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Receptor Modelling - Application to wood burning

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Summary

An overview of current in use receptor models is given in the present report as well as information on their characteristics and limitations. The Chemical Mass Balance (CMB), the Principal Component Analysis (PCA), the Quantitative Bias Trajectory Analysis and the Potential Source Contribution Function (PSCF) receptor methods are described briefly in the current document. In addition, information concerning biomass burning and its particulate matter (PM) emission characteristics are reviewed as well as use of receptor models and chemical analysis techniques in identifying the contribution of wood burning on ambient PM concentrations. Finally, recommendations for source apportionment in Oslo area for wood burning sources are presented where two integrated approaches are proposed.

Receptor Modelling - Application to wood burning

1 Introduction

The general methodology to apportion sources of contaminants in the atmosphere using a mass conservation and mass balance analysis is referred to as receptor modelling. Receptor models are based on the mass balance principle and consequently mass balance analysis with the scope to identify and quantify sources of pollutants in the atmosphere. An extensive dataset of chemical characteristics from ambient samples is needed for determining the contribution of various sources to ambient concentrations using receptor models. After the dataset is constructed a mass balance equation can be written for the m chemical species in the n samples originating from p independent sources (Hopke, 1997):

$$x_{ij} = \sum_{k=1}^p c_{ik} s_{kj} \quad (1)$$

where x_{ij} is the i th elemental concentration measured in the j th sample (ng m^{-3}), c_{ik} is the gravimetric concentration of the i th element in material from the k th source (ng mg^{-1}), and s_{kj} is the airborne total mass concentration of material from the k th source contributing to the j th sample (mg m^{-3}).

Henry (1991) described a number of physical constraints that receptor models must follow for obtaining realistic solutions:

1. The original data must be reproduced by the model. The model must explain the observations.
2. The predicted source compositions must be non-negative. A source cannot have a negative percentage of an element.
3. The predicted source contributions to the aerosol must all be non-negative. A source cannot emit negative mass.
4. The sum of the predicted elemental mass contributions from each source must be less than or equal to total measured mass for each element. The whole is greater than or equal to the sum of its parts.

Seigneur et al. (1997) reviews in detail the recent status on receptor modelling and groups the receptor models into three major categories:

- Models that apportion primary PM using source information.
- Models that apportion primary PM without using source information.
- Models that apportion primary and secondary PM.

There are many techniques available in the different categories including US EPA regulatory tools for PM apportionment (CMB and PCA) as well as recent powerful research tools (e.g. Positive Matrix Factorization, Hybrid methods). Hybrid methods have been applied to apportion the secondary components of PM.

Gray and Cass (1998) have combined modeling of air trajectories combined with receptor modelling to apportion the atmospheric fine carbon particle concentrations in the Los Angeles area. Additionally, ambient data have been used through inverse modelling to improve emission source inventories (Kleeman and Cass, 1999).

In the US EPA's Office of Air Quality Planning and Standards (OAQPS) there are two recommended methods for the PM-10 SIP (State Implementation Plan) guidance document. One important requirement for receptor models is the construction and update of databases on source profiles as well as speciated PM data for PM_{2.5} and PM₁₀.

Biomass burning is one of the major but poorly characterized sources of atmospheric PM and it is believed that it contributes between 14% and 30% of fine particle concentrations in urban areas and account for about 16% of the national PM emission inventories in the United States. Receptor modelling techniques have been applied in a large number of studies (see Appendix A) to characterize and source attribute the ambient PM concentration in various geographical locations (Seigneur et al., 1997). A combination of receptor modelling with GC/MS analysis of source samples for obtaining organic chemical fingerprints (e.g. thermally altered resin acids; syringol and guaiacyl type compounds; plant waxes, etc.) is recently proposed to study the contribution of biomass combustion to ambient fine particle concentrations in the United States.

In the following chapters the major receptor modelling techniques available are summarized and their functionality, use characteristics and limitations are described in brief. In Appendix B a summary of the available receptor models for PM is presented (Seigneur et al., 1997).

Recommendations for source apportionment in Oslo for quantifying the contribution of wood burning on the ambient PM concentrations are presented in Chapter 3. Chemical Mass Balance (CMB) receptor modelling in combination with ambient monitoring and chemical analysis of fine PM samples together with chemical source characterization are expected to give the framework under which a characterization and quantification of the contribution of wood burning on ambient PM concentrations can be performed. More advanced receptor techniques (such as hybrid methods) in combination with traditional methods (PCA and CMB) and more detailed monitoring/chemical analysis and chemical source identification are proposed as a next step in an integrated approach for assessing and quantifying the importance of wood burning contribution to the air quality in Oslo. In addition, in Chapter 3 recent information on biomass burning are reviewed.

2 Receptor Models

2.1 Chemical Mass Balance (CMB) approach

The CMB model is a "multiple regression model" and is the most commonly used for PM source apportionment. Friedlander (1973) described the "ordinary weighted least-squares" solution to the CMB equation in a way that each

concentration of a chemical species at a receptor site can be expressed as a linear sum of products of source profile species and source contributions. Kowalczyk et al. (1978) used a weighted least-squares regression analysis to the CMB modeling where the ambient elemental concentrations are weighted by the inverse of the square of the analytical uncertainty in that measurement. In the recent version of the CMB (CMB 7.0) method an Effective-variance least squares (EVLS) method has been incorporated (Watson et al., 1990a,b). However, the main problem with source profile information is the temporal variability of the chemical emissions from various sources.

In the CMB method the objective of the analysis is to determine the contribution from different sources on the ambient measured samples of PM. The problem is the solution of an equation in the form $\vec{x} = C \vec{s}$ as indicated in equation (1). The equation can be written as

$$\vec{s} = (C^T C)^{-1} C^T \vec{x} \quad (2)$$

and is solved initially with using the least-squares method (Friedlander, 1973). As already mentioned the equation is now solved using advanced numerical techniques.

The assumptions underlying the use of the CMB technique can be summarised as following (EPA, 1996):

1. Compositions of source emissions are constant over the period of ambient and source sampling.
2. Chemical species do not react with each other, i.e., they add linearly.
3. All sources with a potential for significantly contributing to the receptor have been identified and their emissions have been characterized.
4. The source compositions are linearly independent of each other.
5. The number of sources or source categories is less than or equal to the number of chemical species
6. Measurement uncertainties are random, uncorrelated, and normally distributed.

