.03	0.04	0.00	0.02	0.01	0.00	0.03	0.01	0.03	0.02
PENA2M	0.09	0.02	0.00	0.07	0.02	0.00	0.06	0.00	0.03	0.01	0.11	0.04	0.02
M_ETOL	0.04	0.01	0.00	0.02	0.01	0.01	0.00	0.04	0.01	0.03	0.01	0.01	0.01
HEP3ME	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.01
HEXA3M	0.02	0.02	0.01	0.03	0.04	0.00	0.02	0.01	0.01	0.02	0.01	0.03	0.02
PENA3M	0.06	0.01	0.01	0.02	0.00	0.00	0.05	0.01	0.01	0.04	0.15	0.03	0.02
P_ETOL	0.02	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.01	0.01	0.00	0.01	0.01
ACETYL	0.03	0.00	0.00	0.18	0.00	0.08	0.16	0.10	0.00	0.31	0.02	0.06	0.24
BENZE	0.09	0.12	0.06	0.04	0.01	0.05	0.13	0.07	0.03	0.07	0.00	0.04	0.13

Table H.1 - continued 1

N_BUTA	0.34	0.43	0.18	0.09	0.56	0.08	0.81	0.30	0.20	0.46	0.13	0.02	0.09
C2BUTE	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
C2PENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CYHEXA	0.00	0.01	0.01	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.03	0.00
CPENTA	0.01	0.00	0.00	0.02	0.02	0.00	0.01	0.01	0.01	0.00	0.00	0.00	0.01
N_DEC	0.01	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.03	0.02	0.00	0.01	0.01
ETHANE	0.17	0.49	0.28	0.04	0.22	0.28	0.47	0.32	0.22	0.85	0.11	0.18	0.84
ETBZ	0.00	0.04	0.00	0.06	0.08	0.08	0.01	0.04	0.01	0.02	0.01	0.01	0.01
ETHENE	0.09	0.16	0.05	0.06	0.06	0.09	0.27	0.19	0.01	0.32	0.01	0.13	0.24
N_HEPT	0.03	0.00	0.00	0.02	0.02	0.00	0.02	0.01	0.01	0.01	0.00	0.01	0.02
N_HEX	0.02	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.39	0.00	0.01
I_BUTA	0.15	0.11	0.13	0.00	0.17	0.02	0.25	0.09	0.07	0.11	0.05	0.00	0.10
I_PREN	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MP_XYL	0.02	0.11	0.01	0.19	0.27	0.26	0.01	0.13	0.00	0.03	0.03	0.02	0.00
MECYHX	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.01
MCYPNA	0.00	0.03	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.02	0.07	0.03	0.00
N_NON	0.01	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.01
N_PRBZ	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.01
N_OCT	0.02	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.01	0.02
O_XYL	0.01	0.04	0.00	0.06	0.06	0.06	0.00	0.04	0.00	0.02	0.01	0.00	0.02
N_PENT	0.13	0.00	0.05	0.19	0.28	0.01	0.25	0.08	0.10	0.04	0.04	0.01	0.11
N_PROP	0.00	0.14	0.32	0.02	0.58	0.00	0.48	0.45	0.23	0.06	0.10	0.05	0.83
PROPE	0.04	0.06	0.02	0.03	0.01	0.03	0.06	0.05	0.01	0.06	0.01	0.02	0.06
STYR	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00
T2PENE	0.01	0.01	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00

Table H.1 - continued 2

TOLUE	0.30	0.02	1.16	0.32	0.00	0.00	0.00	0.00	0.00	0.68	0.18	0.00	0.00
N_UNDE	0.00	0.01	0.00	0.00	0.02	0.01	0.00	0.00	0.02	0.03	0.01	0.01	0.00
OTHER	0.13	0.14	0.05	0.03	0.10	0.04	0.09	0.13	0.11	0.11	0.03	0.08	0.03

Table H.2 Factor Contributions (avg = 1) from Base Run #7 (Convergent Run) of winter 2006

	Factor1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8	Factor 9	Factor 10	Factor 11	Factor 12	Factor 13
10250BBPX	0.98	1.70	0.90	1.09	1.36	0.03	0.90	0.75	1.03	0.22	0.88	0.99	1.73
11377BFDP	0.51	0.84	0.37	0.01	0.53	0.92	0.62	-0.03	0.45	1.26	0.23	0.77	1.60
11428BFGZ	0.51	0.68	0.54	0.38	0.60	0.70	0.87	0.02	0.11	1.28	0.14	0.59	1.49
11546BFNQ	0.51	0.26	1.83	1.31	0.47	1.35	1.94	1.06	0.94	-0.20	0.43	2.19	0.64
11683BFWD	-0.20	1.92	3.99	3.10	0.28	-0.20	-0.20	-0.20	-0.20	1.52	5.24	6.02	-0.20
11688BFWK	0.35	2.11	0.85	0.48	0.20	0.14	0.70	1.38	0.35	0.19	0.54	0.47	1.88
12135BGWR	1.87	2.66	1.16	3.10	0.88	0.49	2.03	1.56	1.27	0.04	1.01	0.79	-0.20
12380BHLJ	1.58	1.93	0.59	1.17	0.88	0.71	0.78	1.03	0.65	0.92	0.49	1.15	1.31
12439BHPD	0.32	0.21	0.62	0.71	0.43	1.37	1.12	-0.20	0.49	1.37	0.03	1.30	1.46
12533BHTQ	0.93	0.77	0.46	0.75	2.21	0.44	0.78	1.23	3.17	2.56	1.02	-0.16	0.24
12746BJGT	0.64	1.09	0.92	0.13	1.36	0.47	0.84	0.59	0.12	1.66	0.66	0.47	1.79
12889BJPP	2.53	2.65	1.67	1.78	1.05	1.11	0.55	1.85	1.12	0.80	0.82	1.69	0.49
13601BLFM	1.68	1.07	0.93	1.16	2.95	0.75	0.75	0.43	2.88	2.19	1.04	0.15	0.41
13838BLST	1.68	1.15	0.23	1.69	0.35	1.24	0.19	1.39	3.33	1.44	0.47	1.20	0.38
14015BMDF	0.38	1.50	0.57	1.49	0.78	1.59	1.91	2.49	0.64	1.57	0.64	0.75	0.60
14043BMFN	1.01	1.71	1.04	1.04	0.64	0.86	1.50	1.33	0.37	0.66	0.47	0.90	1.34

Table H.2 – continued 1

14602BNMD	0.93	1.51	0.59	0.90	1.14	0.91	2.15	0.92	0.12	1.15	0.33	0.50	0.45
14880BPCK	7.28	-0.20	0.91	1.71	4.71	0.69	-0.20	0.08	-0.19	0.03	2.33	5.72	0.89
14986BPJL	0.47	0.94	0.02	-0.13	1.07	0.30	2.03	0.22	0.28	1.71	0.26	-0.12	0.42
15012BPKR	2.29	0.02	-0.20	6.74	-0.16	1.50	0.41	3.37	1.14	2.41	0.41	1.35	-0.18
15906BRLG	1.40	1.40	-0.14	2.70	0.09	0.80	0.95	0.87	3.20	1.47	0.61	0.55	0.16
15944BRNB	0.99	0.91	0.58	0.66	2.07	0.81	1.11	1.06	1.46	2.30	0.55	-0.09	0.61
16217BSDB	0.32	0.68	1.47	0.47	0.66	0.58	1.42	0.95	0.32	-0.08	0.71	1.31	1.41
16911BTSC	0.14	0.99	1.25	1.16	1.23	-0.20	0.59	1.71	1.60	-0.20	0.82	0.40	1.87
17847BWVR	0.28	0.85	1.34	0.60	0.11	1.20	1.96	1.27	0.16	0.16	0.36	1.70	1.32
18080BXJT	0.63	1.19	1.05	1.04	0.27	0.68	1.14	0.82	-0.03	0.69	0.48	0.48	1.40
18706BYTP	0.30	0.84	0.83	0.89	1.08	0.31	1.78	0.35	0.46	0.91	0.58	0.03	1.36
18725BYVM	-0.20	0.47	1.01	-0.20	0.60	0.65	1.34	0.80	0.17	0.18	0.22	1.69	1.59
19494CBPC	1.39	1.58	0.82	0.01	1.98	0.42	0.80	0.82	1.43	1.67	0.66	-0.08	0.57
19567CBSP	1.51	1.52	0.87	1.68	0.71	0.96	1.17	1.55	0.61	0.78	0.47	1.22	1.04
19796CCGM	-0.14	-0.20	1.88	-0.20	3.85	12.79	-0.20	1.76	-0.20	-0.20	2.82	-0.20	-0.20
19831CCJD	0.61	1.85	1.65	1.22	0.56	0.25	0.39	1.40	0.60	0.28	0.66	0.58	1.80
19833CCJG	0.35	1.94	0.52	0.16	0.33	0.23	0.67	0.64	1.17	0.46	0.63	-0.01	1.26
30003DFKN	0.47	-0.19	-0.20	-0.20	-0.20	2.56	3.73	-0.19	-0.15	-0.19	14.33	1.73	0.89
30182DFVB	0.87	0.40	0.10	1.00	0.53	1.21	1.22	-0.07	-0.20	1.99	-0.04	1.16	1.54
30264DFYY	0.97	0.67	0.53	0.20	1.58	0.62	1.02	0.08	0.40	1.32	0.56	1.06	2.12
31026DHSG	1.81	-0.20	0.85	-0.20	-0.16	0.31	-0.20	4.39	1.80	0.46	0.39	1.65	0.91
31027DHSH	0.26	-0.20	-0.20	0.04	0.16	1.31	0.82	0.54	0.85	2.20	-0.04	1.15	1.85
31049DHTJ	1.26	1.01	0.53	0.30	1.96	0.81	0.20	0.70	2.56	1.77	0.41	0.35	1.20
31487DJTF	2.17	-0.16	7.92	1.24	0.55	1.23	1.21	-0.20	-0.06	1.77	0.50	-0.20	-0.20
31612DKBD	0.45	0.65	0.21	0.05	-0.20	1.24	0.12	0.07	2.61	0.79	-0.19	0.99	1.48

Table H.2 – continued 2

32017DKYL	1.25	1.71	0.44	0.79	1.93	0.32	1.01	0.66	2.18	1.70	0.84	0.06	1.00
32331DLRK	-0.01	0.55	0.86	1.37	1.39	-0.20	1.85	0.63	2.79	0.37	0.83	0.26	1.71
32769DMRG	-0.10	0.30	1.46	-0.03	0.13	0.89	1.60	1.68	1.04	-0.20	0.27	2.35	1.37
32869DMWZ	1.05	1.67	1.70	1.32	1.06	0.45	0.86	0.65	0.81	0.38	0.80	1.00	1.63
33003DNFK	1.04	1.35	0.95	1.39	0.44	0.97	0.91	2.03	0.84	0.74	0.56	1.25	0.72
33696DPTK	1.72	0.98	0.82	1.05	2.46	0.55	-0.20	2.71	2.61	2.58	0.91	-0.16	0.00

Table H.3 Scaled residuals of PMF outputs in winter 2006

	BZ123M	BZ124M	BZ135M	LBUT1E	PA224M	BU22DM	PA234M	BU23DM	PEN23M	PEN24M	O_ETOL
10250BBPX	-0.125	-0.064	-0.129	0.005	-0.233	0.057	-0.11	0.056	0.109	0.034	0.064
11377BFDP	-0.002	0.059	-0.022	0.064	-0.064	0.023	0.086	0.108	0.087	-0.038	0.068
11428BFGZ	-0.104	-0.009	-0.127	0.01	-0.114	0.015	-0.021	0.028	0.042	-0.028	0.113
11546BFNQ	0.203	0.235	-0.069	0.233	0.06	-0.034	-0.236	-0.093	0.083	-0.265	-0.107
11683BFWD	-0.091	0.037	0.024	0.005	0.052	0.008	0.053	-0.003	-0.017	0.299	0.018
11688BFWK	0.071	0.012	0.003	-0.056	-0.002	0.038	-0.119	0.104	0.008	0	-0.036
12135BGWR	-0.118	0.128	-0.006	0.052	0.014	0.012	0.058	0.488	0.246	0.179	0.06
12380BHLJ	0.032	0.087	0.12	0.058	0.226	0.002	0.196	0.104	-0.061	-0.003	0.012
12439BHPD	-0.073	0.001	-0.035	0.039	-0.147	0.029	0.061	0.186	0.17	-0.101	0.101
12533BHTQ	0.185	0.406	-0.362	-0.049	-0.176	0.075	-0.281	-0.154	0.01	-0.125	-0.098
12746BJGT	0.091	0.109	0.005	0.125	0.164	-0.011	-0.025	0.066	-0.005	-0.113	-0.085
12889BJPP	0.064	-0.078	-0.033	-0.05	0.041	-0.006	0.208	0.1	0.013	-0.162	-0.07

