

Air Quality Management through Receptor Modelling

B. Srimuruganandam* and Jithin Jose

School of Civil and Chemical Engineering, VIT-University, Vellore-632014, Tamil Nadu, India;
bsrimuruganandam@vit.ac.in, pauljithinjose@gmail.com

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_{10} and $PM_{2.5}$ 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 plans¹. A well-structured AQMS must be an efficient tool that integrates a various data sets like, source density, emissions intensity, meteorology, geography and receptor informations². 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 agglomeration³.

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 India¹. 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 centers⁴.

*Author for correspondence

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 formation⁵. Without source apportionment it is not possible to control the emissions in an informed way⁶. 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 tasks⁷. 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 compositions¹⁰. These models are highly used where emissions inventories are absent¹¹. 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 APM¹⁴ 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 APM⁶. 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 proposed¹⁸⁻²⁰ 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 approximated¹¹.

Presently for CMB analysis U.S.EPA-CMB version 8.2 Model²³ 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):

$$C_k = \sum_{j=1}^m a_j .s_k \quad i = 1,2,\dots,I \quad \dots(1)$$

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 model¹¹:

- (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 equations²⁴.

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 purpose⁷.

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 repeatedly²³. 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) χ^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)²³.

4.3 Source Apportionment using CMB Model

CMB model have been widely used in source apportionment of $PM_{2.5}$ and PM_{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 1. PM source apportionment studies conducted using CMB model

Location	PM	Species	Sources
Santa Barbara, CA, USA ²²	PM ₁₀	OC, EC, Elements and Ions	Marine = 18-23%; Dust = 25-27%; Vehicles = 30-42%
Cairo, Egypt ²⁵	PM ₁₀ and PM _{2.5}	OC, EC, Elements and Ions	PM ₁₀ : Dust = 36%; Burning = 15%; NH ₄ Cl = 14%; Diesel = 11%; Secondary = 10%; PM _{2.5} : NH ₄ Cl = 30%; Diesel = 23%; Burning = 17%; Secondary = 17%
Thessaloniki, Greece ²⁶	PM ₁₀	Organic compounds, Elements and Ions	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%;
Mira Loma, California ²⁷	PM _{2.5}	OC, EC, Elements and Ions	Secondary nitrate = 41%; Secondary sulphate = 9%; Soil related = 13%; Gasoline vehicles = 5%; Diesel vehicles = 5%; Biomass burning = 1%; Other organics = 13%; Other species = 13%
Beijing, China ²⁸	PM _{2.5}	Organic compounds, Elements, OC, EC	Dust = 20%; Secondary SO ₄ = 17%; Secondary NO ₃ = 10%; Combustion = 7%; Vehicles = 7%; Secondary NH ₄ = 6%; Biomass = 6%; Cigarette smoke = 1%; Vegetative detritus = 1%
Seoul, Korea ²⁹	PM _{2.5}	Elements and Ions	Secondary SO ₄ = 23%; Secondary NO ₃ = 16%; Incineration = 15%; Soil = 13%; Burning = 4%; Combustion = 2.7%, Marine = 1.3%.
Northern China ³⁰	PM ₁₀	TC, EC, Elements and Ions	Soil dust = 10%; Cement = 7%; Coal fly ash = 20%; Vehicular exhaust = 10%; Sulphate = 7%; Nitrate = 2%
New Delhi, India ³¹	Coarse and Fine	Elements	Coarse: Crustal re-suspension = 50.6%; Building material = 13% ; Fine: Crustal re-suspension = 44%; Building material = 15%; Vehicular emissions = 11%
Kolkata, India ³²	TSP and PM ₁₀	TC, OC, Elements and Ions	TSP: Combustion = 37%; Soil = 19%; Diesel = 15%; Dust = 17%; Other = 12%; PM ₁₀ : Combustion = 37%; Soil = 19%; Diesel = 15%; Dust = 17%; Other = 12%
New Delhi, India ³³	Coarse and Fine	Elements	Coarse: Crustal dust = 64%; Vehicular emissions = 29%; Fine: Crustal dust = 35%; Vehicular emissions = 62%
Castello, Spain ³⁴	PM ₁₀	OC, EC, Elements and Ions	Clay = 41%; Industrial 1 = 4%; Industrial 2 = 2%; Vehicular = 13%; Regional = 18%; Marine = 3% ; Soil = 12%; Undetermined = 7%
Izmir, Turkey ³⁵	PM ₁₀ and PM _{2.5}	Elements	Traffic emissions = 80%; Fossil fuel burning = 5%; Mineral industries = 5%; Marine salt = 10%; Soil = 3%
Hyderabad, India ³⁶	PM ₁₀ and PM _{2.5}	Elements	PM ₁₀ : Dust = 40%; Vehicles = 22%; Combustion = 12%; Industrial = 9%; Burning = 7%; Other = 10%; PM _{2.5} : Dust = 26%; Vehicles = 31%; Combustion = 9%; Industrial = 7%; Burning = 6%; Other = 21%
Chennai, India ²⁴	PM ₁₀ and PM _{2.5}	Elements and Ions	PM ₁₀ : Vehicles -Diesel = 52%; Vehicles -Gasoline 16%; Paved road dust = 2.3%; Cooking = 1.5%; Others = trace quantities; PM _{2.5} : Vehicles -Diesel = 65%; Vehicles -Gasoline 8%; Paved road dust = 2.3%; Cooking = 1.5%; Others = trace quantities;
Shanghai, China ³⁷	PM _{2.5}	OM, EC, and Ions	Industrial coal = 11%; Residential gas = 4%; Residential biomass = 11%; Steel manufacture = 1%; Open biomass burning = 5%; Secondary sulfate = 25%; Secondary nitrate = 33%; Dust = 2%.