The main limitations to assessments from these assumptions are that:

1. CMB cannot be used in conditions where PM reactivity and secondary PM formation is appreciable for any component, and
2. source emission compositions are normally not constants. This requires that the source profile represent an average of the composition during the time period of the ambient sampling.

2.2 Principal Component Analysis (PCA) method

Principal Component Analysis (PCA) has the aim to simplify the description of a system by compression of available data into fewer dimensions and with exploring the structure of the relationships between the existing variables. For

example consider a set of samples with different particle contribution from the various sources.

The mass balance for the system can be expressed as (Seigneur et al., 1997):

$$Z = A \cdot F \quad (3)$$

where Z is a matrix of sample vectors, A is the matrix related to the source composition, and F is a matrix related to the contribution of that source type to the variance of that particular measured variable. The PCA method can produce components that have a strong relationship with only one variable. An advantage of the method is that it does not need information for source input as the CMB method. The PCA methodology has been used by Schaug and Larssen (1990) for studying the contribution from various sources in the concentration of ambient particulate matter in Oslo but without studying the contribution from wood burning specifically.

In the PCA model there is a classification of variables into groups which are causes of measured PM levels. These causes are identified as emission sources, chemical reactions and physical changes such as resulting from meteorology. The PCA model needs an extensive amount of measured data at one receptor site at different time periods.

The general procedure in the PCA modelling can be described as (EPA, 1996):

1. Select the chemical species and measurement cases to be included.
2. Calculate the correlation coefficients between the species.
3. Calculate the eigenvectors and eigenvalues of the correlation matrix.
4. Select eigenvectors to be retained.
5. Rotate these eigenvectors into a more physically meaningful space.
6. Interpret the rotated vectors as air pollution sources based on the chemical species with which are highly correlated.

The factor analysis in general can only identify source types and give some insight into the relationships existing among measured compositions. Quantitative apportionment can be achieved by CMB analysis. However, more recently with advanced factor analysis methods such as Absolute Principal Component Analysis (APCA) (Thurston and Sprengler, 1985) and Source Apportionment by Factors with Explicit Constraints (SAFER) (Henry and Kim, 1989) more quantitative apportionment of the various sources can be obtained. In addition, there are some new interesting scientific approaches for factor analysis such as the Positive Matrix Factorization (PMF) (Paatero and Tapper, 1993).

2.3 Quantitative Bias Trajectory Analysis

The Quantitative Bias Trajectory Analysis (Samson and Small, 1984; Keeler, 1987) is an approach that incorporates back trajectories and deposition calculations.

The probability for a depositing tracer to arrive at point x at time t can be expressed as (Lamb and Seinfeld, 1973; Cass, 1981):

$$A(x, t) = \int_{t-\tau}^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} T(x, t | x', t') dx' dt' \quad (4)$$

where $T(x, t | x', t')$ is the potential mass transfer function that is given by

$$T(x, t | x', t') = Q(x, t | x', t') R(t | t') D(x', t') \Lambda(x', t') \quad (5)$$

In the above equation the function $Q(x, t | x', t')$ is the probability of an air parcel located at x' at time t' arriving at the receptor site x at time t , $R(t | t')$ is the probability of the tracer not to be reacted in the time interval, $D(x', t')$ is the probability that the tracer is not removed by dry deposition at the point (x', t') and $\Lambda(x', t')$ is the probability that the tracer is not removed by wet deposition. Finally, the integration is applied to the whole length of the back trajectory. A main problem arising in the above formulation is the identification of the functional forms and values of the various probability components.

Kleeman and Cass (1999) and Gray and Cass (1998) have applied the Quantitative Bias Trajectory Analysis to determine the source contributions to atmospheric fine elemental carbon and fine primary total carbon particle concentrations in the Los Angeles area. The elementary carbon concentration is found to be dominated by emissions from diesel engines. However, the fine primary total carbon concentrations are arising from a great variety of emission sources including vehicles, stationary source fuel oil and gas combustion, industrial processes, paved road dust, fireplaces, cigarettes and food cooking.

2.4 Potential Source Contribution Function

In the Potential Source Contribution Function (PSCF) receptor model air parcel back trajectories ending at a receptor site are calculated using a trajectory model (Ashbaugh et al., 1986; Malm et al., 1986; Cheng et al., 1993). A comprehensive description of the PSCF approach is presented by Hopke (1997) and is briefly repeated here. The trajectories in the PSCF method are represented by segment endpoints which have two coordinates (e.g., latitude and longitude). The geographical area under investigation is divided into an array of grid cells and the cells have indices i and j .

Suppose that during the period of study T there are N number of trajectory endpoints. If there are n segment trajectory endpoints into the ij -th cell (n_{ij}), the probability of this event A_{ij} is given by the expression

$$P[A_{ij}] = \frac{n_{ij}}{N} \quad (6)$$

where $P[A_{ij}]$ is a measure of the residence time.

Suppose also that in the ij -th cell there is a set of m_{ij} segment endpoints of trajectories arriving at a receptor site when the concentrations are higher than the specified values. The corresponding probability for high concentration values is given by

$$P[B_{ij}] = \frac{m_{ij}}{N} \quad (7)$$

Therefore, the PSCF that relates to the residence time of air parcel in the ij -th cell with high concentrations can be expressed as

$$P_{ij} = \frac{P[B_{ij}]}{P[A_{ij}]} = \frac{m_{ij}}{n_{ij}} \quad (8)$$

The PCSF methodology is used mainly for determining the relative contribution of emission sources to the air quality in a pre-specified area. However, there is no method for estimating uncertainties for the PSCF values and this is a considerable limitation of the method. The PCSF methodology has been applied in several studies for sulphur in the United States and Canada (see the review by Seigneur et al., 1997).

3 Biomass Burning

Biomass burning is a source of greenhouse gases such as CO_2 , CH_4 , CO and NMHC. Biomass burning is also producing high concentrations of organic aerosols such as polycyclic aromatic hydrocarbons (PAH) and fatty acids (Ballentine et al., 1996).

Wood burning is a major source of particulate matter in the northwestern United States in winter periods (EPA, 1996). Figure 1 shows the chemical composition of fine particles produced by woodstoves in Denver (Watson and Chow, 1994). Organic carbon (OC) and elemental carbon (EC) are the main constituents from wood burning. Over 90% of the dry mass from wood burning is composed of OC (Mazurek et al., 1991). The OC/EC ratio is ranging from 10:1 to 95:1 with the latest corresponding to flaming conditions.

The CMB methodology was the first to identify and quantify the wood burning contribution for particulate matter concentrations in an urban area in United States (Watson, 1979) (Portland Aerosol Characterization Study, PACS).