Table H.3 – continued 1

13601BLFM	-0.133	-0.231	0.097	0.007	-0.427	-0.095	0.059	-0.057	0.001	-0.157	-0.068
13838BLST	-0.007	-0.164	-0.025	0.133	0.049	-0.003	-0.063	-0.07	-0.025	-0.079	0.018
14015BMDF	0.143	-0.208	-0.053	-0.253	0.2	0.026	-0.118	0.046	-0.156	-0.117	-0.142
14043BMFN	0.014	0.049	0.022	-0.207	-0.142	-0.067	-0.067	-0.223	-0.075	0.077	0.022
14602BNMD	-0.076	-0.001	0.004	0.269	-0.046	-0.03	-0.049	-0.176	-0.094	0.089	-0.018
14880BPCK	0.072	0.008	-0.008	-0.067	0.055	0.043	-0.176	-0.041	-0.079	0.006	-0.029
14986BPJL	-0.216	-0.099	-0.044	0.028	-0.237	0.083	-0.111	0.067	0.062	0.151	0.032
15012BPKR	0.046	-0.041	0.016	0.111	-0.054	-0.029	-0.022	-0.133	0.006	-0.08	-0.03
15906BRLG	-0.019	0.079	0.046	-0.127	0.114	0.077	0	0.051	-0.082	0.022	0.069
15944BRNB	0.061	-0.157	0.063	-0.016	0.066	-0.025	0.083	0.036	-0.13	0.01	0.02
16217BSDB	-0.026	0.007	0.085	0.079	0.078	0.028	-0.014	-0.065	-0.092	-0.068	0.009
16911BTSC	0.086	-0.011	0.118	-0.114	0.205	0.042	0.098	0.118	-0.011	0.073	0.007
17847BWVR	0.013	-0.034	0.01	-0.091	0.176	-0.043	0.215	-0.052	-0.135	-0.011	0
18080BXJT	0.034	0.095	0.008	-0.174	0.081	-0.014	0.061	-0.11	-0.091	0.111	0.022
18706BYTP	-0.154	0.154	0.113	0.234	0.07	-0.038	0.071	-0.122	-0.054	0.235	-0.052
18725BYVM	0.121	-0.004	-0.004	-0.063	-0.244	0.002	-0.205	-0.119	0.053	-0.351	-0.017
19494CBPC	0.19	-0.072	0.088	-0.007	0.267	0.082	0.171	0.059	0.147	0.043	0.156
19567CBSP	0.035	-0.031	0.12	-0.238	-0.04	-0.019	0.149	-0.005	-0.031	0.138	0.041
19796CCGM	-0.05	0.025	-0.005	0.007	-0.002	0.017	0.01	0.014	0.011	0.065	0.018
19831CCJD	0.042	-0.108	-0.144	-0.032	-0.33	0.009	-0.24	-0.061	-0.037	-0.226	-0.03
19833CCJG	0.063	0.127	0.006	0.285	-0.054	-0.003	-0.209	-0.224	-0.048	-0.013	-0.096
30003DFKN	0.031	-0.029	0.004	0	-0.024	-0.012	-0.002	-0.001	0.009	-0.086	-0.002
30182DFVB	-0.096	-0.012	-0.062	-0.011	-0.206	0.027	-0.001	-0.073	0.096	0.009	0.065
30264DFYY	-0.036	0.029	-0.085	0.04	0.248	-0.076	0.024	-0.011	-0.017	0.121	-0.064

Table H.3 – continued 2

31026DHSG	-0.317	0.127	-0.055	0.169	-0.104	0.009	0.103	0.024	0.087	0.344	0.045
31027DHSH	0.125	0.003	0.153	-0.06	0.233	0.041	0.036	0.205	0.057	0.134	-0.056
31049DHTJ	-0.107	-0.011	0.148	-0.099	0.303	-0.101	0.295	-0.05	0.002	0.103	-0.028
31487DJTF	0.028	-0.025	-0.006	-0.051	0.045	0.011	-0.023	0.024	-0.018	0.006	-0.013
31612DKBD	0.069	-0.021	-0.018	0.015	-0.104	-0.016	-0.198	-0.086	-0.111	-0.026	-0.088
32017DKYL	-0.008	0.062	0.098	-0.059	0.214	-0.059	0.072	-0.043	-0.028	0.067	-0.034
32331DLRK	-0.07	-0.089	-0.013	-0.146	0.108	0.064	0.174	0.123	-0.017	0.282	0.065
32769DMRG	-0.016	-0.147	0.054	-0.015	-0.094	-0.036	0.112	0.08	0.018	-0.088	0.088
32869DMWZ	-0.125	-0.087	-0.149	0.317	-0.18	-0.008	-0.08	-0.053	0.111	-0.102	0.027
33003DNFK	0.06	-0.063	-0.003	-0.118	0.037	-0.003	0	-0.059	0.037	-0.108	-0.018
33696DPTK	0.033	0.09	0.042	0.055	-0.108	-0.012	-0.138	0.05	0.029	-0.17	0.114

Table H.3 – continued 3

	IPENTA	HEP2ME	HEXA2M	PENA2M	M_ETOL	HEP3ME	HEXA3M	PENA3M	P_ETOL	ACETYL	BENZE
10250BBPX	-0.061	0.062	0.192	-0.179	0.038	0.123	0.083	-0.211	0.072	0.283	-0.043
11377BFDP	0.088	-0.094	0.032	-0.005	0.045	-0.092	-0.035	0.157	0.046	-0.155	0.24
11428BFGZ	-0.318	0.003	0.047	-0.08	0.139	0.013	-0.026	0.152	0.064	-0.252	0.19
11546BFNQ	-0.362	0.098	0.026	0.357	-0.331	0.197	-0.074	0.551	-0.17	-0.077	0.117
11683BFWD	0.151	0.032	-0.092	-0.333	0.051	-0.035	-0.139	-0.536	0.021	0.098	-0.012
11688BFWK	0.051	-0.006	0.099	0.071	-0.083	0.056	0.072	-0.167	0.005	0.033	0.157
12135BGWR	0.712	-0.028	-0.203	-0.069	-0.063	-0.234	-0.239	-0.086	-0.129	-0.181	-0.484
12380BHLJ	0.152	-0.18	-0.012	0.069	0.053	-0.12	-0.171	0.089	0.03	-0.008	0.188
12439BHPD	0.036	-0.045	0.325	-0.32	-0.005	-0.237	0.018	0.133	-0.126	0.212	-0.085
12533BHTQ	-0.012	0.216	0.322	0.054	-0.38	0.178	0.399	-0.005	-0.048	0.074	0.144
12746BJGT	-0.296	-0.131	-0.062	0.286	-0.099	-0.109	0.175	0.036	0.012	0.109	-0.333
12889BJPP	0.071	-0.151	-0.101	0.096	0.01	-0.061	-0.231	0.138	-0.026	-0.037	-0.286
13601BLFM	-0.041	0.159	0.075	0.068	-0.017	0.43	-0.038	0.35	-0.079	-0.306	0.161
13838BLST	-0.163	-0.1	0.109	0.083	0.188	-0.136	0.4	0.06	0.221	-0.374	0.204
14015BMDF	-0.025	0.025	-0.377	0.477	-0.173	-0.077	-0.188	0.089	-0.021	0.089	-0.812
14043BMFN	-0.327	-0.06	0.236	0.098	0.026	0.031	0.137	0.019	0.031	-0.008	0.578
14602BNMD	0.126	0.069	0.005	-0.096	-0.038	0.037	0.251	-0.105	-0.088	0.204	0.506
14880BPCK	0.052	0.047	-0.004	0.062	-0.033	0.069	0.118	-0.296	0.008	0.092	-0.085
14986BPJL	0.201	0.168	0.152	-0.281	0.264	0.194	0.141	-0.642	0.178	0.305	0.002
15012BPKR	-0.416	0.015	0.137	0.113	0.054	0.152	0.258	0.054	0.115	-0.147	0.152
15906BRLG	-0.073	-0.014	0.019	-0.053	0.11	-0.111	0.064	-0.302	0.147	0.871	-0.143
15944BRNB	-0.165	0.089	-0.183	0.043	0.034	0.103	-0.179	0.195	-0.011	0.088	0.056

Table H.3 – continued 4

16217BSDB	-0.201	0.024	-0.089	0.087	-0.059	0.068	0.073	0.406	0.032	-0.133	0.011
16911BTSC	0.106	-0.166	-0.232	0.085	0.167	-0.292	-0.105	-0.042	0.128	0.045	-0.077
17847BWVR	0.141	-0.023	-0.318	0.186	0.032	0.099	-0.269	0.178	-0.03	-0.03	0.199
18080BXJT	0.26	0.03	0.019	-0.167	0.006	0.016	-0.136	-0.049	0.031	-0.12	0.463
18706BYTP	0.226	0.046	-0.096	-0.192	-0.016	0.02	-0.266	-0.145	0.03	-0.195	-0.316
18725BYVM	0.07	-0.036	0.334	0.167	0.044	-0.034	0.586	0.045	0.12	-0.113	0.263
19494CBPC	0.327	-0.186	-0.053	-0.214	0.205	-0.377	-0.009	0.042	0.273	-0.238	-0.191
19567CBSP	0.042	-0.093	0.097	-0.083	0.155	-0.194	-0.223	0.084	0.026	-0.056	0.535
19796CCGM	0.072	0.02	0.03	-0.105	0.036	-0.012	0.01	-0.215	0.026	0.078	-0.018
19831CCJD	0.149	0.353	0.068	0.049	-0.079	0.407	0.121	0.209	-0.097	0.042	-0.066
19833CCJG	-0.439	0.2	0.213	-0.112	-0.153	0.312	0.292	-0.224	-0.126	0.15	0.029
30003DFKN	-0.076	-0.024	0.009	0.274	-0.006	0.004	0.014	0.747	-0.011	-0.066	0.036
30182DFVB	0.083	0.134	0.069	-0.194	-0.105	0.179	-0.004	0.136	-0.078	-0.325	0.011
30264DFYY	-0.061	0.039	-0.317	0.226	-0.083	-0.105	-0.09	-0.003	-0.013	0.097	-0.271
31026DHSG	0.213	0.216	0.024	-0.411	-0.01	0.006	-0.127	-0.412	-0.039	0.18	-0.142
31027DHSH	0.287	-0.16	-0.173	0.078	-0.009	-0.185	-0.173	-0.371	-0.085	0.343	-0.314
31049DHTJ	-0.345	-0.186	-0.23	0.172	0.066	-0.178	-0.32	0.272	-0.025	0.111	0.162
31487DJTF	-0.015	-0.041	-0.012	0.066	0.023	-0.045	0.04	-0.108	0.026	0.073	-0.053
31612DKBD	0.156	0.201	-0.222	0.156	-0.114	0.258	-0.128	0.109	-0.054	-0.184	-0.115
32017DKYL	-0.331	-0.007	-0.055	0.069	-0.042	-0.06	-0.112	-0.021	-0.084	0.069	-0.194
32331DLRK	0.811	-0.125	0.004	-0.407	0.124	-0.17	-0.16	-0.595	-0.016	0.087	0.015
32769DMRG	-0.461	-0.143	0.194	-0.016	0.203	0.017	0.099	0.12	0.105	-0.06	0.029
32869DMWZ	-0.069	0.138	0.172	-0.118	-0.05	0.066	0.339	-0.036	-0.046	0.03	-0.188
33003DNFK	0.159	-0.067	-0.086	-0.109	-0.005	0.02	0.094	0.093	-0.058	-0.138	-0.096
33696DPTK	-0.024	-0.147	0.128	0.146	-0.011	0.037	-0.024	0.429	-0.183	-0.254	0.352

Table H.3 – continued 5

	N_BUTA	C2BUTE	C2PENE	CYHEXA	CPENTA	N_DEC	ETHANE	ETBZ	ETHENE	N_HEPT	N_HEX
10250BBPX	0.042	0.079	0.071	0.128	-0.046	-0.055	-0.083	0.054	-0.385	0.052	0.077
11377BFDP	0.097	0.01	-0.082	-0.013	0.146	-0.073	0.192	0.211	-0.065	-0.081	-0.014
11428BFGZ	0.084	0.032	-0.006	0.082	0.003	-0.069	0.327	0.109	-0.041	-0.103	0.003
11546BFNQ	-0.152	0.203	-0.042	-0.266	-0.114	0.167	-0.386	0.055	0.386	0.102	-0.213
11683BFWD	0.068	0.027	-0.004	-0.109	0.031	0.036	0.083	-0.014	-0.12	-0.108	0.138
11688BFWK	0.15	0.011	-0.09	-0.073	0.004	-0.079	-0.111	0.041	-0.075	0.076	0.073
12135BGWR	-0.228	0.367	0.199	0.039	-0.093	-0.161	0.275	0.108	0.552	-0.179	0.056
12380BHLJ	0.184	-0.084	-0.045	0.086	-0.013	0.025	0.244	-0.165	-0.256	-0.146	-0.02
12439BHPD	-0.066	0.188	0.313	0.169	-0.265	-0.18	-0.034	0.067	-0.227	-0.064	0.099
12533BHTQ	0.117	0.095	0.163	0.075	-0.147	-0.32	0.023	-0.212	-0.158	0.317	0.147
12746BJGT	-0.114	0.105	0.292	0.022	-0.073	0.07	-0.281	-0.142	0.257	0.138	-0.011
12889BJPP	-0.339	-0.08	0.13	0.147	0.033	-0.211	-0.254	-0.019	0.44	-0.082	-0.074
13601BLFM	0.044	-0.124	-0.24	0.079	0.22	-0.054	0.068	0.031	0.28	-0.014	-0.096
13838BLST	0.154	-0.157	-0.403	-0.273	0.313	0.657	-0.045	-0.121	0.295	0.212	0.064
14015BMDF	-0.369	-0.169	0.08	-0.183	-0.094	0.179	-0.288	0.212	1.385	-0.019	-0.282
14043BMFN	-0.443	-0.106	-0.179	-0.243	0.081	0.226	-0.529	-0.168	0.173	0.04	-0.015
14602BNMD	0.642	-0.021	-0.358	-0.312	0.058	0.177	-0.456	-0.057	-0.189	0.127	-0.018
14880BPCK	0.077	-0.042	0.044	0.011	-0.021	-0.037	0.118	-0.003	-0.133	0.062	0.055
14986BPJL	0.61	-0.007	0.011	0.282	0.144	-0.144	0.709	0.022	-0.873	0.025	0.214
15012BPKR	0.204	-0.069	-0.072	0.081	0.18	-0.007	0.052	-0.083	-0.259	0.133	0.054
15906BRLG	0.152	0.106	0.557	0.372	-0.165	-0.351	0.359	0.118	-0.907	-0.015	0.066
15944BRNB	0.134	-0.148	-0.256	0.087	0.076	0.055	0.073	0.09	-0.296	-0.12	-0.157