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

1. CPCB. Air quality monitoring, Emission inventory & source apportionment studies for Indian cities, Central Pollution Control Board, New Delhi; 2010.
2. Larssen S, Gronskel KE, Hanegraaf MC, Jansen H, Kuik OJ, Oosterhuis FH, Olsthoorn XA. Urban air quality management strategy in Asia-Guidebook. URBAIR. World Bank Publications; 1997.
3. Longhurst JWS, Elsom DM. A theoretical perspective on air quality management in the United Kingdom. Baldasano JM, Brebbia CA, Power H, Zannetti P, editors. Air pollution-II, Vol. 2, Computational Mechanics Inc. Southampton, Boston; 1997.
4. Nagendra SMS, Khare M. Principal component analysis of urban traffic characteristic and meteorological data. *Journal of Transportation Research*. 2003; 8:285-97.
5. U.S.EPA. Air quality criteria for particulate matter. Vol-1, 2 and 3. Research Triangle Park, NC; 2004.
6. Watson JG, Zhu T, Chow JC, Engelbrecht J, Fujita EM, Wilson WE. Receptor modeling application framework for particle source apportionment. *Chemosphere*. 2002; 49:1093-136.
7. Belis CA. European guide on air pollution source apportionment with receptor models joint research centre report EUR 26080 EN; 2014.
8. Colville RN, Gómez-Perales JE, Nieuwenhuijsen MJ. Use of dispersion modelling to assess road-user exposure to PM_{2.5} and its source apportionment. *Atmospheric Environment*. 2003; 37(20):2773-82.
9. Laupsa H, Denby B, Larssen S, Schaug J. Source apportionment of particulate matter (PM_{2.5}) in an urban area using dispersion, receptor and inverse modelling. *Atmospheric Environment*. 2009; 43(31):4733-44.
10. Henry RC, Lewis CW, Hopke PK, Williamson HJ. Review of receptor model fundamentals. *Atmospheric Environment*. 1984; 18:1507-15.
11. Hopke PK. Receptor modeling for air quality management. Amsterdam; 1991.
12. Lai CH, Chen KS, Ho YT, Peng YP, Chou Y. Receptor modeling of source contributions to atmospheric hydrocarbons in urban Kaohsiung, Taiwan. *Atmospheric Environment*. 2005; 39:4543-59.
13. Gu J, Pitz M, Schenlle-Kreis J, Diemer J, Reller A, Zimmermann R, Soentgen J, Stoelzel M, Wichmann HE, Peters A, Cyrus J. Source apportionment of ambient particles: comparison of positive matrix factorization analysis applied to particle size distribution and chemical composition data. *Atmospheric Environment*. 2011; 45:1849-57.
14. Cooper JA, Watson JG. Receptor oriented methods of air particulate source apportionment. *Journal of Air Pollution Control Association*. 1980; 30(10):1116-25.
15. Ramadan Z, Eickhout B, Song Xin-Hua, Buydens LMC, Hopke PK. Comparison of positive matrix factorization and multilinear engine for the source apportionment of particulate pollutants. *Chemometrics and Intelligent Laboratory Systems*. 2003; 66:15-28.
16. Harrison RM, Smith DJT, Luhana L. Source apportionment of atmospheric polycyclic aromatic hydrocarbons collected from an urban location in Birmingham, U.K. *Environmental Science and Technology*. 1996; 30:825-32.
17. Robinson AL, Subramanian R, Donahue NM, Bernardo-Bricker A, Rogge WF. Source apportionment of molecular markers and organic aerosol. *Environmental Science and Technology*. 2006; 40:7811-19.
18. Winchester JW, Nilfong GD. Water pollution in Lake Michigan by trace elements from aerosol fallout. *Water Air Soil Pollution*. 1971; 1:50-64
19. Hidy GM, Friedlander SK. The nature of Los Angeles aerosol. *Proceedings of 2nd IUAPPA Clean Air Congress*, Washington DC; 1972.
20. Kneip TJ, Kleinman MT, Eisenbud M. Relative contribution of emission sources to the total airborne particulates in New York city. *Proceedings of 3rd IUAPPA Clean Air Congress*; 1972.
21. Gordon GE. Receptor models. *Environmental Science and Technology*. 1980; 14:792-800.
22. Chow JC, Watson JG, Ono DM, Mathai CV. PM₁₀ standards and nontraditional particulate source controls: A summary of the A&WMA/EPA international specialty con-