Parameters which determine the proportionality between EC and OC are the combustion stage, stove type and fuelwood condition (EPA, 1996). The most abundant trace element from wood burning is the Potassium (K) (Watson and Chow, 1994). Li and Kamens (1993) used successfully polycyclic aromatic hydrocarbons as source signatures (organic tracers) in receptor modelling for wood burning. Li and Kamens (1993) found almost entirely on soot particles the following PAH: benz(a)anthracene, chrysene, benzo(e)pyrene, benzo(b)-

fluoranthene, benzo(b)fluoranthene, benzo(a)pyrene, benzo(ghi)perylene, indeno-(123,cd)pyrene and coronene.

Furthermore, a number of organic chemical fingerprints A GC/MS analysis of source samples for obtaining organic chemical fingerprints (e.g. thermally altered resin acids; syringol and guaiacyl type compounds; plant waxes, etc.) were used for identifying biomass burning sources in the United States.

Furthermore, methyl chloride (CH_3Cl) is used as a tracer for wood burning but with accuracies around $\pm 50\%$ (Khalil et al., 1983). In recent apportionment studies in the US ambient concentrations of biomass tracer compounds (e.g. thermally altered resin acids; syringol and guaiacyl type compounds, plant waxes) were used for identifying wood burning sources (EPA, 1996). In Figure 2 we present the results by Ballentine et al. (1996) concerning different PAH in aerosols during a field burn of sugar cane.

Particle emissions from wood burning are concentrated mainly in the fine sizes. Dasch (1982) found a mass median diameter close to $0.17 \mu\text{m}$ from burning hardwood, softwood and synthetic logs. An overview of the PM emission characteristics from various sources is presented in Figure 3 (Houck et al., 1989, 1990).

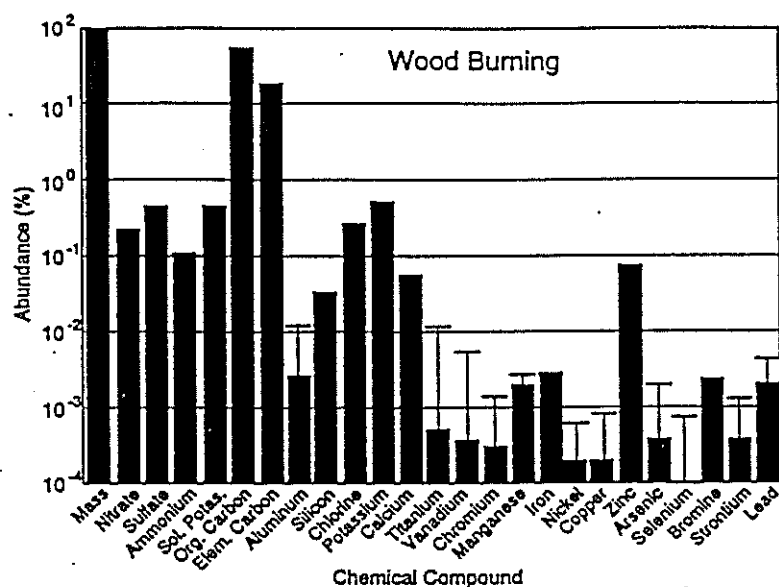


Figure 1; Chemical abundances for $\text{PM}_{2.5}$ emissions from wood burning in Denver, CO. solid bars represent fractional abundances, and the error bars represent variability in species abundances. Error bars represent detection limits when there are no solid bars.

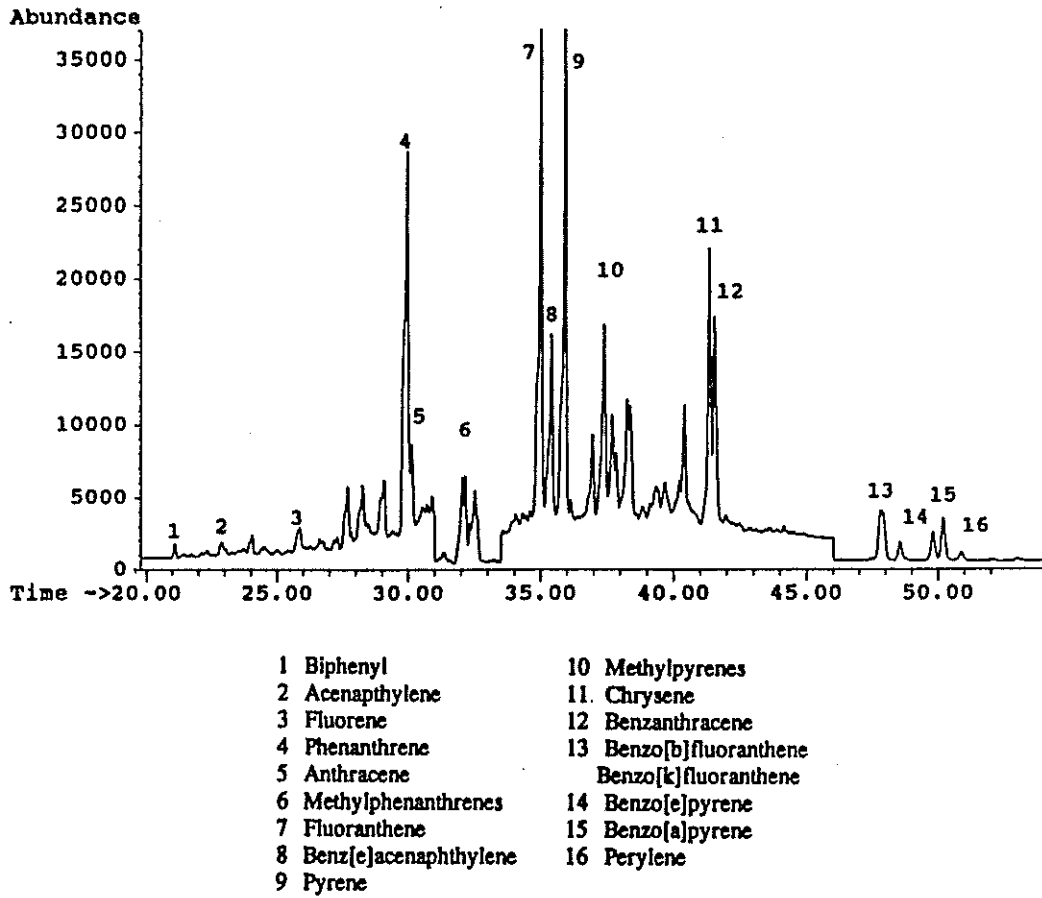


Figure 2: GC-MS trace in selected ion mode of PAH in aerosols collected during a field burn of sugar cane.