Table H.3 – continued 6

16217BSDB	0.117	-0.152	-0.083	0.211	0.141	-0.067	0.501	-0.005	-0.196	0.029	-0.073
16911BTSC	-0.125	-0.024	-0.007	0.034	0.128	0.032	0.456	0.178	-0.187	-0.042	-0.076
17847BWVR	-0.063	-0.158	-0.132	0.157	0.009	-0.11	0.072	-0.048	0.028	-0.1	-0.185
18080BXJT	0.062	-0.067	-0.156	-0.128	0.058	-0.015	0.239	-0.066	-0.101	-0.093	0.016
18706BYTP	-0.035	-0.072	-0.029	-0.014	0.14	0.1	0.967	-0.005	-0.073	-0.104	0.022
18725BYVM	0.095	-0.057	0.023	0.17	-0.008	-0.133	0.431	0.049	-0.315	0.293	0.134
19494CBPC	-0.217	0.132	0.242	-0.036	0.224	0.182	0.509	0.195	0.154	-0.032	0.092
19567CBSP	-0.392	-0.126	-0.185	-0.159	-0.247	0.087	-0.149	-0.157	0.009	-0.201	-0.055
19796CCGM	0.089	0.046	0.066	0.013	0.003	-0.036	0.072	-0.073	-0.143	-0.024	0.469
19831CCJD	0.166	-0.018	0.117	0.227	-0.229	-0.106	0.205	-0.004	-0.059	0.11	-0.054
19833CCJG	0.275	0.079	0.077	0.059	0.085	-0.058	-0.106	-0.148	-0.374	0.194	0.162
30003DFKN	-0.06	-0.024	-0.041	0.004	-0.01	0.011	-0.049	0.017	0.082	0.024	-0.345
30182DFVB	0.048	0.108	-0.023	-0.026	-0.013	0.022	0.055	0.148	0.366	-0.011	0.029
30264DFYY	-0.111	0.059	-0.023	-0.121	0.029	0.029	-0.429	0.013	0.318	-0.058	-0.107
31026DHSG	0.223	0.191	0.129	-0.051	-0.022	-0.029	0.067	0.028	-0.201	-0.195	0.139
31027DHSH	-0.288	0.133	0.183	-0.092	-0.021	-0.019	-0.475	-0.186	0.515	-0.038	0.036
31049DHTJ	0.013	-0.071	-0.208	-0.098	-0.034	0.279	-0.503	-0.074	0.046	-0.158	-0.193
31487DJTF	-0.005	-0.029	0.025	0.003	-0.02	-0.005	-0.061	-0.004	-0.037	0.017	0.016
31612DKBD	-0.046	-0.179	-0.253	-0.055	0.036	-0.01	0.554	0.145	0.186	-0.024	-0.171
32017DKYL	-0.305	0.037	0.427	-0.05	-0.464	0.009	-0.674	-0.14	0.548	-0.034	0.024
32331DLRK	0.059	0.013	0.027	-0.279	0.03	0.027	-0.485	-0.078	0.359	-0.28	0.148
32769DMRG	0.056	-0.023	0.091	0.395	0.012	-0.047	-0.009	-0.094	-0.255	0.092	0.099
32869DMWZ	0.211	0.197	-0.074	-0.092	0.137	0.178	-0.451	-0.027	0.143	0.303	0.083
33003DNFK	-0.198	-0.075	-0.029	-0.045	0.068	-0.002	-0.19	0.169	0.402	0.086	-0.012
33696DPTK	-0.243	-0.02	-0.204	0.011	-0.091	-0.136	0.264	0.161	-0.015	-0.008	-0.104

Table H.3 – continued 7

	I_BUTA	I_PREN	MP_XYL	MECYHX	MCYPNA	N_NON	N_PRBZ	N_OCT	O_XYL	N_PENT	N_PROP
10250BBPX	0.787	-0.039	-0.146	0.536	0.086	0.119	0.051	-0.02	0.001	-0.028	-0.307
11377BFDP	-0.363	-0.11	-0.013	-0.077	-0.117	-0.182	0.049	-0.115	-0.169	-0.12	0.075
11428BFGZ	-0.121	-0.092	-0.1	-0.025	-0.071	-0.038	0.1	-0.005	0.037	0.499	-0.206
11546BFNQ	0.023	-0.028	0.57	-0.025	-0.168	-0.335	-0.087	-0.212	-0.424	-0.128	0.315
11683BFWD	-0.055	-0.04	-0.019	0.148	0.917	0.011	0.008	0.149	-0.115	0.118	-0.057
11688BFWK	-0.179	-0.177	-0.046	0.075	-0.064	-0.053	-0.012	-0.037	-0.127	-0.12	0.006
12135BGWR	-0.713	-0.162	-0.135	0.196	-0.094	0.24	0.027	0.232	0.016	0.101	0.026
12380BHLJ	-0.542	0.182	0.066	-0.275	-0.106	-0.25	-0.036	-0.24	0.223	-0.173	0.285
12439BHPD	-0.171	0.181	-0.18	0.335	-0.126	0.618	0.067	0.059	0.036	0.24	-0.113
12533BHTQ	0.131	-0.054	-0.074	0.083	-0.249	0.116	-0.081	0.25	0.134	-0.204	-0.137
12746BJGT	0.187	0.093	0.196	-0.191	-0.222	-0.298	-0.073	-0.109	-0.048	-0.269	0.536
12889BJPP	-0.047	0.241	-0.012	-0.135	-0.056	0.397	-0.069	-0.079	0.203	-0.122	0.167
13601BLFM	0.07	0.038	0.028	-0.034	-0.097	0.11	-0.025	0.089	0.122	0.006	-0.317
13838BLST	-0.148	0.08	-0.113	-0.286	-0.175	-0.292	0.065	-0.595	0.182	-0.028	0.003
14015BMDF	0.426	-0.08	0.62	0.308	0.185	0.256	-0.13	0.124	-0.351	-0.278	0.184
14043BMFN	1.284	0.473	0.055	-0.409	-0.011	-0.22	-0.041	-0.101	0.1	0.048	-0.015
14602BNMD	-0.047	0.079	0.17	0.281	0.225	0.033	-0.055	0.172	-0.208	-0.2	-0.03
14880BPCK	0.255	-0.102	-0.005	0.075	0.121	0.021	-0.006	0.175	-0.062	-0.097	-0.088
14986BPJL	0.496	-0.184	-0.259	0.364	0.232	0.07	0.069	0.339	0.046	-0.012	-0.4
15012BPKR	0.059	-0.039	-0.157	-0.34	-0.188	-0.148	0.005	-0.05	0.176	-0.04	0.001
15906BRLG	0.494	-0.071	0.035	0.324	0.071	-0.278	0.084	-0.006	-0.26	-0.326	0.086
15944BRNB	0.276	0.091	0.056	-0.186	0.105	-0.057	0.001	-0.009	0.189	-0.053	-0.063
16217BSDB	-0.21	0.115	0.046	-0.401	-0.223	-0.069	0.044	-0.144	0.099	0.049	-0.065

Table H.3 – continued 8

16911BTSC	0.134	-0.05	0.033	-0.328	0.098	0.032	0.056	-0.237	-0.052	-0.165	0.138
17847BWVR	-0.122	-0.185	0.105	-0.287	0.087	-0.13	0.068	-0.134	0.283	-0.161	0.166
18080BXJT	-0.399	-0.141	0.031	-0.185	0.161	-0.034	-0.015	0.072	-0.063	0.162	-0.096
18706BYTP	-0.258	0.01	0.031	0.048	0.226	0.008	-0.007	0.162	-0.136	0.57	-0.301
18725BYVM	0.035	-0.064	-0.172	-0.345	-0.37	-0.182	0.002	-0.028	0.158	-0.3	-0.052
19494CBPC	-0.637	-0.017	-0.149	-0.357	-0.09	-0.388	0.207	-0.305	-0.162	-0.021	0.288
19567CBSP	0.092	0.199	0.102	-0.249	0.086	0.072	-0.01	-0.215	0.076	0.521	-0.036
19796CCGM	-0.019	-0.035	-0.296	0.118	0.123	-0.005	0.016	0.086	-0.077	0.061	-0.058
19831CCJD	0.168	0.077	0.063	0.493	-0.076	0.078	-0.007	0.355	0.115	-0.204	-0.222
19833CCJG	0.458	-0.123	-0.056	0.039	0.01	0.06	0.016	0.202	-0.077	0.275	-0.264
30003DFKN	0.007	0.039	0.018	-0.089	-0.406	0	-0.005	-0.077	0.056	-0.049	0.042
30182DFVB	-0.282	0.018	-0.203	0.321	-0.01	0.128	0.077	0.115	0.102	0.285	-0.205
30264DFYY	0.07	0.035	0.222	0.056	0.071	-0.052	-0.082	-0.038	-0.198	-0.177	0.314
31026DHSG	-0.223	-0.058	-0.075	0.906	0.303	0.171	0.014	0.559	-0.243	0.24	-0.262
31027DHSH	0.121	-0.034	0.109	0.119	0.126	0.122	-0.042	-0.055	-0.055	-0.28	0.311
31049DHTJ	-0.066	0.075	0.273	-0.289	0.046	0.06	-0.043	-0.447	0.125	0.063	0.404
31487DJTF	0.167	-0.024	-0.014	-0.002	0.003	0.011	-0.015	-0.019	0.009	-0.097	0.046
31612DKBD	0.115	-0.079	0.094	-0.118	0.189	0.138	-0.118	0.721	-0.045	-0.017	-0.233
32017DKYL	-0.279	-0.077	0.097	-0.038	-0.067	-0.028	-0.068	-0.11	-0.071	0.497	0.515
32331DLRK	-0.471	0.087	-0.184	0.407	0.397	0.209	-0.015	0.41	-0.045	0.166	0.036
32769DMRG	0.126	0.119	-0.188	-0.358	-0.327	-0.089	0.075	-0.413	0.332	0.244	0.053
32869DMWZ	0.203	-0.1	-0.105	0.397	-0.055	-0.032	0.007	0.001	0.016	-0.209	-0.099
33003DNFK	-0.013	-0.013	-0.215	-0.093	0.036	0.18	-0.016	0.017	0.133	-0.025	-0.006
33696DPTK	-0.11	0.012	0.022	-0.15	-0.2	-0.072	0.062	-0.119	0.1	0.107	-0.109

Table H.3- continued 9

Site	PROPE	STYR	T2PENE	TOLUE	N_UNDE	OTHER
10250BBPX	-0.119	-0.202	0.106	-0.08	-0.109	-0.033
11377BFDP	-0.064	-0.3	-0.115	0.024	0.114	-0.05
11428BFGZ	0.016	-0.376	-0.008	0.001	-0.08	-0.05
11546BFNQ	0.32	-0.014	-0.1	0.051	0.34	0.129
11683BFWD	-0.058	-0.132	-0.028	-0.08	-0.2	-0.028
11688BFWK	0.152	0.322	-0.121	0.007	0.246	0.065
12135BGWR	-0.164	0.077	0.249	0.067	-0.043	0.025
12380BHLJ	-0.128	-0.096	-0.12	0.06	0.069	0.021
12439BHPD	-0.15	0.368	0.378	-0.002	-0.049	0.022
12533BHTQ	-0.179	0.003	0.372	-0.032	0.206	0.158
12746BJGT	-0.072	0.059	0.509	0.08	0.165	0.031
12889BJPP	0.05	0.251	0.148	0.07	0.386	0.07
13601BLFM	0.121	0.048	-0.417	-0.044	0.189	-0.069
13838BLST	0.375	0.166	-0.639	0.042	-0.257	-0.04
14015BMDF	-0.096	0.621	0.208	0.011	-0.076	0.024
14043BMFN	0.084	-0.153	-0.252	-0.055	0.041	0.042
14602BNMD	-0.088	-0.132	-0.495	-0.04	-0.078	-0.091
14880BPCK	-0.145	0.056	0.107	-0.044	-0.123	0.033
14986BPJL	-0.346	-0.421	0.069	-0.085	-0.601	-0.106
15012BPKR	0.228	-0.052	-0.05	0.021	0.047	-0.043
15906BRLG	-0.54	-0.347	0.873	-0.049	-0.034	-0.014
15944BRNB	0.118	0.062	-0.432	-0.032	0.01	0.024
16217BSDB	0.034	0.326	-0.118	0.024	-0.001	0.016

Table H.3- continued 10

16911BTSC	-0.326	0.087	-0.115	0	-0.307	0.02
17847BWVR	-0.18	-0.132	-0.183	0.021	0.359	0.024
18080BXJT	-0.04	0.005	-0.271	-0.005	-0.05	0.009
18706BYTP	0.135	-0.146	0.029	-0.027	-0.666	0.019
18725BYVM	-0.222	-0.096	0.064	-0.004	-0.048	-0.005
19494CBPC	0.08	-0.167	0.143	0.1	-0.357	-0.031
19567CBSP	0.176	0.095	-0.29	-0.017	0.049	-0.01
19796CCGM	-0.058	-0.076	0.095	-0.015	-0.118	-0.014
19831CCJD	-0.492	-0.448	0.213	-0.08	-0.133	-0.028
19833CCJG	0.379	0.277	0.174	-0.03	-0.047	0.092
30003DFKN	0.038	0.05	-0.058	0.012	0.082	0.002
30182DFVB	0.062	-0.064	-0.073	-0.009	-0.136	0.015
30264DFYY	0.404	0.101	-0.014	0.03	0.348	-0.002
31026DHSG	-0.154	-0.264	0.209	-0.048	-0.343	-0.106
31027DHSH	-0.143	0.114	0.134	0.015	0.267	0.11
31049DHTJ	0.15	0.207	-0.308	0.059	0.25	-0.171
31487DJTF	-0.033	0.069	0.065	0.003	0.019	-0.002
31612DKBD	-0.149	-0.035	-0.314	-0.031	-0.426	0.06
32017DKYL	0.18	0.147	0.787	0.095	0.443	-0.088
32331DLRK	-0.039	0.133	-0.014	0	0.039	-0.009
32769DMRG	0.349	-0.159	0.191	0.03	0.144	-0.084
32869DMWZ	0.356	0.112	-0.147	-0.021	-0.026	-0.067
33003DNFK	0.203	0.243	-0.003	0.015	0.079	-0.019
33696DPTK	0.048	-0.202	-0.251	0.002	0.243	0.134

Table H.4 PMF Outputs Diagnostics of winter 2006 (Best run is highlighted in yellow shade)

Run #	Q(Robust)	Q(True)	Converged	# Steps
1	84.371	84.3704	Yes	260
2	84.6984	84.6953	Yes	295
3	84.8394	84.8391	Yes	274
4	84.3757	84.3752	Yes	257
5	84.983	84.9816	Yes	289
6	84.2713	84.2708	Yes	309
7	84.1623	84.1619	Yes	376
8	85.2006	85.1996	Yes	299
9	85.4705	85.468	Yes	261
10	84.9635	84.9624	Yes	240
11	84.3745	84.3735	Yes	243
12	84.2252	84.2248	Yes	238
13	84.8246	84.8235	Yes	280
14	84.8138	84.813	Yes	282
15	85.0873	85.0862	Yes	280
16	84.4376	84.4367	Yes	289
17	85.0121	85.0112	Yes	286
18	85.0473	85.0435	Yes	271
19	85.2683	85.2667	Yes	283
20	84.7257	84.7254	Yes	317

Table H.5 Factor Profiles (conc. of species) from Base Run #18 (Convergent Run) PMF of summer 2006