- ference. *Journal of Air and Waste Management Association*. 1993; 43:74–84.
23. Coulter CT. EPA-CMB8.2-User's manual, Air Quality Modeling Group Emissions, Monitoring and Analysis Division Office of Air Quality Planning and Standards; Research Triangle Park, NC; 2004.
 24. Srimuruganandam B, Nagendra SMS. Source characterization of PM_{10} and $PM_{2.5}$ mass using a chemical mass balance model at urban roadside. *Science of the Total Environment*. 2012; 433:8–19.
 25. Abu-Allaban M, Gertler AW, Lowenthal DH. A preliminary apportionment of the sources of ambient PM_{10} , $PM_{2.5}$ and VOCs in Cairo. *Atmospheric Environment*. 2002; 36:5549–57.
 26. Samara C, Kouimtzi TH, Tsiouridou R, Kaniass G, Simeonov V. Chemical mass balance source apportionment of PM_{10} in an industrialized urban area of Northern Greece. *Atmospheric Environment*. 2003; 37:41–54.
 27. Sawant AA, Na K, Zhu X, Cocker DR. Chemical characterization of outdoor $PM_{2.5}$, gas-phase compounds in Mira Loma, California. *Atmospheric Environment*. 2004; 38:5517–28.
 28. Zheng M, Salmon LG, Schauer JJ, Zeng L, Kiang CS, Zhang Y, Cass GR. Seasonal trends in $PM_{2.5}$ source contributions in Beijing, China. *Atmospheric Environment*. 2005; 39:3967–76.
 29. Park SS, Kim YJ. Source contributions to fine particulate matter in an urban atmosphere. *Chemosphere*. 2005; 59:217–26.
 30. Bi X, Feng Y, Wu J, Wang Y, Zhu T. Source apportionment of PM_{10} in six cities of northern China. *Atmospheric Environment*. 2007; 41:903–12.
 31. Srivastava A, Jain K. Seasonal trends in coarse and fine particle sources in Delhi by the chemical mass balance receptor model. *Journal of Hazardous Materials*. 2007; 144:283–91.
 32. Gupta AK, Karar K, Srivastava A. Chemical mass balance source apportionment of PM_{10} and TSP in residential and industrial sites of an urban region of Kolkata, India. *Journal of Hazardous Materials*. 2007; 142:279–87.
 33. Srivastava A, Jain VK. Source apportionment of suspended particulate in a clean area of Delhi: a note. *Transportation Research, Part D*. 2008; 13:59–63.
 34. Viana M, Pandolfi M, Minguillon MC, Querol X, Alastuey A, Monfort E, Celades I. Inter-comparison of receptor models for PM source apportionment: Case study in an industrial area. *Atmospheric Environment*. 2008; 42:3820–32.
 35. Yatkin S, Bayram A. Source apportionment of PM_{10} and $PM_{2.5}$ using positive matrix factorization and chemical mass balance in Izmir, Turkey. *Science of the Total Environment*. 2008; 390:109–123.
 36. Gummeneni S, Yusup YB, Chavali M, Samadi SZ. Source apportionment of particulate matter in the ambient air of Hyderabad city, India. *Atmospheric Research*. 2011; 101(3):752–64.
 37. Hua Y, Cheng Z, Wang S, Jiang J, Chen D, Cai S, Fu X, Fu Q, Chen C, Xu B, Yu J. Characteristics and source apportionment of $PM_{2.5}$ during a fall heavy haze episode in the Yangtze River Delta of China. *Atmospheric Environment*; 2015 Dec; 123(B):380–91.