Air Quality Management through Receptor Modelling

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Abstract

Background: One of the major risk factors to human health is air pollution. It contains a complex mixture of gaseous and particulate pollutants which possesses dynamic properties due to the combination of anthropogenic activities and meteorological conditions. The precise characteristics of the ambient air pollutants in a given locale depend on the source origin, which in-turn is a function of economic, social and technological factors. Hence it is very essential to identify the source origins. Methods: Receptor models have been widely used in source identification and their contribution of Airborne Particulate Matter (APM). Chemical Mass Balance model (CMB) is one among them. This paper presents a critical brief reappraisal of the source apportionment of APM through CMB model. Findings: The review shows that CMB model have been frequently used and proved to be an important tool in source apportionment studies without any pre requisite of source and meteorological data sets. Applications: Source apportionment through CMB model is one among the way to control and manage the PM$\text{10}$ and PM$\text{2.5}$ emissions in an informed way.

Keywords: Air Quality, CMB Model, Management, Particulate Matter, Receptor Modelling, Source Apportionment

1. Introduction

Air Quality Management (AQM) is defined as the regulation of source emissions in the ambient air in order to achieve specified National Ambient Air Quality Standards (NAAQS). Thus the following key factors should be given more importance to develop an effective Air Quality Management Strategy (AQMS) for non-attainment areas (i) source identification; (ii) assessment of source emissions; (iii) prioritization of source emissions; (iv) evaluation of various options in source emission control; and (v) appropriate action plans. A well-structured AQMS must be an efficient tool that integrates a various data sets like, source density, emissions intensity, meteorology, geography and receptor informations. The source density of emission sources and their intensity of releases from individual sources are the most directly amenable to human managerial intervention. Hence, theory suggests that to improve air quality, one should first address the source density and emission intensity. Such a response needs the management of urban environment and the factors influencing its agglomeration.

This theoretical framework provides information which would enable local administrator to prepare appropriate strength for management of local air quality. Over the past few years, several government administrators, legislators and the general public have shown stark increase in interest in transgressing air quality. This forced the governing bodies to bring forward laws for protecting the environment from emission sources. Air (Prevention and Control of Pollution) Act, 1981, Environment (Protection) Act, 1988, the Motor Vehicles Act, 1988 and Central Motor Vehicle Rules, 1989 are the most important among them. Also implementation of NAAQS and emission standards were made to control air pollution in India. However, fast urbanization, lack in effective public transport system and traffic congestion led decline of local ambient air quality, predominantly near traffic intersections and at busy urban centers.
Presently the air quality and emissions policies/regulations are mainly based on the measured mass of fine PM (PM$_{2.5}$) and coarse PM (PM$_{10}$) concentrations. The study of particle concentrations exposure to the receptor is important to elucidate the APM sources and the mechanisms associated with their formation$^5$. Without source apportionment it is not possible to control the emissions in an informed way$^6$. Hence in this paper, we present a critical brief reappraisal of the source apportionment of APM through receptor model viz. Chemical Mass Balance (CMB) model.

2. Source Apportionment of PM

APM generated with different source origins has different physicochemical characteristics, which may, in turn, result in different health effects. Thus, the identification and quantification of source emissions is very important in order to establish the relationship between APM exposures of specific sources to its health outcomes. Source apportionment techniques were extensively used for this purpose. In general, the techniques were used to quantify the source contribution of each origin to APM concentrations based on its physicochemical characteristics and their temporal co-variation. This can be done by first by identification of the source origins and then by apportioning the measured APM to these sources. Emission inventories, source and receptor models are the three main approaches to achieve the above said tasks$^7$. Many studies reported on source apportionment of urban sites using dispersion models$^{8,9}$. However, receptor models are the one which have widely used in many of the source apportionment studies and hence, receptor models are the prime emphasis of this review.

3. Receptor Models

Receptor models represent the statistical evaluation of ambient measurements at different times and locations. Hence it forms a subcategory of apportionment techniques and apportions the species based on the measured data and the knowledge on sources compositions$^{10}$. These models are highly used where emissions inventories are absent$^{11}$. Many of these models not require a presupposed knowledge on source-composition. Receptor models also include the models that use both gaseous and APM data's. Recently, these models have been accepted as one of the main tool in the development of effective and efficient AQM plans$^{12,13}$.