	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8	Factor 9	Factor 10	Factor 11	Factor 12	Factor 13
BZ123M	0.00	0.05	0.01	0.01	0.00	0.02	0.00	0.01	0.02	0.02	0.01	0.01	0.02
BZ124M	0.01	0.26	0.02	0.02	0.00	0.09	0.01	0.06	0.06	0.10	0.08	0.03	0.11
BZ135M	0.00	0.07	0.00	0.00	0.01	0.02	0.00	0.01	0.02	0.02	0.02	0.01	0.03
DETBZ1	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
DETBZ2	0.01	0.02	0.01	0.01	0.00	0.01	0.00	0.01	0.02	0.02	0.01	0.01	0.01
LBUT1E	0.03	0.02	0.03	0.01	0.07	0.02	0.01	0.00	0.01	0.00	0.02	0.04	0.01
PENTE1	0.01	0.00	0.01	0.00	0.02	0.01	0.00	0.00	0.01	0.01	0.00	0.01	0.00
PA224M	0.01	0.00	0.02	0.02	0.06	0.00	0.00	0.01	0.01	0.01	0.03	0.05	0.01
BU22DM	0.02	0.00	0.01	0.02	0.00	0.01	0.01	0.03	0.01	0.02	0.01	0.02	0.00
PA234M	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.01	0.00	0.01	0.01	0.01
BU23DM	0.01	0.01	0.02	0.03	0.02	0.01	0.00	0.04	0.01	0.03	0.02	0.02	0.02
PEN23M	0.02	0.01	0.01	0.01	0.03	0.01	0.00	0.02	0.01	0.01	0.01	0.02	0.01
PEN24M	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
O_ETOL	0.00	0.06	0.00	0.00	0.00	0.02	0.00	0.01	0.01	0.02	0.02	0.01	0.02
IPENTA	0.61	0.19	0.02	0.00	0.55	0.25	0.31	0.85	0.48	0.26	0.01	0.47	0.13
HEP2ME	0.01	0.02	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.02	0.01	0.00
HEXA2M	0.05	0.02	0.01	0.02	0.04	0.03	0.01	0.06	0.03	0.03	0.03	0.01	0.01
PENA2M	0.03	0.03	0.06	0.12	0.09	0.07	0.02	0.20	0.06	0.17	0.12	0.11	0.16
M_ETOL	0.00	0.14	0.00	0.01	0.01	0.05	0.00	0.04	0.03	0.05	0.05	0.02	0.05
HEP3ME	0.01	0.02	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.00
HEXA3M	0.06	0.02	0.02	0.03	0.04	0.04	0.01	0.07	0.03	0.02	0.04	0.02	0.02
PENA3M	0.03	0.04	0.02	0.05	0.15	0.06	0.01	0.07	0.03	0.12	0.07	0.04	0.17
P_ETOL	0.00	0.07	0.01	0.01	0.00	0.02	0.00	0.02	0.02	0.02	0.02	0.01	0.03

Table H.5 - continued 1

ACETYL	0.04	0.05	0.14	0.06	0.02	0.02	0.03	0.05	0.01	0.03	0.00	0.03	0.03
BENZE	0.07	0.05	0.12	0.04	0.16	0.03	0.05	0.05	0.07	0.05	0.03	0.04	0.03
N_BUTA	0.25	0.10	0.11	0.00	0.47	0.09	0.21	0.30	0.23	0.24	0.00	0.27	0.01
C2BUTE	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
C2PENE	0.01	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00
CYHEXA	0.05	0.01	0.00	0.01	0.00	0.02	0.00	0.01	0.00	0.00	0.02	0.00	0.01
CPENTA	0.00	0.00	0.01	0.03	0.00	0.00	0.01	0.08	0.03	0.01	0.03	0.05	0.02
N_DEC	0.01	0.01	0.00	0.07	0.00	0.03	0.02	0.00	0.13	0.01	0.00	0.00	0.06
ETHANE	0.32	0.23	0.74	0.41	0.30	0.09	0.19	0.16	0.31	0.15	0.00	0.21	0.09
ETBZ	0.00	0.00	0.08	0.03	0.04	0.00	0.14	0.03	0.05	0.07	0.18	0.02	0.09
ETHENE	0.14	0.09	0.33	0.15	0.10	0.00	0.07	0.06	0.01	0.01	0.02	0.06	0.12
N_HEPT	0.04	0.02	0.00	0.03	0.03	0.04	0.01	0.06	0.01	0.00	0.05	0.04	0.02
N_HEX	0.00	0.04	0.05	0.07	0.20	0.07	0.00	0.00	0.00	0.12	0.11	0.05	0.30
I_BUTA	0.20	0.00	0.00	0.00	0.00	0.00	0.52	0.00	0.00	0.00	0.27	0.16	0.18
I_PREN	0.00	0.00	0.14	0.00	0.00	0.37	0.04	0.00	0.00	0.00	0.00	0.08	0.00
MP_XYL	0.01	0.02	0.22	0.06	0.13	0.05	0.39	0.12	0.16	0.20	0.51	0.04	0.26
MECYHX	0.01	0.03	0.00	0.01	0.02	0.01	0.00	0.01	0.00	0.00	0.02	0.01	0.01
MCYPNA	0.01	0.01	0.04	0.04	0.04	0.03	0.01	0.02	0.00	0.06	0.03	0.02	0.06
N_NON	0.01	0.02	0.01	0.01	0.02	0.01	0.00	0.00	0.04	0.01	0.01	0.01	0.01
N_PRBZ	0.00	0.04	0.01	0.00	0.01	0.02	0.00	0.01	0.01	0.01	0.02	0.01	0.02
N_OCT	0.01	0.03	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.02	0.01	0.00
O_XYL	0.02	0.02	0.06	0.03	0.02	0.03	0.09	0.06	0.05	0.07	0.13	0.02	0.07
N_PENT	0.31	0.10	0.00	0.01	0.41	0.14	0.20	0.77	0.35	0.09	0.04	0.33	0.06
N_PROP	0.07	0.03	0.00	1.40	0.71	0.14	1.23	0.00	0.00	0.01	0.00	0.00	0.00
PROPE	0.07	0.05	0.07	0.01	0.13	0.03	0.03	0.00	0.03	0.01	0.01	0.01	0.03

Table H.5 - continued 2

STYR	0.01	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00
T2PENE	0.01	0.00	0.00	0.01	0.00	0.02	0.00	0.01	0.01	0.04	0.00	0.00	0.00
TOLUE	0.46	0.02	0.00	0.04	1.13	0.35	0.52	0.28	0.64	0.12	1.26	0.07	0.36
N_UNDE	0.03	0.02	0.01	0.00	0.01	0.05	0.02	0.01	0.14	0.00	0.02	0.03	0.07
OTHER	0.28	0.28	0.11	0.24	0.46	0.34	0.15	0.16	0.21	0.05	0.15	0.37	0.06

Table H.6 Factor Profiles (% of species total) from Base Run #18 (Convergent Run) of summer 2006

	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8	Factor 9	Factor 10	Factor 11	Factor 12	Factor 13
BZ123M	2.2	28	3	4.9	0.5	11	0.7	5.6	9.2	13	8.5	4.5	9.4
BZ124M	1.5	31	2.2	2.8	0	11	1	7.4	6.7	11	9.1	3	13
BZ135M	1.3	33	0	0.6	2.8	11	0.7	6.4	8.3	11	9.4	3.2	12
DETBZ1	3	19	8.7	9	1.2	7.7	1.3	4.2	10	14	7.8	6.4	7.5
DETBZ2	5.2	17	9.9	9.3	2.6	6.7	1.8	4.3	11	14	7.4	6.3	4.9
LBUT1E	11	7.9	10	5	22	8.4	4	1.3	5.1	1.5	7.1	12	4.4
PENTE1	7.7	4.2	8.2	5.4	21	7	4.6	2.7	7.7	11	6.6	12	2.1
PA224M	3.9	1.2	7.3	6.3	26	0	1.6	4.5	5.6	4.1	13	20	5.8
BU22DM	11	3.2	5.4	12	2.2	5.3	4.2	23	3.5	10	5.9	15	0
PA234M	4.8	4.6	4.1	2.3	31	0.9	1.5	0	8.3	5.6	13	17	6.4
BU23DM	4	2.3	7.4	11	6.8	3.5	2	16	5.2	14	8.1	10	9.9
PEN23M	11	3.8	4.6	5.2	17	6.2	2.3	12	7.2	6.6	9.1	10	4.3
PEN24M	4	1.9	9.7	11	12	3	1.4	8	6.6	13	10	14	6.3
O_ETOL	1.4	32	1.2	2	2.1	11	0.8	7.3	7.3	10	9.4	4.2	12

Table H.6 – continued 1

IPENTA	15	4.5	0.5	0	13	6	7.6	21	12	6.4	0.3	11	3
HEP2ME	8.4	15	4.3	5.7	9.4	12	2.1	8.3	6.2	5.9	13	6.6	3.7
HEXA2M	15	5	4	5	12	9.5	3.1	16	7.4	8.1	7.3	4.1	3.3
PENA2M	2.8	2.7	5	9.8	7.3	5.2	1.4	16	4.7	14	9.5	8.6	13
M_ETOL	0.1	31	0.9	2	2.2	11	0.5	7.9	6.8	11	11	4.1	12
HEP3ME	6.8	14	2.5	5.2	11	10	0	11	8.9	11	12	5	2
HEXA3M	14	4.5	5.3	6.4	9.3	9	3.2	18	5.9	5.1	8.5	5.6	5.1
PENA3M	3.6	4.9	2.8	5.6	17	7.6	0.7	7.8	3	14	8.3	4.6	20
P_ETOL	0.7	29	2.6	2.8	1.3	9.8	1.3	9.1	6.5	9.1	11	5.4	12
ACETYL	8.5	9.9	26	11	3.3	4.4	6.3	10	2.5	6.2	0.3	6.4	4.8
BENZE	9.3	6.3	16	4.8	20	4.1	5.8	6.9	8.3	5.8	3.5	5.3	4.2
N_BUTA	11	4.5	4.6	0.2	21	3.8	9.3	13	10	10	0	12	0.6
C2BUTE	9.6	7.1	2.5	3.1	22	6.8	3.4	3.8	8.7	22	3.8	7.1	0
C2PENE	9.5	2.9	5.5	13	3.2	11	2	8.7	5.3	34	1.7	2.1	1.4
CYHEXA	41	5.2	0.3	12	0	12	0	4.1	0	1.4	14	2.6	7
CPENTA	0	0	3.8	9.8	0	1.4	4.2	30	9.7	3.4	12	17	8.7
N_DEC	1.6	3.6	0	22	0	8.9	4.9	0	38	2.4	0.8	0	18
ETHANE	10	7.2	23	13	9.3	2.8	5.9	5.1	9.8	4.6	0	6.7	2.8
ETBZ	0	0	11	3.6	6.1	0.5	19	4.8	6.3	8.9	25	2.8	12
ETHENE	12	7.7	28	13	8.7	0	6.1	5.1	1	1.1	2	5	10
N_HEPT	12	5.3	0.5	7.4	9.3	11	1.6	19	4	0	15	11	5.6
N_HEX	0	3.8	4.6	6.8	20	7.4	0	0.3	0	12	11	4.7	30
I_BUTA	15	0	0	0	0	0	39	0	0	0	20	12	14
I_PREN	0	0	22	0	0	58	6.4	0	0.2	0.4	0	13	0
MP_XYL	0.6	0.8	10	2.6	6.2	2.2	18	5.7	7.5	9.2	24	1.9	12

Table H.6 – continued 2

MECYHX	10	24	0	5.6	12	11	0.4	5.2	1.7	1	16	5.8	7.4
MCYPNA	3.2	2.6	9.7	12	10	7.5	2.3	4.7	1.2	16	8.8	6	16
N_NON	8.6	11	3.8	4.1	8.8	5.9	1.7	1.6	26	7.8	7.6	4.6	8.8
N_PRBZ	1.9	25	3.1	2.6	4.9	9.5	1.2	8	8.2	8.6	10	5.7	11
N_OCT	6.4	20	4.2	5.9	9.2	7	0.3	8.3	8.7	7.2	14	7.3	1
O_XYL	2.3	3.5	9.4	4.4	3.2	4.7	14	8.6	7.8	9.8	20	2.8	10
N_PENT	11	3.7	0	0.5	14	4.9	7.1	27	12	3.1	1.6	12	2.2
N_PROP	1.9	0.7	0	39	20	3.9	34	0	0	0.3	0	0	0
PROPE	15	12	16	2.5	27	6.2	6.3	0.4	5.9	1.4	1.1	1.2	5.3
STYR	10	7.8	15	0.5	23	10	4	0	5.5	0	10	6.3	6.9
T2PENE	12	2.8	3.5	11	4.3	14	2.3	8.5	5.7	36	0	0	0.7
TOLUE	8.9	0.3	0	0.7	22	6.6	9.8	5.4	12	2.4	24	1.4	6.9
N_UNDE	8.4	5.3	2.6	0	2	12	4.5	1.6	34	0.1	4.3	7.5	18
OTHER	9.8	9.6	3.8	8.5	16	12	5.2	5.7	7.2	1.9	5.3	13	2.1

Table H.7 Factor Contributions (avg = 1) from Base Run #18 (Convergent Run) of summer 2006