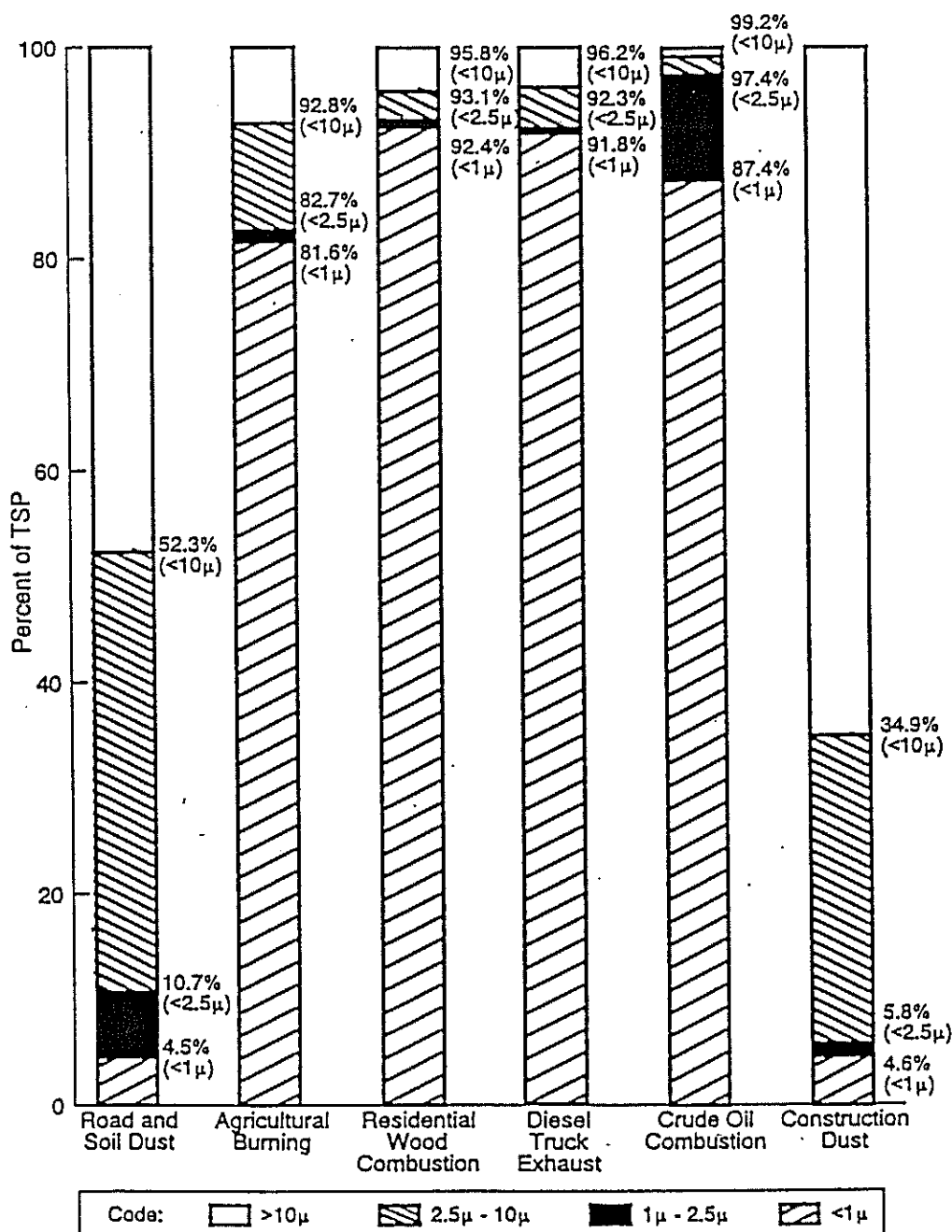


Figure 3: Size distribution of California source emissions, 1986.

Measurements including of chemical analysis and size distribution characteristics for wood burning has been performed by many researchers (e.g. Susott et al., 1991; Radke et al., 1991). Measurements of particulate emissions from prescribed chaparral fires with a helicopter using filters was performed by Cofer et al. (1988). It is important to note that the products from forest fire emissions can be identified in the air even after prolonged periods of time (Ferrare et al., 1990).

Using the CMB methodology it was found that vegetative burning which includes agricultural fires, wildfires, prescribed burning and residential wood combustion to be important in various locations in United States as shown in Appendix A. Additionally, the residential wood combustion was identified as the main source since the contribution of vegetative burning was higher in winter and was identified to be a local problem with no significant regional contribution.

4 Recommendations for Source Apportionment in Oslo for wood burning sources

As discussed previously there are available a number of techniques for source apportionment. The CMB and hybrid methodologies (such as the Quantitative Bias Trajectory Analysis) have been successfully applied to investigate the contribution of wood burning on the ambient PM concentration in several studies (see also Chapter 3). The objective to quantify the contribution of wood burning sources to atmospheric fine particle concentrations in Oslo is a feasible task and can be met combining receptor modelling techniques together with source profile information, extensive measurement studies for fine PM and chemical analysis of the ambient samples. Since biomass burning has large emission uncertainties it is better characterized through receptor modelling than episodic (dispersion) modelling. However, when quantification of the emission inventories are established the modelling through an episodic three dimensional air quality model will be another alternative for examining the contribution of wood burning sources in the air quality in the Oslo area.

Because of the various limitations that different receptor models have (see Chapter 2) we recommend the use of a combination of methods together with an extensive monitoring programme and chemical analysis of PM samples. We propose an approach in two steps for studying the contribution of wood burning to the air quality in Oslo area.

The first step can be seen as the starting point in studying the importance of wood burning. The CMB receptor model will be used in combination with chemical signature of wood burning measurements in Oslo area (source profile information), ambient measurements of PM in two sites in Oslo (a period of several months in winter) and chemical analysis of the samples. An important task in the current approach is the determination of the regional background particulate matter values and their chemical composition, since they are contributing significantly to the ambient urban concentrations. This approach is expected to be completed over a period of one year in which extended measurements in a winter period will be performed.

The second step which will offer an integrated investigation of the contribution of biomass combustion to ambient fine particle concentrations in Oslo will include a combination of several receptor modelling techniques (such as CMB and PCA methods), extended field experiments over two winter periods in Oslo, use of organic chemical tracer techniques for source samples and fine particle samples from the measurement sites as well as construction of an emission inventory for wood burning in greater Oslo area. The completion of this approach will require two years including measurements in two winter periods. An outline of the proposed approaches is given in the following subsections.