Receptor models are broadly classified into two; microscopic models and chemical models. In microscopic methods the analysis of morphological features of APM$^{14}$ were done using optical microscope, Scanning Electron Microscope (SEM) and automated SEM analyses. Most cases the results are not quantitative and hence it’s not feasible for large-scale use. On the other hand, the chemical methods use APM chemical composition in identification and apportionment of each source origins of APM.

Various techniques have been used for source apportionment of APM$^6$. Presupposed knowledge on each of the sources and their corresponding profiles determines the selection of the appropriate technique. CMB analysis, enrichment Factor Analysis (FA), times series analysis, multivariate factor analysis species series analysis and Multilinear Engine (ME) analysis are the major techniques used in this category.$^{14,15}$ These methods employ the elemental concentration of heavy metals, concentration of elemental and organic carbon and concentration of ionic species for the identification of sources. APM is a complex mixture of species (both inorganic and organic), a wide range of indicator species were used. Perhaps the most subjective and the least quantitative aspect of the entire modeling process is the interpretation of factors predicted by receptor models. For selection of their source origins, researchers are forced to search vast libraries of APM source composition similar to those in their source factors. Receptor model’s never guarantees a single source type. Therefore, identification and quantization of organic molecular markers for source apportionment is turning into a promising field of research in recent years.$^{16,17}$

4. Chemical Mass Balance Model

CMB was first proposed$^{18-20}$ for both identification and quantification of source contributions at receptor concentrations. This model is robust and relatively easy to apply$^{21,22}$ and based on the mass conservation of individual chemical species or markers viz. organic compounds, elements and ions. These concentrations and compositions at “receptor” were expressed in linear sum of products of source profile abundances and their contributions. The proportions must be different for each of the source emissions and changes between source and receptor proportions are negligible or can be approximated$^{21}$.
Presently for CMB analysis U.S.EPA-CMB version 8.2 Model\textsuperscript{22} is used globally for source identification at receptors. The measured data is apportioned to source profiles using effective variance least squares algorithm. The concentration of species \( i \) at a receptor site \( k \), \( C_{ik} \), can be expressed as in equation (1):

\[
C_k = \sum_{j=1}^{m} a_{ij} s_{jk} \quad i = 1,2,\ldots I \quad \ldots. (1)
\]

where, \( a_{ij} \) is the relative concentration of species \( i \) from source \( j \), and \( s_{jk} \) is the contribution of source \( j \) to receptor site \( k \). The model solves for source contributions \( s_{jk} \) from predicted concentrations \( C_{ik} \) at receptor site \( k \). For a unique solution the number of sources (\( m \)) must be lesser than or equal to the number of species (\( I \)).

The following assumptions were made to formulate the CMB model:\textsuperscript{11}

(i) During sampling the composition of source emission were constant.
(ii) Species are conservative.
(iii) Potential sources have been identified and characterized.
(iv) Source profiles are linearly independent of each other.
(v) Number of species is greater than or equal to the number of sources.
(vi) Uncertainties are random, uncorrelated and normally distributed.

4.1 Methodological Framework
The study should be planned in advance according to the objectives of the study, available resources, data collection methods, instruments, model and software to be used, extraction and analytical methods, input source emission data and availability of local source profiles. The steps can be followed to obtain proper source contributions from CMB model are (i) identification source contributions and species; (ii) selection of sources and species; (iii) estimation of the fraction of species in all source profiles; (iv) uncertainty estimation in both ambient and source profiles; and finally, (v) solution in terms of source contribution to the CMB equations\textsuperscript{24}.

Selection of indicator species and source profile is the important step in CMB model. Indicator species refers to the mixer of elements and ions used for the source identification. A number of case scenarios have to be investigated using previous source apportionment studies conducted at the study site or similar sites to find the right species for the right sources. Examining diagnostic ratios between species can help to eliminate outlier profiles. By understanding the trends and relationships among species that would impact CMB analysis through preliminary data analysis also helps for this purpose\textsuperscript{7}.