Species	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8	Factor 9	Factor 10	Factor 11	Factor 12	Factor 13
10250BBPX	2.19	1.23	1.82	1.88	1.57	-0.20	-0.07	0.59	0.56	0.81	1.56	1.66	1.57
11000BDHQ	1.61	1.05	1.82	1.45	1.25	0.62	0.83	0.54	1.33	1.15	0.95	0.10	0.49
11377BFDP	2.33	0.74	0.07	1.41	1.71	1.63	0.25	-0.20	1.80	0.34	0.50	0.17	2.53
11428BFGZ	0.78	0.90	1.47	1.14	0.47	1.03	0.29	0.28	0.77	0.17	0.57	2.04	0.62
11546BFNQ	-0.20	-0.20	-0.20	-0.20	0.50	-0.20	17.38	-0.20	-0.20	2.07	7.81	-0.20	0.50
11683BFWD	0.40	2.54	0.88	0.94	0.40	0.74	0.64	0.34	0.95	0.78	0.47	1.79	0.66
11688BFWK	-0.20	0.59	2.14	-0.15	-0.20	5.37	1.25	1.16	-0.05	3.38	0.59	0.60	-0.18
12380BHLJ	1.35	1.11	0.83	0.14	2.55	0.27	1.35	1.05	1.68	1.23	1.40	0.91	-0.20
12439BHPD	0.39	0.54	2.45	0.10	1.07	2.02	1.08	0.99	0.61	1.16	0.36	0.44	0.41
12533BHTQ	1.27	1.36	0.54	1.09	1.13	0.43	-0.20	1.52	1.09	2.30	0.47	0.09	5.24
12746BJGT	-0.16	-0.20	2.11	0.29	0.44	4.03	0.93	-0.07	-0.20	-0.07	-0.20	2.08	-0.13
12753BJHC	-0.20	1.53	-0.19	5.58	1.94	1.67	2.56	0.14	1.46	0.16	-0.20	-0.20	-0.20
12889BJPP	0.44	1.20	2.30	0.71	0.73	0.28	0.48	0.41	1.09	0.81	1.47	0.43	-0.17
13601BLFM	-0.20	-0.04	0.11	1.65	-0.20	1.32	0.31	4.20	8.69	-0.20	0.76	0.59	3.45
13838BLST	1.83	1.13	2.05	1.17	1.29	-0.05	0.29	1.13	0.53	0.26	1.19	-0.09	0.80
14015BMDF	1.21	0.69	0.71	0.37	2.13	0.30	1.39	0.79	1.82	1.50	0.18	0.77	0.17
14602BNMD	0.87	0.71	0.31	0.36	1.67	0.17	1.72	0.74	0.52	0.31	-0.18	0.40	-0.20
14880BPCK	1.36	1.35	1.40	1.07	0.65	-0.10	0.47	-0.09	0.51	0.00	0.73	1.79	-0.02
14986BPJL	3.92	1.08	-0.20	1.39	-0.20	0.33	0.99	-0.15	-0.20	-0.20	0.65	2.45	1.34
15012BPKR	3.11	0.81	-0.20	1.63	1.95	0.84	-0.20	1.09	1.66	1.05	3.25	-0.20	-0.12
15906BRLG	1.45	0.41	-0.19	1.96	1.77	0.75	0.37	2.79	-0.05	4.96	0.14	0.54	5.11
15944BRNB	0.71	0.72	1.27	1.19	1.10	1.38	0.14	-0.19	2.05	0.32	2.02	2.70	-0.20
16217BSDB	0.77	0.86	1.45	1.07	1.35	1.15	-0.12	2.19	0.27	0.27	2.34	0.65	0.49

Table H.7 – continued

16911BTSC	1.39	0.83	1.44	0.70	0.67	-0.16	0.79	0.79	0.92	0.53	0.29	0.27	0.51
17847BWVR	0.68	1.36	2.22	0.70	0.88	0.25	0.65	0.65	0.84	0.44	-0.07	0.87	0.73
18080BXJT	0.97	0.68	1.21	0.83	0.90	0.60	0.44	0.79	0.35	-0.11	0.54	1.01	0.66
18706BYTP	0.73	0.16	0.77	-0.20	0.25	1.80	2.09	0.67	1.44	-0.20	0.51	1.34	1.19
18725BYVM	0.48	0.95	1.99	0.33	0.09	2.42	0.93	0.86	0.48	2.47	0.59	0.68	-0.20
19567CBSP	0.38	0.78	1.28	0.56	0.80	1.26	0.81	0.67	0.90	0.34	0.01	1.17	0.85
19796CCGM	1.22	1.41	0.68	1.06	0.97	0.33	0.62	0.82	0.89	1.33	1.20	0.90	2.14
19831CCJD	1.60	0.00	1.65	1.04	0.90	2.34	0.75	0.90	-0.18	1.93	0.74	1.20	0.36
30003DFKN	1.18	0.45	0.08	1.78	1.03	0.25	0.30	-0.06	1.03	2.98	0.94	4.83	-0.16
30182DFVB	0.96	0.95	1.39	1.35	0.93	0.59	0.00	1.13	0.84	-0.01	1.21	1.15	0.58
30264DFYY	0.59	0.49	0.82	0.96	1.13	0.86	0.69	1.18	0.67	0.59	0.18	1.94	0.66
31026DHSG	-0.17	9.00	-0.20	1.20	0.98	1.03	-0.20	1.96	0.16	1.64	3.36	-0.07	3.62
31027DHSH	-0.04	0.32	2.15	0.50	1.09	2.32	0.90	0.85	0.12	-0.17	0.29	1.81	0.36
31049DHTJ	0.08	-0.19	-0.20	1.57	1.37	1.34	-0.10	6.96	2.52	-0.17	3.79	-0.19	1.48
31487DJTF	1.27	0.30	1.47	1.14	0.97	2.02	-0.10	-0.19	0.22	-0.20	1.46	0.97	0.00
31612DKBD	0.87	1.46	1.78	0.66	0.45	-0.01	0.50	0.20	0.66	0.53	0.48	0.57	0.24
32017DKYL	2.69	-0.12	0.23	1.31	1.28	0.31	0.87	3.57	0.15	4.18	0.57	1.12	1.50
32331DLRK	1.08	1.32	0.56	-0.03	1.41	0.68	1.63	1.08	2.73	1.59	-0.20	-0.02	0.53
32769DMRG	1.47	2.11	0.31	0.96	0.47	0.37	0.18	-0.02	0.68	0.71	1.00	1.74	1.31
32869DMWZ	0.90	0.53	1.35	0.64	1.56	0.39	0.87	0.87	0.34	0.58	-0.08	2.27	1.11
33003DNFK	0.40	0.67	1.16	0.83	0.22	1.37	0.51	0.16	2.77	-0.04	0.24	0.96	1.04
33696DPTK	1.22	1.40	0.06	0.86	1.63	0.91	-0.18	2.06	-0.11	3.44	1.05	0.86	4.50

Table H.8 PMF Outputs Diagnostics of Summer 2006

Run #	Q(Robust)	Q(True)	Converged	# Steps
1	226.578	226.578	Yes	390
2	226.637	226.636	Yes	264
3	226.54	226.54	Yes	268
4	226.621	226.621	Yes	328
5	226.542	226.542	Yes	290
6	226.577	226.576	Yes	288
7	226.573	226.573	Yes	296
8	226.72	226.72	Yes	314
9	226.552	226.551	Yes	354
10	226.58	226.579	Yes	260
11	226.537	226.537	Yes	278
12	226.637	226.636	Yes	321
13	226.62	226.619	Yes	259
14	226.533	226.533	Yes	233
15	226.641	226.641	Yes	345
16	226.663	226.662	Yes	312
17	226.576	226.575	Yes	261
18	226.533	226.533	Yes	263
19	226.543	226.543	Yes	276
20	226.568	226.567	Yes	378

Appendix H: PCA Outputs

Appendix I.1 PCA loadings, eigenvalues, and variance explained of 20 components before rotation of winter 2006

	PC1	**PC2**	**PC3**	**PC4**	**PC5**	**PC6**	**PC7**	**PC8**	**PC9**
BZ123M	0.17	-0.10	0.01	-0.13	0.02	-0.02	0.02	0.13	0.00
BZ124M	0.15	-0.11	-0.03	-0.22	0.05	-0.02	0.00	0.20	-0.03
BZ135M	0.16	-0.10	-0.01	-0.19	0.06	-0.02	0.02	0.15	-0.04
LBUT1E	0.15	-0.07	-0.04	0.06	-0.24	0.06	-0.02	0.03	-0.10
P1E2ME	0.12	-0.05	-0.17	-0.01	-0.36	0.08	-0.27	0.01	0.06
PENTE1	0.10	-0.11	-0.12	0.04	-0.37	-0.01	-0.36	0.06	0.03
PA224M	0.14	0.14	-0.16	0.03	0.17	-0.08	-0.03	-0.20	-0.09
BU22DM	0.17	0.07	-0.12	0.06	0.03	-0.04	-0.03	-0.13	-0.01
PA234M	0.14	0.18	-0.08	0.02	0.18	-0.13	-0.02	-0.10	-0.14
BU23DM	0.16	0.21	0.02	0.02	-0.04	-0.11	-0.01	0.00	-0.08
PEN23M	0.16	0.14	-0.03	0.02	0.01	-0.04	0.08	-0.14	0.06
PEN24M	0.13	0.25	-0.04	-0.08	-0.15	0.09	0.11	-0.09	0.26
O_ETOL	0.16	-0.12	0.01	-0.19	0.04	-0.04	0.03	0.15	-0.03
IPENTA	0.16	0.03	-0.02	0.17	0.09	-0.14	-0.01	-0.05	0.02
HEP2ME	0.16	-0.01	-0.14	-0.13	0.13	0.00	-0.04	-0.06	-0.02

Table I.1 – continued 1

HEXA2M	0.16	0.12	-0.05	-0.04	0.04	-0.01	0.10	-0.19	0.13
PENA2M	0.13	0.32	0.08	-0.05	-0.09	-0.11	-0.02	0.12	-0.15
M_ETOL	0.16	-0.09	-0.03	-0.18	0.03	-0.01	0.03	0.10	-0.06
HEP3ME	0.17	-0.01	-0.10	-0.09	0.11	-0.05	0.01	-0.15	-0.04
HEXA3M	0.17	0.08	-0.08	-0.07	0.02	-0.02	0.06	-0.18	0.06
PENA3M	0.08	0.36	0.20	-0.05	-0.09	-0.11	-0.02	0.23	-0.17
P_ETOL	0.16	-0.10	-0.04	-0.19	0.00	-0.01	0.03	0.09	-0.06
ACETYL	0.10	-0.14	0.10	-0.12	-0.17	-0.07	0.48	-0.04	-0.21
BENZE	0.14	0.01	-0.16	0.16	-0.06	0.25	0.14	0.00	-0.08
N_BUTA	0.14	-0.01	0.10	0.25	0.08	-0.16	0.01	0.08	0.06
C2BUTE	0.15	-0.06	0.01	0.26	-0.12	-0.13	-0.04	-0.03	-0.02
C2PENE	0.15	-0.06	-0.03	0.17	-0.20	-0.13	-0.03	-0.03	0.02
CYHEXA	0.08	0.26	-0.18	-0.15	-0.12	0.31	0.04	-0.01	0.07
CPENTA	0.16	-0.03	-0.07	0.03	-0.01	-0.06	0.02	-0.10	-0.08
N_DEC	0.13	-0.15	0.18	-0.16	-0.07	-0.15	-0.15	0.07	0.19
ETHANE	0.11	-0.11	0.26	0.11	0.08	-0.03	0.20	0.14	0.27
ETBZ	0.11	-0.10	0.29	-0.02	0.07	0.29	-0.14	-0.29	-0.05
ETHENE	0.12	-0.07	0.05	0.09	-0.02	0.16	0.42	0.17	-0.19
N_HEPT	0.17	0.02	-0.11	-0.05	0.07	-0.06	0.01	-0.16	-0.03

Table I.1 – continued 2

N_HEX	0.05	0.29	0.37	-0.08	-0.05	0.10	-0.17	0.05	-0.15
I_BUTA	0.13	0.09	0.04	0.26	0.19	-0.03	-0.01	0.12	0.14
I_PREN	0.16	-0.09	0.06	0.12	-0.06	0.12	0.13	-0.08	-0.01
MP_XYL	0.12	-0.09	0.28	-0.01	0.07	0.29	-0.14	-0.28	-0.06
MECYHX	0.12	0.04	-0.24	-0.06	0.21	0.19	-0.17	0.19	0.06
MCYPNA	0.08	0.37	0.21	-0.10	-0.18	0.04	0.00	0.13	0.04
N_NON	0.16	-0.07	0.09	-0.11	0.10	-0.04	-0.13	0.05	0.14
N_PRBZ	0.16	-0.11	0.02	-0.18	0.02	-0.06	0.02	0.06	-0.04
N_OCT	0.14	-0.03	-0.14	-0.21	0.17	-0.02	-0.15	0.06	0.06
O_XYL	0.13	-0.12	0.27	-0.03	0.03	0.27	-0.12	-0.23	-0.05
N_PENT	0.16	0.00	0.01	0.14	0.14	-0.11	-0.02	-0.09	-0.03
N_PROP	0.05	0.07	0.01	0.30	0.38	0.16	-0.12	0.27	-0.07
PROPE	0.16	-0.08	-0.03	0.09	-0.09	0.20	0.16	0.06	-0.15
STYR	0.11	-0.08	-0.09	0.20	-0.01	0.34	-0.12	0.34	-0.10
T2BUTE	0.15	-0.06	0.03	0.25	-0.12	-0.16	-0.07	-0.03	-0.01
T2PENE	0.15	-0.07	-0.02	0.16	-0.21	-0.14	-0.04	-0.03	0.01
TOLUE	0.08	0.10	-0.03	0.04	-0.05	0.19	0.21	0.04	0.65
N_UNDE	0.12	-0.13	0.30	-0.05	0.05	-0.17	-0.07	0.10	0.20
Eigenvalue	31.05	3.91	3.24	2.71	2.27	1.57	1.44	1.25	1.03
Variance Explained (%)	59.72	7.51	6.23	5.22	4.36	3.02	2.76	2.41	1.98