4.1 First step in studying the contribution of wood burning on Oslo air quality (Completion Period : 1 year)

As a first step in studying the effect of wood burning in Oslo area the CMB model combined with a monitoring and chemical characterization study are proposed.

The following steps are proposed for performing a CMB receptor modelling in Oslo area:

- Source profile characterization of wood burning and possible from other major source categories (use of syringol and guaiacyl type compounds as tracers). NILU has adequate laboratory capabilities using the GC/MS method to identify these compounds. The same methodology is used in the United States recently.
- Analysis of a limited number of samples (around 10 samples) using the Carbon-14 technique for identifying the source of the carbon material in the filters parallel to the chemical analysis with the GC/MS (Ramdahl et al., 1984).
- Background particulate matter chemical characterization in Oslo.
- Chemical speciated PM concentrations in a couple of measurement sites in Oslo area for an extended winter period (4 months). One of the sites has to be located in the suburbs of Oslo and the other in the city centre but not very close to a main highway. Chemical species such as syringol and guaiacyl type compounds will be used as tracers.
- CMB receptor modelling using data from the measurement campaign.

At NILU the CMB 7.0 and CMB 8.0 versions from the CMB model are available for performing source apportionment modelling when the necessary emission and measurement data are available. In addition, the GC/MS technique for identification of the organic tracers (syringol and guaiacyl type compounds) is also available at NILU.

4.2 Integrated Methodology for studying the contribution of wood burning on Oslo air quality (Completion Period: 2 years)

An integrated study on the wood burning problem in Oslo requires the use of a combination of receptor modeling techniques combined with extensive monitoring and chemical characterization of ambient fine particulate matter.

The necessary components of the proposed study are the following:

- Source profile characterization of wood burning and possible from other major source categories.
- Background particulate matter chemical characterization in Oslo.
- Chemical speciated PM concentrations in a couple of measurement sites in Oslo area for two extended winter period (8 months). Chemical species such as syringol and guaiacyl type compounds will be used as tracers.
- Analysis of a limited number of samples (around 20 samples) using the Carbon-14 technique for identifying the source of the carbon material in the filters parallel to the chemical analysis with the GC/MS (Ramdahl et al., 1984).
- CMB and PCA receptor modelling using data from the measurement campaign.
- Chemical analysis of the ambient samples for determining specific organic components (e.g. thermally altered resin acids).

5 Conclusions

The quantitative evaluation of the contribution of wood burning sources in Oslo area is a feasible task with the combination of measurement studies and source apportionment modelling techniques. The use of appropriate chemical tracers (such as syringol and guaiacyl type compounds) in conjunction with a Carbon-14 technique will be the required steps for experimentally identifying wood burning sources. In the modelling side the CMB technique is mainly recommended for source apportionment together with the PCA methodology.

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Appendix A

Receptor Model Source Contributions to PM10 based on the CMB Methodology (Seigneur et al., 1997)



Table 3-2. Receptor Model Source Contributions to PM-10.

Sampling Site	Time Period	Primary Geological	Primary Construction	Primary Motor Vehicle Exhaust	Primary Vegetative Burning	Secondary Ammonium Sulfate	Secondary Ammonium Nitrate	Misc. Source				Measured PM-10 Concentration	
								1	2	3	4		
Central Phoenix, AZ (Chow et al., 1991)	Winter 1989-1990	33.0	0.0	25.0	2.3	0.2	2.8	0.0	0.0	0.0	0.0	0.0	64.0
Corona de Tucson, AZ (Chow et al., 1992a)	Winter 1989-1990	17.0	0.0	1.6	0.0	1.9	0.0	0.0	0.0	0.0	0.0	0.0	19.1
Craycroft, AZ (Chow et al., 1992a)	Winter 1989-1990	13.0	0.0	8.3	0.0	0.7	0.6	1.2 ^a	0.0	0.0	0.0	0.0	23.4
Downtown Tucson, AZ (Chow et al., 1992a)	Winter 1989-1990	26.0	5.1	14.0	0.0	1.0	0.2	1.3 ^a	0.0	0.0	0.0	0.0	48.0
Hayden 1, AZ (Garfield) (Ryan et al., 1988)	1986	5.0	2.0 ^b	0.0	0.0	4.0	0.0	74.0 ^c	5.0 ^d	1.0 ^e	0.0	0.0	105.0
Hayden 2, AZ (Jail) (Ryan et al., 1988)	1986	21.0	4.0 ^b	0.0	0.0	4.0	0.0	28.0 ^c	0.0	1.0 ^e	0.0	0.0	59.0
Orange Grove, AZ (Chow et al., 1992a)	Winter 1989-1990	20.0	0.0	15.0	0.0	0.4	0.4	0.0	0.0	0.0	0.0	0.0	34.2
Phoenix, AZ (Estrella Park) (Chow et al., 1991)	Winter 1989-1990	37.0	0.0	10.0	0.9	1.6	0.0	0.0	0.0	0.0	0.0	0.0	55.0
Phoenix, AZ (Gunnery Rg.) (Chow et al., 1991)	Winter 1989-1990	20.0	0.0	5.5	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	27.0
Phoenix, AZ (Pinnacle Pk.) (Chow et al., 1991)	Winter 1989-1990	7.0	0.0	2.9	1.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0	12.0
Rillito, AZ (Tianukos et al., 1992)	1988	42.7	13.8 ^b	1.2 ^f	0.0	0.0	0.0	11.6 ^d	0.0	0.0	0.0	0.0	79.5
Scottsdale, AZ (Chow et al., 1991)	Winter 1989-1990	25.0	0.0	19.0	7.4	0.6	3.6	0.0	0.0	0.0	0.0	0.0	55.0
West Phoenix, AZ (Chow et al., 1991)	Winter 1989-1990	30.0	0.0	25.0	10.0	0.4	3.1	0.0	0.0	0.0	0.0	0.0	69.0
Anaheim, CA (Gray et al., 1988)	1986	21.2	0.0	4.1 ^f	0.0	7.0	9.8	0.4 ^f	1.4 ^g	8.2 ^h	0.0	0.0	52.1
Anaheim, CA (Summer) (Watson et al., 1994)	Summer 1987	11.4	0.0	8.5	0.0	9.0	2.9	0.0 ^f	6.5 ^h	0.0	0.0	0.0	51.3
Anaheim, CA (Fall) (Watson et al., 1994)	Fall 1987	13.2	0.0	37.2	0.0	3.7	38.5	0.0 ^f	3.1 ^h	0.0	0.0	0.0	104.0
Azusa, CA (Summer) (Watson et al., 1994)	Summer 1987	34.9	0.0	15.9	0.0	11.4	6.1	0.0 ^f	5.7 ^h	0.0	0.0	0.0	92.1
Bakersfield, CA (Magliano, 1988)	1986	27.4	3.0	5.5	9.6 ^f	5.6	0.0	0.5 ^f	0.0	0.0	0.0	0.0	67.6
Bakersfield, CA (Chow et al., 1992b)	1988-1989	42.9	1.6	7.7	6.5	5.5	12.7	1.0 ^m	1.5 ⁿ	0.6 ^o	0.0	0.0	79.6
Burbank, CA (Gray et al., 1988)	1986	21.3	0.0	6.1 ^f	0.0	7.2	10.2	0.1 ^f	0.9 ^h	9.8 ^h	0.0	0.0	56.6
Burbank, CA (Summer) (Watson et al., 1994)	Summer 1987	14.0	0.0	17.0	0.0	12.4	6.5	0.0 ^f	5.7 ^h	0.0	0.0	0.0	72.3
Burbank, CA (Fall) (Watson et al., 1994)	Fall 1987	11.0	0.0	39.1	0.0	3.1	25.1	0.0 ^f	1.9 ^h	0.0	0.0	0.0	94.8
Chula Vista 1, CA (Bayside) (Cooper et al., 1988)	1986	6.7	0.0	0.8	0.0	7.5	0.0	0.4 ^f	2.7 ^h	2.0 ^h	0.0	0.0	28.8
Chula Vista 2, CA (Del Ray) (Cooper et al., 1988)	1986	8.2	0.3	1.5	0.0	8.9	0.0	0.6 ^f	1.8 ^h	0.0	0.0	0.0	31.1
Chula Vista 3, CA (Cooper et al., 1988)	1986	9.7	0.3	1.4	0.0	8.2	0.0	0.6 ^f	1.7 ^h	0.0	0.0	0.0	29.6
Claremont, CA (Summer) (Watson et al., 1994)	Summer 1987	19.4	0.0	14.4	0.0	9.5	6.3	0.0 ^f	4.7 ^h	0.0	0.0	0.0	70.0
Crows Landing, CA (Chow et al., 1992b)	1988-1989	32.2	0.0	2.2	3.4	2.8	6.5	0.5 ^m	1.5 ⁿ	1.2 ^h	0.0	0.0	52.5