4.2 CMB Analysis and Validation
After selecting each sources or several or composite profiles based on the specificity of the study area and the markers at the receptor the U.S.EPA CMB model of version 8.2 is usually run repeatedly\textsuperscript{23}. Best combinations can be selected based on the quality of the CMB solutions. Also the sensitivity of the results to the choice of the source profiles and the related uncertainties can be assessed.

Performance of CMB analysis usually evaluated by six parameters (i) \( T \) statistics (ratio of source contribution to standard error and this value should be >2.0); (ii) \( R^2 \) (fraction of the variance between measured and species concentrations should be between 0 to 1); (iii) correlation coefficient (>0.6); (iv) \( \chi^2 \) (weighed sum of squares of differences between estimated and measured fitting markers and should be < 4); (v) % mass (predicted/measured mass concentration percent value and it should be between 80–120%) and (vi) \( R/U \) ratio (ratio of residual to uncertainty and should be < 2)\textsuperscript{23}.

4.3 Source Apportionment using CMB Model
CMB model have been widely used in source apportionment of PM\textsubscript{2.5} and PM\textsubscript{10} concentrations measured across the globe. Table 1 summarizes the source apportionment studies conducted at various parts of the world using CMB model in the past decade. There are several differences between the sources estimated. The differences reflect the nature of the source origin which are important in production of the fine and coarse PM. Further limited studies were alone examined the spatial variability of source contributions at different sites within an urban area by using CMB model.