Table I.1 – continued 3

	PC10	PC11	PC12	PC13	PC14	PC15	PC16	PC17	PC18	PC19	PC20
BZ123M	-0.03	-0.11	-0.03	-0.14	-0.06	0.04	0.13	0.10	-0.13	0.06	-0.13
BZ124M	0.04	-0.15	-0.11	-0.10	-0.13	0.05	0.01	0.08	-0.07	0.02	0.00
BZ135M	0.04	-0.06	-0.09	-0.13	-0.14	0.01	0.11	0.01	-0.05	-0.05	0.11
LBUT1E	0.09	0.16	-0.03	-0.03	-0.23	0.15	-0.39	-0.12	0.01	-0.21	-0.29
P1E2ME	-0.02	0.21	0.14	0.02	0.05	0.00	0.10	0.28	0.01	-0.01	-0.25
PENTE1	0.05	0.22	0.30	0.13	-0.17	0.15	0.05	0.10	0.10	-0.07	0.43
PA224M	-0.06	0.27	-0.14	-0.07	0.07	0.11	0.20	0.01	-0.16	-0.23	0.16
BU22DM	0.01	-0.06	0.03	0.02	0.15	-0.08	0.12	-0.01	0.06	-0.13	0.08
PA234M	0.02	0.33	-0.16	-0.06	0.03	0.03	0.15	-0.04	-0.11	-0.24	0.18
BU23DM	0.03	-0.01	0.03	0.00	0.05	-0.06	0.06	-0.12	0.04	-0.07	-0.02
PEN23M	-0.17	0.04	0.01	0.08	-0.17	0.02	-0.03	-0.18	-0.10	0.07	0.00
PEN24M	-0.28	-0.04	-0.02	0.06	-0.20	-0.04	-0.04	-0.23	0.12	0.18	0.23
O_ETOL	0.04	-0.09	-0.06	-0.07	-0.15	-0.06	0.01	-0.01	-0.04	-0.03	0.12
IPENTA	0.06	-0.19	0.04	-0.06	0.09	0.08	0.05	-0.11	0.30	-0.18	0.00
HEP2ME	0.11	0.09	0.03	0.14	-0.04	0.00	-0.04	0.02	-0.01	0.14	-0.21
HEXA2M	-0.19	0.02	0.08	0.01	-0.17	0.05	-0.02	0.01	-0.04	0.22	0.01
PENA2M	0.09	-0.01	0.08	-0.03	0.07	-0.04	0.04	-0.01	-0.01	-0.01	-0.13
M_ETOL	0.06	-0.05	-0.06	-0.09	-0.12	-0.07	0.06	-0.02	-0.03	-0.03	0.11
HEP3ME	0.09	0.12	0.10	0.06	-0.03	-0.02	0.02	0.01	-0.04	0.13	-0.24
HEXA3M	-0.13	-0.01	0.14	0.00	-0.10	0.08	-0.01	0.07	-0.07	0.18	-0.03
PENA3M	0.15	0.04	0.04	-0.03	0.03	-0.03	0.00	0.00	-0.04	0.00	-0.15
P_ETOL	0.06	-0.10	-0.01	-0.08	-0.07	-0.07	0.06	0.01	-0.03	-0.04	0.06
ACETYL	0.11	-0.04	0.26	0.34	0.23	-0.02	-0.11	0.18	-0.03	0.02	0.34

Table I.1 – continued 4

BENZE	0.11	0.15	-0.06	-0.31	0.11	-0.38	-0.21	-0.03	0.03	0.11	0.02
N_BUTA	0.09	-0.08	-0.06	-0.18	-0.15	0.26	-0.05	0.19	0.27	0.12	0.06
C2BUTE	0.00	-0.16	-0.25	0.05	-0.09	0.12	-0.17	-0.13	-0.07	-0.05	0.03
C2PENE	-0.08	-0.12	-0.22	0.17	0.11	-0.28	0.18	0.05	-0.15	0.00	-0.05
CYHEXA	-0.33	-0.29	-0.15	-0.16	0.14	0.06	-0.06	0.43	0.16	-0.28	-0.03
CPENTA	0.05	-0.26	0.35	-0.05	0.02	-0.09	-0.01	-0.16	0.21	-0.07	-0.10
N_DEC	-0.24	0.09	0.08	-0.24	0.36	0.01	-0.21	-0.12	0.03	-0.20	0.06
ETHANE	-0.08	0.29	0.00	0.17	-0.34	-0.24	0.27	0.15	0.33	-0.25	-0.19
ETBZ	0.04	-0.07	-0.06	0.06	-0.01	0.06	0.05	0.03	0.00	-0.05	0.03
ETHENE	-0.22	0.15	-0.12	0.22	0.17	0.39	0.05	0.02	0.08	-0.07	-0.12
N_HEPT	0.01	0.02	0.21	-0.01	0.03	0.13	-0.01	0.17	-0.19	0.09	-0.16
N_HEX	0.17	0.04	-0.05	0.07	0.05	0.01	0.00	0.06	-0.04	-0.04	0.06
I_BUTA	0.18	0.09	-0.02	-0.13	0.09	0.10	-0.05	0.42	0.02	0.35	0.18
I_PREN	0.07	0.19	-0.07	-0.24	0.10	-0.31	-0.11	0.00	0.15	0.13	0.10
MP_XYL	0.04	-0.06	-0.06	0.04	0.00	0.08	0.04	0.05	-0.03	-0.02	0.01
MECYHX	0.14	-0.01	-0.22	0.37	-0.03	-0.05	-0.31	-0.02	0.04	-0.03	0.15
MCYPNA	-0.03	-0.03	0.01	0.07	-0.09	-0.05	-0.04	-0.08	0.06	0.16	0.04
N_NON	-0.16	0.19	-0.09	0.11	0.29	-0.01	-0.02	-0.21	0.11	0.14	0.04
N_PRBZ	0.03	-0.05	-0.01	-0.05	-0.12	-0.07	0.05	-0.02	-0.06	-0.08	0.12
N_OCT	0.11	0.02	-0.07	0.28	0.24	0.00	-0.10	-0.02	0.32	0.09	-0.16
O_XYL	0.06	-0.07	0.02	0.03	-0.07	-0.08	0.03	-0.01	0.01	0.02	-0.03
N_PENT	0.05	-0.20	0.22	-0.06	0.07	0.04	0.00	-0.07	0.16	-0.11	-0.01
N_PROP	-0.28	-0.08	0.37	0.17	-0.10	-0.25	-0.20	0.09	-0.27	-0.21	0.04

Table I.1 – continued 5

PROPE	0.00	0.17	0.06	-0.13	-0.04	0.07	-0.11	-0.16	-0.14	-0.03	-0.05
STYR	-0.10	-0.08	0.09	-0.05	0.14	0.16	0.45	-0.30	0.00	0.26	0.01
T2BUTE	0.00	-0.17	-0.21	0.11	-0.06	0.15	-0.16	-0.01	-0.12	0.02	0.01
T2PENE	-0.06	-0.15	-0.18	0.20	0.13	-0.29	0.16	0.12	-0.17	0.06	-0.09
TOLUE	0.46	-0.07	0.09	0.02	0.14	0.12	0.09	-0.12	-0.30	-0.24	-0.03
N_UNDE	-0.24	0.08	0.07	-0.09	0.14	0.07	-0.17	0.05	-0.26	0.08	-0.08
Eigenvalue	0.67	0.53	0.45	0.35	0.28	0.22	0.19	0.16	0.13	0.10	0.09
Variance Explained (%)	1.29	1.02	0.86	0.67	0.55	0.43	0.36	0.31	0.25	0.20	0.17

Appendix I.2 PCA score of winter 2006

Site	**PC1**	**PC2**	**PC3**	**PC4**	**PC5**	**PC6**	**PC7**	**PC8**	**PC9**
10250BBPX	0.04	0.79	-1.00	1.16	0.56	-0.14	-0.60	-0.51	0.05
11377BFDP	-7.46	0.24	0.56	-1.16	0.44	-1.03	0.79	-0.94	-0.02
11428BFGZ	-7.13	0.21	0.19	-0.81	0.10	-1.06	0.68	-1.23	-0.05
11546BFNQ	-2.52	1.36	-1.17	0.61	0.10	0.81	0.04	-0.92	-0.76
11683BFWD	3.84	5.32	0.84	-3.14	-3.84	1.76	1.77	-0.48	3.40
11688BFWK	-4.31	-0.30	-1.45	0.61	-1.29	1.27	-1.41	0.93	-0.45
12135BGWR	7.77	-0.20	-1.41	3.49	-2.71	-0.19	-1.25	-0.48	-0.64
12380BHLJ	1.83	-0.45	-0.45	0.56	-0.70	0.31	0.37	-0.06	-0.27
12439BHPD	-5.41	-0.04	0.08	-0.68	-0.77	-0.64	0.40	-1.12	0.09
12533BHTQ	3.53	-1.87	1.62	0.19	0.77	-1.99	-0.38	0.90	1.31
12746BJGT	-1.94	-0.38	0.35	1.13	0.15	-0.13	0.80	0.41	0.00
12889BJPP	9.05	-0.85	-0.98	1.14	-1.16	1.64	-0.17	1.05	0.23
13601BLFM	6.15	-1.07	1.68	0.94	1.54	-1.36	0.02	0.08	1.28
13838BLST	2.94	-2.04	-0.16	-2.21	-1.95	-0.35	-1.33	0.65	0.29
14015BMDF	4.03	-1.77	0.97	1.48	0.15	1.92	2.19	2.00	-1.18
14043BMFN	0.80	-0.15	-0.53	1.57	0.04	1.12	1.21	0.07	-0.61
14602BNMD	-0.06	-0.23	-0.26	2.03	-0.54	-0.17	0.62	-0.69	-0.78
14880BPCK	19.41	4.19	-4.23	-1.68	4.01	-1.20	-1.18	-2.71	-0.27
14986BPJL	-6.04	0.11	0.49	0.88	0.07	-2.24	0.51	-1.05	0.13
15012BPKR	12.80	-3.64	-0.51	-3.71	-2.69	0.11	2.19	-1.19	-1.91
15906BRLG	3.21	-1.79	-0.10	-0.59	-3.18	-2.44	-1.20	-0.55	0.32
15944BRNB	1.75	-1.46	1.45	0.55	0.94	-0.65	0.70	0.48	0.45
16217BSDB	-5.21	1.17	-1.27	0.35	-0.09	1.06	-0.84	-0.17	-0.35
16911BTSC	-3.64	0.48	-0.45	0.24	2.06	0.50	-0.86	0.40	-0.25

Appendix I.2 – continued

17847BWVR	-3.79	0.93	-0.83	0.38	0.18	1.24	0.76	-0.03	-0.67
18080BXJT	-4.59	0.25	-0.44	0.03	0.14	0.24	0.67	-0.47	-0.48
18706BYTP	-3.84	0.14	0.05	1.50	-0.10	-0.69	0.30	-0.65	-0.11
18725BYVM	-8.57	1.38	-0.58	-0.53	1.20	0.39	0.43	-0.76	-0.27
19494CBPC	0.47	-0.90	0.84	1.36	0.26	-1.44	-0.21	0.32	0.64
19567CBSP	2.65	-0.36	-0.54	0.44	0.28	1.03	1.20	0.06	-0.73
19796CCGM	2.52	-1.70	7.77	-0.67	1.45	3.87	-2.75	-3.00	-0.14
19831CCJD	-1.80	0.03	-1.01	-0.01	0.33	0.81	-0.35	0.07	0.38
19833CCJG	-5.97	-0.59	-1.22	0.41	-2.70	-0.23	-2.99	0.27	0.04
30003DFKN	4.12	8.63	5.09	-0.40	-1.11	-1.74	-0.58	2.78	-2.30
30182DFVB	-2.97	-0.45	0.24	-0.70	-0.32	-0.84	1.97	-1.24	-0.42
30264DFYY	-1.64	0.34	0.13	0.71	1.38	-0.30	1.08	-0.19	-0.38
31026DHSG	-1.36	-1.09	-2.83	-4.94	2.34	1.09	-1.52	3.04	-0.46
31027DHSH	-5.73	-1.05	0.86	-2.23	0.43	-0.88	1.84	0.29	-0.39
31049DHTJ	0.44	-1.11	1.30	-0.28	1.72	-0.74	-0.11	0.66	0.57
31487DJTF	0.54	1.32	-1.22	2.15	0.94	1.44	1.17	0.77	3.74
31612DKBD	-8.47	-0.66	-0.31	-3.15	-0.62	-1.00	-1.91	-0.21	0.78
32017DKYL	3.42	-1.18	0.60	2.02	-0.23	-1.14	-0.47	0.73	0.21
32331DLRK	-1.20	0.36	-0.37	1.73	1.61	-0.68	-0.64	0.18	-0.16
32769DMRG	-5.66	1.18	-1.32	-0.62	0.42	1.42	-0.06	0.28	-0.32
32869DMWZ	1.27	0.11	-1.62	1.65	-1.43	0.72	-1.47	-0.03	0.08
33003DNFK	0.53	-0.54	-0.54	-0.54	0.09	1.08	0.44	0.54	-0.63
33696DPTK	6.19	-2.68	1.68	-1.26	1.74	-0.57	0.13	1.72	1.00

Appendix I.3 PCA T-Squared of winter 2006

Site	T-Squared
10250BBPX	45.02128
11377BFDP	45.02128
11428BFGZ	45.02128
11546BFNQ	45.02128
11683BFWD	45.02128
11688BFWK	45.02128
12135BGWR	45.02128
12380BHLJ	45.02128
12439BHPD	45.02128
12533BHTQ	45.02128
12746BJGT	45.02128
12889BJPP	45.02128
13601BLFM	45.02128
13838BLST	45.02128
14015BMDF	45.02128
14043BMFN	45.02128
14602BNMD	45.02128
14880BPCK	45.02128
14986BPJL	45.02128
15012BPKR	45.02128
15906BRLG	45.02128
15944BRNB	45.02128
16217BSDB	45.02128
16911BTSC	45.02128
17847BWVR	45.02128
18080BXJT	45.02128
18706BYTP	45.02128
18725BYVM	45.02128
19494CBPC	45.02128
19567CBSP	45.02128
19796CCGM	45.02128
19831CCJD	45.02128
19833CCJG	45.02128
30003DFKN	45.02128
30182DFVB	45.02128
30264DFYY	45.02128

Table I.3 – continued

31026DHSG	45.02128
31027DHSH	45.02128
31049DHTJ	45.02128
31487DJTF	45.02128
31612DKBD	45.02128
32017DKYL	45.02128
32331DLRK	45.02128
32769DMRG	45.02128
32869DMWZ	45.02128
33003DNFK	45.02128
33696DPTK	45.02128

Appendix I.4 PCA loadings, eigenvalues, and variance explained of 20 components before rotation of summer 2006