Table 3-2. Receptor Model Source Contributions to PM-10 (continued).

Sampling Site	Time Period	Primary Geographical	Primary Construction	Primary Motor Vehicle Exhaust	Primary Vegetative Burning	Secondary Ammonium				Secondary Ammonium Nitrate	Misc. Source 1	Misc. Source 2	Misc. Source 3	Misc. Source 4	Measured PM-10 Concentration
						Sulfate	Sulfate	Sulfate	Sulfate						
Downtown Los Angeles, CA (Gray et al., 1988)	1986	23.8	0.0	6.4 ¹	0.0	7.6	11.2	0.0	1.3 ¹	7.9 ¹	0.0	0.0	0.0	60.2	
Downtown Los Angeles, CA (Summer) (Watson et al., 1994)	Summer 1987	12.7	0.0	16.2	0.0	13.0	4.4	0.0 ¹	6.5 ¹	0.0	0.0	0.0	0.0	67.6	
Downtown Los Angeles, CA (Fall) (Watson et al., 1994)	Fall 1987	9.4	0.0	41.1	0.0	3.9	27.5	0.0 ¹	1.8 ¹	0.0	0.0	0.0	0.0	98.6	
Fellows, CA (Chow et al., 1992b)	1988-1989	29.0	1.4	2.1	3.4	5.1	7.5	7.0 ^m	1.4 [*]	1.4 ¹	0.0	0.0	0.0	54.6	
Fresno, CA (Magliano, 1988)	1986	17.1	0.7	4.0	9.2 ¹	1.8	0.0	0.1 ¹	0.0	0.0	0.0	0.0	0.0	48.1	
Fresno, CA (Chow et al., 1992b)	1988-1989	31.8	0.0	6.8	5.1	3.6	10.4	0.3 ^m	1.0 [*]	0.1 [*]	0.0	0.0	0.0	71.5	
Hawthorne, CA (Summer) (Watson et al., 1994)	Summer 1987	7.5	0.0	5.6	0.0	15.0	0.6	0.0 ¹	7.0 [*]	0.0	0.0	0.0	0.0	45.9	
Hawthorne, CA (Fall) (Watson et al., 1994)	Fall 1987	8.9	0.0	35.1	0.0	5.1	20.4	0.0 ¹	3.7 [*]	0.0	0.0	0.0	0.0	85.1	
Indio, CA (Kim et al., 1992)		33.0	3.0	4.4	7.1	3.6	4.1	0.2 ¹	1.0 [*]	0.0	0.0	0.0	0.0	58.0	
Kern Wildlife Refuge, CA (Chow et al., 1992b)	1988-1989	15.1	2.0	2.2	4.0	3.3	1.5	0.5 ^m	1.5 [*]	0.7 ¹	0.0	0.0	0.0	47.8	
Lennox, CA (Gray et al., 1988)	1986	16.0	0.1	4.6 ¹	0.0	7.6	7.9	0.2 ¹	3.1 ¹	7.6 ¹	0.0	0.0	0.0	46.9	
Long Beach, CA (Gray et al., 1988)	1986	20.7	0.0	5.1 ¹	0.0	8.0	9.2	0.1 ¹	2.0 [*]	6.4 ¹	0.0	0.0	0.0	51.9	
Long Beach, CA (Summer) (Watson et al., 1994)	Summer 1987	11.1	0.0	6.3	0.0	10.9	0.8	0.1 ¹	2.2 [*]	0.0	0.0	0.0	0.0	46.1	
Long Beach, CA (Fall) (Watson et al., 1994)	Fall 1987	11.3	0.0	42.8	0.0	3.8	23.2	0.0 ¹	2.7 [*]	0.0	0.0	0.0	0.0	96.1	
Magnolia, CA (Chow et al., 1992c)	1988	31.7	0.0	11.2	0.0	4.9	19.7	0.3 ¹	1.2 [*]	1.2 [*]	0.0	0.0	0.0	66.0	
Palm Springs, CA (Kin et al., 1992)		16.4	1.4	2.3	5.1	3.7	4.2	0.1 ¹	0.5 [*]	0.0	0.0	0.0	0.0	35.1	
Riverside, CA (Chow et al., 1992c)	1988	32.6	0.0	7.0	0.0	4.8	21.4	0.3 ¹	1.3 [*]	1.1 [*]	0.0	0.0	0.0	64.0	
Rubidoux, CA (Gray et al., 1988)	1986	43.1	4.0 ¹	5.6 ¹	0.0	6.4	21.3	0.3 ¹	1.0 [*]	5.9 ¹	0.0	0.0	0.0	87.4	
Rubidoux, CA (Summer) (Watson et al., 1994)	Summer 1987	34.9	4.5	17.3	0.0	9.5	27.4	0.0 ¹	5.1 [*]	0.0	0.0	0.0	0.0	114.8	
Rubidoux, CA (Fall) (Watson et al., 1994)	Fall 1987	19.2	16.1	30.3	0.0	2.1	31.6	0.0 ¹	1.1 [*]	0.0	0.0	0.0	0.0	112.0	
Rubidoux, CA (Chow et al., 1992c)	1988	48.0	0.0	10.2	0.0	5.3	21.7	0.4 ¹	1.5 [*]	5.7 [*]	0.0	0.0	0.0	87.0	
San Nicolas Island, CA (Summer) (Watson et al., 1994)	Summer 1987	1.6	0.0	0.9	0.0	3.7	0.5	0.0 ¹	4.3 ¹	0.0	0.0	0.0	0.0	17.4	