5. Conclusions
Management and safeguard of ambient air quality assumes priori knowledge of the state of the environment.
<table>
<thead>
<tr>
<th>Location</th>
<th>PM</th>
<th>Species</th>
<th>Sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>Santa Barbara, CA, USA</td>
<td>PM$_{10}$</td>
<td>OC, EC, Elements and Ions</td>
<td>Marine = 18-23%; Dust =25-27%; Vehicles =30-42%</td>
</tr>
<tr>
<td>Cairo, Egypt</td>
<td>PM$<em>{10}$ and PM$</em>{2.5}$</td>
<td>OC, EC, Elements and Ions</td>
<td>PM$_{10}$: Dust = 36%; Burning = 15%; NH$<em>4$Cl = 14%; Diesel = 11%; Secondary = 10%; PM$</em>{2.5}$: NH$_4$Cl = 30%; Diesel = 23%; Burning = 17%; Secondary = 17%</td>
</tr>
<tr>
<td>Thessaloniki, Greece</td>
<td>PM$_{10}$</td>
<td>Organic compounds, Elements and Ions</td>
<td>TC: Geological sources = 11-22%; Fuel oil emissions = 35–70%; Vehicle exhaust = 40–99%; Elements: Industrial Sources = 1-51%; Geological sources = 6-10%; Vehicle exhaust = 1–4%; Ions: Industrial Sources = 1-87%; Geological sources = 2-4%; Vehicle exhaust = 5-9%;</td>
</tr>
<tr>
<td>Mira Loma, California</td>
<td>PM$_{2.5}$</td>
<td>OC, EC, Elements and Ions</td>
<td>Secondary nitrate = 41%; Secondary sulphate = 9%; Soil related = 13%; Gasoline vehicles = 5%; Diesel vehicles =5%; Biomass burning = 1%; Other organics = 13%; Other species = 13%</td>
</tr>
<tr>
<td>Beijing, China</td>
<td>PM$_{2.5}$</td>
<td>Organic compounds, Elements, OC, EC</td>
<td>Dust = 20%; Secondary SO$_4$ = 17%; Secondary NO$_3$ = 10%; Combustion = 7%; Vehicles = 7%; Secondary NH$_4$Cl = 30%; Diesel = 23%; Burning = 17%; Secondary = 17%; Vegetative detritus = 1%</td>
</tr>
<tr>
<td>Seoul, Korea</td>
<td>PM$_{2.5}$</td>
<td>Elements and Ions</td>
<td>Secondary SO$_4$ = 23%; Secondary NO$_3$ = 16%; Incineration = 15%; Soil = 13%; Burning = 4%; Combustion = 2.7%, Marine = 1.3%.</td>
</tr>
<tr>
<td>Northern China</td>
<td>PM$_{10}$</td>
<td>TC, EC, Elements and Ions</td>
<td>Soil dust = 10%; Cement = 7%; Coal fly ash = 20%; Vehicular exhaust = 10%; Sulphate = 7%; Nitrate = 2%</td>
</tr>
<tr>
<td>New Delhi, India</td>
<td>Coarse and Fine</td>
<td>Elements</td>
<td>Coarse: Crustal re-suspension = 50.6%; Building material = 13%; Fine: Crustal re-suspension = 44%; Building material = 15%; Vehicular emissions = 11%</td>
</tr>
<tr>
<td>Kolkata, India</td>
<td>TSP and PM$_{10}$</td>
<td>TC, OC, Elements and Ions</td>
<td>TSP: Combustion = 37%; Soil = 19%; Diesel = 15%; Dust = 17%; Other = 12%; PM$_{10}$: Combustion = 37%; Soil = 19%; Diesel = 15%; Dust = 17%; Other = 12%</td>
</tr>
<tr>
<td>New Delhi, India</td>
<td>Coarse and Fine</td>
<td>Elements</td>
<td>Coarse: Crustal dust = 64%; Vehicular emissions = 29%; Fine: Crustal dust = 35%; Vehicular emissions = 62%</td>
</tr>
<tr>
<td>Castello, Spain</td>
<td>PM$_{10}$</td>
<td>OC, EC, Elements and Ions</td>
<td>Clay = 41%; Industrial 1 = 4%; Industrial 2 = 2%; Vehicular = 13%; Regional =18%; Marine = 3%; Soil = 12%; Undetermined = 7%</td>
</tr>
<tr>
<td>Hyderabad, India</td>
<td>PM$<em>{10}$ and PM$</em>{2.5}$</td>
<td>Elements</td>
<td>PM$<em>{10}$: Dust = 40%; Vehicles = 22%; Combustion = 12%; Industrial = 9%; Burning = 7%; Other = 10%; PM$</em>{2.5}$: Dust = 26%; Vehicles = 31%; Combustion = 9%; Industrial = 7%; Burning = 6%; Other = 21%</td>
</tr>
<tr>
<td>Chennai, India</td>
<td>PM$<em>{10}$ and PM$</em>{2.5}$</td>
<td>Elements and Ions</td>
<td>PM$<em>{10}$: Vehicles -Diesel = 52%; Vehicles -Gasoline 16%; Paved road dust = 2.3%; Cooking = 1.5%; Others = trace quantities; PM$</em>{2.5}$: Vehicles -Diesel = 65%; Vehicles -Gasoline 8%; Paved road dust = 2.3%; Cooking = 1.5%; Others = trace quantities;</td>
</tr>
<tr>
<td>Shanghai, China</td>
<td>PM$_{2.5}$</td>
<td>OM, EC, and Ions</td>
<td>Industrial coal = 11%; Residential gas = 4%; Residential biomass = 11%; Steel manufacture = 1%; Open biomass burning = 5%; Secondary sulfate = 25%; Secondary nitrate = 33%; Dust = 2%.</td>
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It involves both cognitive and interpretative aspects. AQM requires tools that are able to extrapolate the field data both temporally and spatially. Environmental conservation and preservation can only be obtained by systematic planning of emission reduction either through mathematical or by receptor models which are capable of linking the emission source origins to the concentrations at receptor. There exist innumerable and diverse models that may be utilized for the aforementioned purposes. Source apportionment through receptor models is one among the way to control the emissions in an informed way. This paper presents a critical brief reappraisal of concept, theory and application of the source apportionment of APM through CMB. The study also showed that the CMB model have been frequently used and proved to be a most useful tool in source identification and their contribution in APM composition without any prerequisite of source and meteorological data sets.

6. References

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