	PC1	**PC2**	**PC3**	**PC4**	**PC5**	**PC6**	**PC7**	**PC8**	**PC9**
BZ123M	0.00	-0.02	0.00	0.02	0.07	0.02	0.00	-0.04	0.04
BZ124M	0.03	-0.10	-0.05	0.12	0.41	0.13	-0.01	-0.26	0.25
BZ135M	0.01	-0.03	-0.01	0.03	0.11	0.04	-0.01	-0.07	0.07
P1E2ME	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	-0.02
PENTE1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	-0.02
PA224M	0.01	-0.01	0.01	0.01	0.00	0.01	-0.04	0.01	-0.05
BU22DM	0.01	-0.02	0.01	0.00	0.01	-0.01	0.01	0.01	-0.02
PA234M	0.00	0.00	0.00	0.00	0.00	0.01	-0.02	0.01	-0.01
BU23DM	0.01	-0.03	0.02	0.01	0.05	0.00	0.01	0.00	-0.03
PEN23M	0.01	-0.01	0.01	0.00	0.01	0.01	-0.01	0.00	-0.02
PEN24M	0.00	-0.01	0.01	0.00	0.01	0.00	0.00	0.01	-0.02
O_ETOL	0.01	-0.02	-0.01	0.03	0.08	0.03	-0.01	-0.05	0.05
IPENTA	0.18	-0.49	0.43	-0.14	-0.04	-0.24	-0.08	0.10	-0.16
HEP2ME	0.00	-0.01	0.00	0.01	0.02	0.01	0.01	-0.02	0.01
HEXA2M	0.01	-0.04	0.02	0.01	0.02	0.01	0.01	-0.03	-0.03
PENA2M	0.06	-0.17	0.11	0.05	0.30	0.03	0.03	-0.07	-0.12
M_ETOL	0.02	-0.06	-0.02	0.06	0.21	0.07	-0.01	-0.13	0.13
HEP3ME	0.00	-0.01	0.00	0.01	0.02	0.01	0.01	-0.02	0.01
HEXA3M	0.02	-0.05	0.02	0.01	0.02	0.01	0.01	-0.04	-0.02
PENA3M	0.04	-0.12	0.06	0.06	0.30	0.06	-0.08	-0.11	-0.17
P_ETOL	0.01	-0.03	-0.01	0.03	0.10	0.03	0.00	-0.06	0.06
ACETYL	0.01	-0.01	0.01	0.01	0.09	0.04	0.06	0.03	-0.04

Table I.4 – continued 1

BENZE	0.02	-0.04	0.01	0.01	0.02	0.07	-0.01	0.04	-0.08
N_BUTA	0.11	-0.14	0.18	-0.09	0.02	-0.09	-0.11	0.12	-0.42
C2BUTE	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	-0.02
C2PENE	0.00	-0.01	0.01	0.00	0.02	0.00	0.01	0.00	-0.03
CYHEXA	0.00	-0.01	0.00	0.01	0.01	0.01	-0.05	-0.01	-0.04
CPENTA	0.02	-0.05	0.03	0.00	0.00	-0.02	0.04	-0.01	0.07
N_DEC	0.02	-0.05	0.07	0.00	0.00	0.06	0.09	-0.03	0.28
ETHANE	0.03	-0.06	0.14	-0.04	0.12	0.53	0.26	0.73	0.05
ETBZ	0.12	0.01	-0.09	-0.04	0.12	-0.10	0.07	0.09	0.08
ETHENE	0.01	-0.01	-0.01	0.02	0.17	0.14	-0.09	0.10	-0.04
N_HEPT	0.02	-0.04	0.00	0.02	0.01	0.01	0.01	-0.06	0.01
N_HEX	0.04	-0.12	0.04	0.09	0.42	0.11	-0.16	-0.14	-0.24
I_BUTA	0.30	0.19	-0.25	-0.13	0.16	-0.50	-0.22	0.31	-0.07
I_PREN	-0.02	0.04	-0.05	-0.01	0.01	-0.13	0.83	-0.21	-0.40
MP_XYL	0.31	-0.02	-0.24	-0.08	0.34	-0.27	0.27	0.18	0.26
MECYHX	0.00	-0.01	-0.01	0.02	0.04	0.03	-0.02	-0.04	0.02
MCYPNA	0.01	-0.03	0.02	0.02	0.11	0.02	0.00	-0.01	-0.11
N_NON	0.01	-0.02	0.01	0.00	0.01	0.02	0.00	0.00	0.07
N_PRBZ	0.01	-0.02	-0.01	0.02	0.06	0.02	0.00	-0.03	0.04
N_OCT	0.01	-0.01	-0.01	0.02	0.03	0.03	-0.01	-0.03	0.03
O_XYL	0.08	-0.02	-0.05	0.00	0.11	-0.06	0.10	0.02	0.07
N_PENT	0.14	-0.40	0.32	-0.10	-0.18	-0.18	0.14	-0.10	0.42
N_PROP	0.59	0.58	0.51	0.05	-0.01	0.14	0.01	-0.17	0.02
PROPE	0.01	-0.01	-0.01	0.02	0.03	0.06	-0.07	-0.02	-0.04

Table I.4 – continued 2

STYR	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	-0.01
T2PENE	0.00	-0.01	0.02	0.00	0.03	0.00	0.02	0.00	-0.07
TOLUE	0.60	-0.32	-0.49	0.03	-0.34	0.36	-0.04	-0.15	-0.12
N_UNDE	0.01	-0.05	0.03	0.00	-0.01	0.00	0.08	-0.01	0.20
OTHERS	0.06	-0.07	0.05	0.95	-0.11	-0.21	0.03	0.20	-0.01
Eigenvalue	21.31	5.61	1.16	0.91	0.59	0.48	0.22	0.18	0.15
Variance Explained (%)	68.94	18.16	3.76	2.95	1.90	1.55	0.72	0.59	0.48

Table I.4 – continued 3

	PC10	**PC11**	**PC12**	**PC13**	**PC14**	**PC15**	**PC16**	**PC17**	**PC18**	**PC19**	**PC20**
BZ123M	0.07	0.04	-0.02	-0.01	-0.05	-0.02	0.06	0.04	0.02	-0.01	0.08
BZ124M	0.48	0.24	0.09	-0.02	-0.11	-0.03	-0.04	-0.01	-0.04	-0.16	-0.03
BZ135M	0.13	0.07	0.00	0.00	-0.04	0.01	-0.02	0.01	-0.02	0.07	-0.01
P1E2ME	-0.01	0.00	-0.01	0.00	-0.01	0.00	0.02	-0.01	0.01	0.01	-0.01
PENTE1	0.00	0.01	-0.01	-0.01	-0.02	0.01	0.00	-0.02	0.03	0.02	0.00
PA224M	-0.02	0.02	0.03	0.05	-0.02	-0.08	0.10	-0.13	0.26	0.52	-0.14
BU22DM	-0.01	0.02	0.06	-0.06	-0.03	-0.02	0.10	-0.03	0.00	0.02	-0.04
PA234M	0.00	0.01	-0.01	0.01	-0.01	-0.02	0.00	0.01	0.10	0.16	-0.04
BU23DM	-0.04	0.01	0.04	-0.02	-0.01	-0.03	0.11	0.04	-0.03	0.06	-0.08
PEN23M	-0.01	0.01	0.02	-0.01	0.01	-0.01	0.05	0.00	0.15	0.03	0.04

Table I.4 – continued 4

PEN24M	-0.01	0.01	0.01	0.01	0.01	-0.03	0.05	-0.02	0.07	0.08	-0.04
O_ETOL	0.10	0.05	0.00	-0.02	-0.03	0.00	0.00	-0.02	0.00	0.04	0.02
IPENTA	0.36	-0.11	0.05	-0.14	0.47	0.10	-0.02	-0.07	-0.07	0.05	-0.05
HEP2ME	0.03	0.02	0.03	-0.02	0.01	-0.02	-0.01	-0.01	0.11	0.01	-0.04
HEXA2M	-0.04	0.03	0.04	-0.07	0.05	0.06	0.11	0.15	0.23	-0.22	0.25
PENA2M	-0.28	-0.07	0.13	-0.15	-0.08	-0.03	0.45	0.28	-0.23	0.12	-0.24
M_ETOL	0.23	0.13	0.02	-0.04	-0.07	0.00	0.00	-0.02	0.00	0.16	0.01
HEP3ME	0.02	0.03	0.01	-0.03	0.01	-0.01	0.01	0.05	0.09	-0.02	-0.04
HEXA3M	-0.06	0.00	0.10	-0.10	0.03	0.07	0.22	0.00	0.28	-0.27	0.33
PENA3M	-0.17	-0.16	-0.11	-0.06	-0.07	0.10	-0.11	0.31	-0.14	-0.08	0.01
P_ETOL	0.10	0.05	0.02	-0.01	-0.03	0.00	0.02	-0.03	-0.01	0.10	0.00
ACETYL	-0.02	0.11	0.22	0.18	0.12	-0.08	0.16	0.06	-0.20	0.35	0.70
BENZE	0.00	0.21	-0.05	0.49	-0.03	0.79	0.19	-0.10	-0.03	-0.03	-0.10
N_BUTA	0.01	0.51	-0.36	0.24	-0.29	-0.38	0.06	-0.03	0.09	-0.11	0.02
C2BUTE	0.01	0.02	-0.01	0.00	-0.01	0.00	-0.01	0.05	0.02	-0.01	-0.02
C2PENE	0.00	0.02	0.00	0.00	0.00	0.00	0.02	0.09	-0.03	-0.08	-0.02
CYHEXA	0.01	-0.02	0.03	-0.05	0.12	0.06	0.09	0.27	0.56	0.04	-0.14
CPENTA	-0.08	-0.02	0.10	-0.05	-0.10	-0.07	0.24	-0.29	-0.04	0.12	-0.09
N_DEC	0.07	-0.30	-0.29	0.33	0.00	-0.13	0.27	0.29	0.07	0.14	-0.06
ETHANE	0.12	-0.07	0.00	-0.14	-0.17	0.04	-0.06	0.00	0.04	-0.01	0.02
ETBZ	-0.10	0.10	-0.04	0.02	0.07	-0.03	0.01	-0.15	0.07	0.19	0.02
ETHENE	-0.15	-0.01	0.59	0.49	0.25	-0.30	-0.07	-0.08	0.02	-0.23	-0.22

Table I.4 – continued 5

N_HEPT	-0.04	-0.02	0.12	-0.16	-0.06	0.07	0.30	-0.25	0.34	-0.11	0.09
N_HEX	-0.20	-0.41	-0.19	0.04	-0.11	0.06	-0.29	-0.38	0.12	0.04	0.12
I_BUTA	0.29	-0.28	0.21	0.08	-0.36	0.05	0.06	0.11	0.03	-0.01	0.03
I_PREN	0.17	-0.12	0.11	0.10	-0.08	-0.01	-0.09	0.00	0.06	0.01	-0.06
MP_XYL	-0.31	0.24	-0.22	-0.06	0.33	0.03	-0.10	-0.04	0.02	0.00	-0.05
MECYHX	0.08	0.03	0.06	-0.03	-0.01	-0.03	-0.04	-0.11	0.16	-0.01	-0.06
MCYPNA	-0.05	-0.02	0.01	0.01	0.02	-0.03	0.08	-0.02	0.08	0.00	0.13
N_NON	0.04	-0.03	-0.08	0.10	0.00	-0.02	0.03	0.11	0.12	0.05	-0.10
N_PRBZ	0.06	0.03	0.00	-0.01	-0.03	0.01	0.01	-0.02	0.02	0.05	0.02
N_OCT	0.07	0.06	0.03	-0.03	0.01	-0.05	0.02	-0.06	0.11	0.01	-0.19
O_XYL	-0.08	0.06	-0.04	-0.08	0.05	-0.02	0.08	0.05	0.05	-0.24	0.04
N_PENT	-0.27	0.01	0.22	0.11	-0.46	0.04	-0.25	0.02	0.07	-0.02	0.06
N_PROP	0.00	0.01	0.01	-0.02	0.04	0.01	-0.01	-0.02	-0.01	0.00	0.00
PROPE	0.02	0.06	0.04	0.16	0.11	0.05	-0.41	0.38	0.27	0.21	0.11
STYR	0.01	0.00	0.01	0.02	0.02	0.03	0.00	-0.05	0.01	0.01	0.04
T2PENE	-0.01	0.04	-0.01	0.00	0.01	0.00	0.03	0.23	-0.08	-0.21	-0.02
TOLUE	0.02	-0.05	0.00	-0.02	-0.01	-0.04	0.01	0.02	-0.06	0.01	0.00
N_UNDE	0.14	-0.33	-0.32	0.34	0.14	-0.20	0.17	-0.16	0.02	-0.21	0.12
OTHERS	0.00	0.02	-0.01	0.02	0.00	-0.01	-0.02	0.00	0.00	-0.01	0.00
Eigenvalue	0.09	0.06	0.04	0.03	0.03	0.01	0.01	0.01	0.00	0.00	0.00
Variance Explained (%)	0.28	0.21	0.14	0.10	0.08	0.04	0.04	0.02	0.01	0.01	0.01

Appendix I.5 PCA score of summer 2006

	PC1	**PC2**	**PC3**	**PC4**	**PC5**	**PC6**	**PC7**	**PC8**	**PC9**
10250BBPX	3.51	0.34	0.50	-2.05	-2.82	1.98	-2.16	0.82	0.67
11000BDHQ	0.58	0.07	0.76	-1.29	-0.63	2.19	1.01	1.66	-0.41
11377BFDP	1.22	-0.11	0.33	-0.08	-1.19	-0.98	2.74	-0.26	-0.08
11428BFGZ	-3.03	-0.30	0.19	-0.41	0.18	-0.81	1.60	0.82	0.78
11546BFNQ	7.89	9.84	8.11	2.23	2.10	0.19	-0.26	-0.77	0.41
11683BFWD	-1.80	-2.06	0.55	0.54	0.77	-0.58	1.16	-0.22	0.64
11688BFWK	0.65	-1.41	-0.63	-1.77	5.15	-0.82	0.81	0.56	-1.47
12380BHLJ	2.29	1.64	0.35	-0.52	-2.43	-0.01	0.89	0.31	-1.31
12439BHPD	-2.08	-0.09	0.79	-1.51	0.48	1.55	-0.24	0.81	-1.03
12533BHTQ	5.49	-1.82	-0.46	-0.34	0.09	1.19	-0.31	-1.63	1.13
12746BJGT	-7.59	-0.37	-0.20	-0.13	2.37	-0.16	-0.48	0.61	-0.62
12753BJHC	-0.50	0.45	0.69	-0.10	0.01	1.73	1.23	0.11	0.62
12889BJPP	-3.54	-0.42	0.78	-0.10	-0.28	1.25	-0.21	0.44	0.07
13601BLFM	8.84	0.22	-4.88	6.71	0.18	3.28	0.92	0.02	0.25
13838BLST	-1.16	-0.03	1.20	-0.96	-1.79	1.42	-1.22	1.83	-0.75
14015BMDF	-0.32	1.47	-0.60	-0.62	-1.56	0.40	1.73	-0.86	-0.57
14602BNMD	-7.30	0.74	-0.20	1.02	-0.37	-1.16	-0.52	-2.36	-0.84
14880BPCK	-5.36	-0.85	0.80	0.10	-0.83	0.24	-1.36	-0.57	1.02
14986BPJL	-3.60	0.00	-0.24	0.68	-0.99	-1.56	-1.63	-0.60	0.00
15012BPKR	3.95	0.89	-0.33	0.11	-3.22	-2.51	-0.21	-1.27	-2.54
15906BRLG	10.91	0.43	-1.97	-3.72	1.24	0.35	-0.12	-1.49	1.73
15944BRNB	0.73	0.98	0.10	0.03	-1.00	-0.78	2.11	2.55	-0.10
16217BSDB	0.98	0.07	-0.01	-0.23	-0.41	-1.28	-1.24	0.94	0.27
16911BTSC	-5.56	-0.29	-0.23	0.69	0.02	0.53	-1.11	-1.42	-0.02