Table 3.2 Receptor Model Source Contributions to PM-10 (continued).

Sampling Site	Time Period	$\mu\text{g}/\text{m}^3$										Measured PM-10 Concentration
		Primary Geological	Primary Construction	Primary Motor Vehicle Exhaust	Primary Vegetative Burning	Secondary Ammonium Sulfate	Secondary Ammonium Nitrate	Misc. Source 1	Misc. Source 2	Misc. Source 3	Misc. Source 4	
Stockton, CA (Chow et al., 1992b)	1989	34.4	0.5	5.2	4.8	3.1	7.0	0.7 ^m	1.8 ⁿ	0.0 ^t	0.0	62.4
Upland, CA (Gray et al., 1988)	1986	25.4	0.4 ^l	4.1 ^l	0.0	6.4	14.5	0.6 ^l	7.8 ^l	0.0	58.0	
Telluride 1, CO (Central) (Dresser and Baird, 1988)	Winter 1986	32.0	0.0	0.0	98.7	0.0	-	61.3 ^p	0.0	0.0	208.0	
Telluride 2, CO (Society Turn) (Dresser and Baird, 1988)	Winter 1986	12.1	0.0	0.0	7.3	0.0	-	7.3 ^p	0.0	0.0	27.0	
Pocatiello, ID (Houck et al., 1992)	1990	8.3	7.5 ^q	0.1	0.0	0.0	0.0	0.0	0.0	84.1 ^r	100.0	
S. Chicago, IL (Hopke et al., 1988)	1986	27.2	2.4	2.8	0.0	15.4 ^l	-	15.1 ^l	2.2 ^l	0.0	80.1	
S.E. Chicago, IL (Vermette et al., 1992)	1988	14.7 ^l	0.0	0.9 ^l	0.0	7.7	-	0.8 ^l	0.3 ^l	1.1 ^m	41.0	
Reno, NV (Non-sweeping) (Chow et al., 1990)	Winter 1987	9.7	0.0	8.7	0.1	0.6	0.2	0.0	0.0	0.0	20.4	
Reno, NV (Sweeping) (Chow et al., 1990)	Winter 1987	11.8	0.0	11.0	1.2	0.8	0.2	0.0	0.0	0.0	24.9	
Reno, NV (Chow et al., 1988)	1986-1987	14.9	0.0	10.0	1.9	1.3	0.6	0.0	0.0	0.0	30.0	
Sparks, NV (Chow et al., 1988)	1986-1987	15.1	0.0	11.6	13.4	2.7	0.9	0.0	0.0	0.2 ^l	41.0	
Verdi, NV (Chow et al., 1988)	1986-1987	7.8	0.0	4.0	1.1	0.9	0.1	0.0	0.0	0.0	15.0	
Follansbee, OH (Skidmore et al., 1992)	1991	10.0	0.0	35.0	0.0	16.0	-	9.3 ^l	0.0	0.0	66.0	
Mingo, OH (Skidmore et al., 1992)	1991	12.0	0.0	14.0	4.1	15.0	-	3.4 ^l	11.0 ^l	0.0	60.0	
Sewage Plant, OH (Skidmore et al., 1992)	1991	22.0	0.0	12.0	0.0	13.0	-	6.6 ^l	8.7 ^l	0.0	62.0	
Steubenville, OH (Skidmore et al., 1992)	1991	8.3	0.0	14.0	0.8	14.0	-	3.8 ^l	5.0 ^l	0.0	46.0	
WTOV Tower, OH (Skidmore et al., 1992)	1991	7.4	0.0	16.0	0.2	15.0	-	3.4 ^l	7.9 ^l	0.0	49.0	

^lSmelter background aerosol.

^mCement plant sources, including kiln stacks, gypsum pile, and kiln area.

ⁿCopper ore.

^oCopper tailings.

^pCopper smelter building.

^qHeavy-duty diesel exhaust emission.

^rBackground aerosol.

^sMarine aerosol, road salt, and sea salt plus sodium nitrate.

^tMotor vehicle exhaust from diesel and leaded gasoline.

^uResidual oil combustion.

^vSecondary organic carbon.

^wBiomass burning.

^xPrimary crude oil.

^yNaCl + NaNO₃.

^zLime.

^{aa}Road sanding material.

^{ab}Asphalt industry.

^{ac}Phosphorus/phosphate industry.

^{ad}Regional sulfate.

^{ae}Steel mills.

^{af}Refuse incinerator.

^{ag}Local road dust, coal yard road dust, steel haul road dust.

^{ah}Incineration.

^{ai}Unexplained mass.

Appendix B

Available Receptor Modeling Methods for PM

(Seigneur et al., 1997)



Table T-9. Summary of the Receptor Modeling Methods that are Available for PM Source Identification and Apportionment.