Table I. 5 - continued

17847BWVR	-4.01	-0.80	0.39	-0.21	-0.35	1.94	-0.62	-0.10	0.42
18080BXJT	-5.23	-0.13	0.03	0.32	-0.13	-1.20	-0.23	-0.25	1.11
18706BYTP	-4.86	0.42	-0.32	2.68	1.04	-0.67	0.00	0.34	-0.12
18725BYVM	-1.64	-1.18	-0.27	-1.03	2.72	0.23	-0.21	0.35	-0.73
19567CBSP	-4.68	-0.47	-0.22	0.53	0.72	0.19	-0.04	-0.56	0.13
19796CCGM	1.22	-0.76	0.44	0.05	-0.54	0.03	0.23	-0.72	0.22
19831CCJD	-0.18	0.83	-0.57	-2.53	1.06	0.64	-0.32	0.12	-1.01
30003DFKN	3.00	2.00	-2.13	-2.04	-0.45	-1.56	1.50	0.05	0.87
30182DFVB	-1.80	-0.16	0.18	0.11	-0.82	-1.85	0.95	1.66	2.61
30264DFYY	-2.52	0.82	-0.75	-0.40	0.13	-1.52	1.01	0.19	0.94
31026DHSG	15.01	-9.75	5.57	1.60	0.08	-0.98	-0.37	0.47	-0.57
31027DHSH	-4.13	0.13	0.23	-0.16	0.47	0.55	-1.06	1.71	-0.32
31049DHTJ	9.26	2.23	-4.03	3.37	0.76	-2.63	-2.68	2.07	-0.07
31487DJTF	-5.06	-0.30	0.56	-0.20	-0.06	-0.76	-0.58	0.23	-0.16
31612DKBD	-6.11	-1.37	0.50	0.55	0.27	0.48	-0.75	-0.93	0.88
32017DKYL	7.76	2.20	-3.20	-3.05	0.83	0.04	-1.25	-0.47	-0.81
32331DLRK	-0.43	0.24	-0.72	1.02	-0.35	0.87	1.70	-0.87	-1.98
32769DMRG	-2.01	-1.92	0.71	0.88	-0.45	-1.20	-0.10	-1.38	-0.02
32869DMWZ	-2.16	0.76	-0.46	-0.39	-1.00	0.57	-0.96	0.18	0.10
33003DNFK	-4.64	-1.08	-0.60	2.36	0.66	1.00	0.50	-0.51	0.02
33696DPTK	8.00	-1.09	-0.78	-1.76	0.34	0.17	0.17	-1.59	0.64

Appendix I.6 PCA T-Squared of summer 2006

site	T-Squared
10250BBPX	43.0222
11000BDHQ	43.0222
11377BFDP	43.0222
11428BFGZ	43.0222
11546BFNQ	43.0222
11683BFWD	43.0222
11688BFWK	43.0222
12380BHLJ	43.0222
12439BHPD	43.0222
12533BHTQ	43.0222
12746BJGT	43.0222
12753BJHC	43.0222
12889BJPP	43.0222
13601BLFM	43.0222
13838BLST	43.0222
14015BMDF	43.0222
14602BNMD	43.0222
14880BPCK	43.0222
14986BPJL	43.0222
15012BPKR	43.0222
15906BRLG	43.0222
15944BRNB	43.0222
16217BSDB	43.0222
16911BTSC	43.0222
17847BWVR	43.0222
18080BXJT	43.0222
18706BYTP	43.0222
18725BYVM	43.0222
19567CBSP	43.0222
19796CCGM	43.0222
19831CCJD	43.0222
30003DFKN	43.0222
30182DFVB	43.0222
30264DFYY	43.0222
31026DHSG	43.0222
31027DHSH	43.0222

Table I.6 – continued

31049DHTJ	43.0222
31487DJTF	43.0222
31612DKBD	43.0222
32017DKYL	43.0222
32331DLRK	43.0222
32769DMRG	43.0222
32869DMWZ	43.0222
33003DNFK	43.0222
33696DPTK	43.0222

Appendix I: Species with Absolute Loadings Equal or Greater Than 0.26 in Any Components before Species Exclusion

Table J.1 Winter 2006

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
BZ123M	0.25	0.00	-0.01	0.03	-0.01	0.02	0.02	0.02	0.02
BZ124M	0.32	0.02	-0.05	-0.04	0.03	0.06	0.00	0.02	-0.03
BZ135M	0.29	0.01	-0.02	-0.02	0.04	0.03	0.02	-0.01	-0.03
LBUT1E	0.05	0.04	0.04	-0.06	-0.26	-0.01	0.17	0.01	-0.02
P1E2ME	0.03	-0.01	0.02	-0.22	-0.42	0.14	-0.04	0.04	0.09
PENTE1	0.03	0.00	0.02	-0.16	-0.49	0.13	-0.10	0.09	-0.02
PA224M	-0.05	0.03	-0.01	0.02	0.04	0.05	-0.02	-0.37	-0.03
PA234M	-0.02	0.13	-0.04	0.06	0.06	0.03	-0.02	-0.32	-0.08
PEN24M	-0.05	0.11	-0.01	-0.07	-0.02	-0.02	0.01	-0.08	0.42
O_ETOL	0.30	0.01	-0.02	-0.01	0.02	-0.01	0.01	0.01	-0.03
PENA2M	0.03	0.41	-0.08	0.00	-0.03	-0.01	0.01	-0.07	-0.01
M_ETOL	0.26	0.01	0.00	-0.05	0.01	0.01	0.04	-0.04	-0.03
HEP3ME	0.09	-0.05	0.04	-0.03	0.02	-0.02	-0.01	-0.27	-0.01
PENA3M	0.04	0.52	-0.08	0.04	0.01	-0.01	0.00	0.05	-0.04
P_ETOL	0.27	0.00	-0.01	-0.07	-0.01	0.00	0.05	-0.04	-0.03
ACETYL	0.18	0.02	-0.03	-0.02	0.04	-0.44	0.35	0.00	-0.02
BENZE	-0.05	-0.04	0.02	-0.03	-0.07	0.12	0.36	-0.07	0.08
N_BUTA	-0.02	0.04	-0.04	0.35	-0.08	0.01	0.00	-0.03	-0.03
C2BUTE	-0.07	0.00	-0.01	0.19	-0.27	-0.04	0.05	-0.06	-0.05
C2PENE	-0.02	0.00	-0.04	0.11	-0.31	-0.06	0.03	-0.04	0.01
CYHEXA	-0.01	0.12	0.00	-0.28	0.04	0.18	0.14	-0.05	0.32
N_DEC	0.23	0.00	0.08	0.09	-0.13	-0.07	-0.26	0.12	0.08
ETHANE	0.10	-0.05	0.05	0.37	0.07	-0.09	0.03	0.18	0.19

Table J.1 – continued

ETBZ	-0.04	-0.02	0.54	-0.01	0.02	-0.01	0.01	-0.04	0.00
ETHENE	0.12	0.04	-0.04	0.11	0.10	-0.09	0.48	0.09	0.00
N_HEPT	0.05	-0.03	0.01	-0.01	-0.02	-0.02	0.00	-0.26	0.02
N_HEX	-0.03	0.46	0.27	-0.02	0.05	0.02	-0.06	0.09	-0.04
I_BUTA	-0.06	0.04	-0.03	0.34	0.02	0.19	0.01	-0.05	0.07
MP_XYL	-0.04	-0.02	0.53	-0.02	0.02	0.01	0.02	-0.04	0.00
MECYHX	0.12	-0.03	-0.04	-0.07	0.08	0.42	0.02	-0.08	0.03
MCYPNA	-0.01	0.44	0.02	-0.03	0.00	-0.01	-0.02	0.10	0.20
N_PRBZ	0.26	0.00	0.02	-0.02	0.00	-0.05	-0.01	-0.04	-0.03
O_XYL	0.00	-0.02	0.49	-0.02	-0.01	-0.01	0.04	-0.01	-0.01
N_PROP	-0.05	0.05	0.01	0.30	0.16	0.44	0.11	0.03	-0.16
PROPE	0.06	-0.01	0.07	-0.01	-0.08	0.03	0.35	0.01	0.00
STYR	0.07	0.01	0.03	0.03	-0.12	0.41	0.28	0.19	-0.06
T2BUTE	-0.06	0.02	0.00	0.20	-0.29	-0.04	0.01	-0.05	-0.05
T2PENE	-0.01	0.01	-0.03	0.10	-0.31	-0.07	0.03	-0.04	0.00
TOLUE	-0.05	-0.15	-0.04	0.13	0.06	0.08	0.02	0.11	0.65
N_UNDE	0.19	0.02	0.11	0.27	-0.02	-0.08	-0.23	0.14	0.05
Eigenvalue	34.45	3.98	3.25	2.79	2.30	1.59	1.45	1.28	1.06
Variance Explained (%)	61.51	7.10	5.81	4.98	4.11	2.84	2.59	2.29	1.89

Table J.2 Summer 2006

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
BZ123M	0.00	-0.28	-0.03	0.00	0.02	-0.03	-0.01	0.00	0.01
BZ124M	0.00	-0.30	-0.02	-0.01	0.03	0.01	0.00	0.00	-0.01
BZ135M	-0.01	-0.34	-0.02	0.01	0.00	0.01	0.01	-0.01	0.00
P1E2ME	-0.03	0.07	0.01	-0.01	0.04	-0.66	0.02	-0.05	0.04
PENTE1	-0.07	0.01	0.04	-0.03	-0.04	-0.63	-0.02	0.01	-0.03
PA224M	0.12	0.05	-0.01	0.11	-0.61	0.02	-0.03	0.00	-0.01
BU22DM	0.42	0.07	-0.05	-0.09	0.03	-0.02	-0.07	0.04	0.03
PA234M	-0.17	-0.07	0.04	0.04	-0.59	-0.06	0.00	-0.08	-0.01
PEN24M	0.24	0.00	-0.02	-0.09	-0.34	0.00	0.04	0.05	-0.02
O_ETOL	0.00	-0.34	-0.02	0.02	0.01	0.00	-0.01	0.00	0.00
M_ETOL	0.00	-0.33	0.00	0.03	-0.01	0.01	-0.02	-0.01	0.00
P_ETOL	0.02	-0.31	0.01	0.05	-0.01	0.02	-0.01	-0.01	0.01
N_BUTA	0.11	-0.01	0.09	-0.33	-0.16	0.02	0.04	0.03	-0.08
C2BUTE	-0.01	0.00	-0.01	-0.46	-0.10	0.10	-0.06	0.07	0.02
C2PENE	0.07	0.00	-0.05	-0.44	0.07	-0.09	-0.04	-0.02	0.01
CPENTA	0.33	0.06	0.06	0.14	0.02	0.07	0.08	-0.04	0.03
N_DEC	0.01	-0.01	-0.14	0.08	0.02	0.01	0.53	-0.05	0.00
ETBZ	0.02	-0.02	0.46	0.01	0.00	-0.01	-0.01	-0.02	-0.02
I_BUTA	0.06	0.00	0.42	-0.02	-0.01	0.01	-0.03	0.05	-0.04
MP_XYL	0.00	-0.02	0.46	0.00	0.01	-0.01	0.01	-0.03	0.00
N_NON	0.00	-0.06	0.02	-0.02	-0.02	0.02	0.46	-0.04	0.00
N_PRBZ	0.00	-0.30	0.02	0.06	-0.01	-0.01	0.01	-0.01	0.02
O_XYL	0.02	-0.02	0.44	0.00	0.04	-0.01	0.01	-0.03	0.02

Table J.2 – continued

PROPE	-0.65	0.04	0.01	-0.16	-0.07	0.18	0.04	-0.10	0.10
STYR	-0.08	-0.02	0.02	-0.02	0.01	0.04	-0.01	0.94	0.02
T2PENE	0.02	0.00	-0.05	-0.48	0.09	-0.09	-0.03	-0.04	0.01
TOLUE	-0.08	0.08	0.33	0.01	0.02	0.01	0.03	0.04	0.03
N_UNDE	-0.03	0.01	0.05	0.01	0.03	-0.12	0.62	0.15	-0.01
OTHERS	0.07	-0.02	0.01	0.01	-0.01	0.00	0.00	0.00	0.98
Eigenvalue	30.0	5.8	3.9	3.3	2.2	1.8	1.5	1.2	0.896
Variance Explained (%)	53.5	10.4	7.0	5.8	3.9	3.2	2.7	2.1	1.6

Appendix J: Species with loadings greater than 0.1 in one or more component of PCA without Z score

Table K.1 Winter 2006

	PC1	PC2	PC3
IPENTA		-0.44	
N_BUTA		-0.63	0.11
ETHANE		-0.23	
ETHENE		-0.14	
I_BUTA		-0.18	
MP_XYL		-0.17	0.26
N_PENT		-0.27	
N_PROP	-0.11	-0.28	
OTHER		-0.18	
N_HEX		0.21	0.87
TOLUE	0.99		
PENA2M			0.19
PENA3M			0.29
MCYPNA			0.12
Eigenvalue	3.80	1.60	0.96
Variance explained (%)	51.2	21.5	12.9

Table K.2 Summer 2006

	PC1	PC2	PC3	PC4
BZ124M				0.16
IPENTA		-0.68		
PENA2M		-0.20		
PENA3M		-0.12		
N_BUTA		-0.26		
ETHANE		-0.14		
ETBZ	0.15			
N_HEX		-0.11		0.12
I_BUTA	0.39	0.19		
MP_XYL	0.40			
MECYHX				
N_PENT		-0.54		
N_PROP	0.18	-0.11	0.90	-0.30
TOLUE	0.73		-0.11	0.39
OTHERS	-0.29		0.40	0.81
Eigenvalue	21.3	5.6	1.2	0.91
Variance Explained (%)	68.9	18.2	3.8	3.0

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