Model	EPA Model Available	Requires Source Information	Quantitative Apportionment	Source Location Information	Apportions Secondary Aerosol	Other Advantages	Other Disadvantages
Chemical Mass Balance (least-squares) (CMB)	yes	yes	yes propagation	no	no	Easy to use, includes errors in source compositions, accepted by OAQPS	Can misspecify sources; does not include variability in source compositions; Sensitive to collinearity
Partial Least Squares	no	yes	yes	no	no	Identifies completeness of source profile set	Requires specialized software
Artificial Neural Networks (Backpropagation)	no	yes	yes	no	no	Least sensitive to collinearity	Requires specialized software; can be time consuming
Genetic Algorithm	no	no	no	no	yes	uncertain	Requires specialized software; can be time consuming
Principal Components Analysis (PCA)	no	no	no	no	no	Easy to use, identification of source types; identification of unusual samples, recognized by OAQPS	Depends on correlation that can be driven by meteorology or collocation
Absolute Principal Components Analysis	no	no	yes	no	no	Estimates source profiles and contributions;	Propagates error in centering and uncentering of data; assumes that all sources have been identified
Target Transformation Factor Analysis	no	no	yes	no	no	Does not center; estimates uncertainties	Assumes that all sources have been identified

Table T-9. Summary of the Receptor Modeling Methods that are Available for PM Source Identification and Apportionment (continued).

Model	EPA Model Available	Requires Source Information	Quantitative Apportionment	Source Location Information	Apportions Secondary Aerosol	Other Advantages	Other Disadvantages
SAFER	no	no	yes	no	no	Includes external constraints and other information	Assumes that all sources have been identified
Positive Matrix Factorization	no	no	yes	no	sometimes	Treats missing and detection limit data well; estimates uncertainties	Assumes that all sources have been identified; for secondary apportionment, requires correlation with other species (black carbon, MSA, etc.)
Artificial Neural Networks (Kohonen)	no	no	Can lead to one	yes	uncertain	Provides a map that can be related to geographical distribution of sources	Better if multiple source locations; need at least 35 samples per site; time consuming
Empirical Orthogonal Function Analysis	no	no	sometimes	yes	yes	Easy to use, can estimate source contributions.	Requires sufficiently large spatial extent in sampling sites.
Residence Time Analysis	no	no	no	yes	yes	Provides likely source areas	Needs sufficient nos. of samples
Area of Influence Analysis	no	no	no	yes	yes	Provides likely source areas	Needs sufficient nos. of samples

Table T-9. Summary of the Receptor Modeling Methods that are Available for PM Source Identification and Apportionment (continued).

Model	EPA Model Available	Requires Source Information	Quantitative Apportionment	Source Location Information	Apportions Secondary Aerosol	Other Advantages	Other Disadvantages
Quantitative Trajectory Bias Analysis	no	no	yes	yes	yes	Incorporates wet and dry deposition; combines measurements from multiple sites	Requires detailed information of precipitation along trajectory
Potential Source Contribution Function	no	no	no	yes	yes	Provides likely source areas	Needs sufficient nos. of samples
PSCF with Apportionment	no	yes	yes	yes	yes	Provides likely source areas	Needs sufficient nos. of samples; depends on quality of emissions inventory
Residence Time Weighted Concentration	no	no	Possibly	yes	yes	Provides likely source areas and estimates of their relative contributions	Needs sufficient nos. of samples

Table T-10. Summary of the Receptor Modeling Methods, Data Requirements, and Software to Implement Them

Model	Information Required		Other Data Requirements	Software Availability	Ease of Use
	Source Profiles	# of Ambient Samples			
Chemical Mass Balance	Yes	≥ 1	None	EPA TTN2000 WWW Site	Easy
Partial Least Squares	Yes	≥ 1	None	SCAN ¹ , UnScrambler ² , SIMCA ³	Moderate
Artificial Neural Networks (Backpropagation)	Yes	≥ 1	None	MATLAB ⁴	Difficult
Genetic Algorithm	Yes	≥ 1	None	MATLAB	Difficult
Simulated Annealing	Yes	≥ 1	None	MATLAB	Difficult
Artificial Neural Networks (Kohonen)	No	≥ 30 to 40; more is better	None	Anonymous FTP at sun.mes.clarkson.edu;/pub /topkepk	Moderate to Difficult
Principal Components Analysis	No	≥ 30 to 40; more is better	None	Most standard statistical packages	Moderate
Absolute Principal Components Analysis	No	≥ 30 to 40; more is better	Total sample mass	Most standard statistical packages	Moderate

Table T-10. Summary of the Receptor Modeling Methods, Data Requirements, and Software to Implement Them
(continued)

Model	Information Required		Other Data Requirements	Software Availability	Ease of Use
	Source Profiles	# of Ambient Samples			
Target Transformation Factor Analysis	No	≥ 30 to 40; more is better	Total sample mass	Available from P.K. Hopke	Difficult
SAFER	No	≥ 30 to 40; more is better	Total sample mass; any other elemental relationships	Available from R.C. Henry	Difficult
Positive Matrix Factorization	No	≥ 30 to 40; more is better	Total sample mass; estimates of uncertainty for each datum point	Available from Pentti Paatero	Difficult
Empirical Orthogonal Function Analysis	No	Multiple sites; ≥ 30 samples per site	None	Most standard statistical packages	Easy
RMAPS (SAFER)	No	Multiple sites; ≥ 30 samples per site	Any other spatial relationships	Available from R.C. Henry	Difficult
Residence Time Analysis	No	≥ 40	Back trajectories *	No directly available software	Easy if trajectories are available

Table T-10. Summary of the Receptor Modeling Methods, Data Requirements, and Software to Implement Them (continued)

Model	Information Required		Other Data Requirements	Software Availability	Ease of Use
	Source Profiles	# of Ambient Samples			
Quantitative Trajectory Bias Analysis	No	≥ 20, better with multiple site data	Back trajectories, precipitation data along path of back trajectory	No directly available software	Difficult
Area of Influence Analysis	No	≥ 35	Back trajectories	No directly available software	Easy if trajectories are available
Potential Source Contribution Function	No	≥ 35	Back trajectories	No directly available software	Easy if trajectories are available
PSCF with Apportionment	Yes; gridded emission inventory	≥ 35	Back trajectories	No directly available software	Easy if trajectories are available
Residence Time Weighted Concentration	No	≥ 35	Back trajectories	No directly available software	Easy if trajectories are available
¹ Commercial program available from Minitab, Inc.					
² Commercial program available from Camo USA					
³ Commercial program available from Umetrics, Inc.					
⁴ Commercial program available from The Math Works, Inc.					

