World Journal of Environmental Research

Volume 7, Issue 2, (2017) 52-60

www.wjer.eu

A review on top-down and bottom-up approach for air pollution studies

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Suggested Citation:

Abulude, F. O ., Bahloul, M., Olubayode, S. A. & Adeoya, E. A. (2017). A review on top-down and bottom-up approach for air pollution studies . *World Journal on Environ mental Research . 7*(2), 52-60.

Received Jun e 17, 2017; revised Septemb er 28, 2017; accepted Decemb er 28, 2017

Selection and peer review under responsibility of Prof. Dr. Haluk Soran, Near East University.

Abstract

It is a well-known fact that pollution is a global problem and must be holistically tackled. In doing this, adequate knowledge of the sources of pollution is important; therefore, the aim of this paper is to review source apportionment with reference to top-down and bottom-up methods. In this paper, dispersion modelling, emissions inventory and sampling methods are discussed. Also, analytical methods involved in top-down source apportionment are mentioned. The two techniques are needed to evaluate pollutants and their sources. Based on these two approaches, pollution control strategy is developed and decisions can be made on deciding the right approach to solve or reduce the pollution problems.

Keywords : PM_{10}, TSP, pollutants, element ma rkers, epidemiologi cal, dispersion modelling.

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1. Introduction

Air quality has gained a lot of attention in developing and developed countries of the world due to its impacts on man, animals and materials. These impacts depend on the pollutant type, its concentration in air, length of exposure, other pollutants in the air and individual susceptibility (Pope & Dockery, 2006). Epidemiological studies by the Health Effects Institute (2004) have shown that ambient particulate matter (PM) levels lead to an increased risk of mortality and morbidity.

PM is one of the problematic pollutants of concern in Europe and other continents (Harrison, Stedman & Derrent, 2008). The classification of the particles in the air is done by size and chemical composition, which are known as PM or aerosols. The different sizes of aerosols are as follows:

- Total Suspended Particulates (TSP, with aerodynamic diameter < ~30 microns (μm)).
- PM_{10} (with an aerodynamic diameter of less than 10μm also referred to as coarse).
- $PM_{2.5}$ (with an aerodynamic diameter of less than 2.5μm also referred to as fine).
- Ultrafine PM is that with a diameter of fewer than 0.1 μm.

Few of the particles could originate from volcanoes, dust storms, forest and grassland fires, living vegetation, sea spray and human activities like industrial emissions and land-use change (Guttikunda, 2008). The sizes of PM affect the atmospheric lifetime, spatial distributions, indoor–outdoor ratios, variability and wealth impacts of particles.

Aerosol in terms of mechanisms of emissions is classified as primary and secondary particles emitted directly from sources such as burning, road traffic, windblown soil, industrial activities, carbon, organic compounds, metal, and metal oxides and ions into the atmosphere, while secondary particles are through the chemical transformation of gaseous. Volatile organic compounds, sulphur dioxide (SO_2), ammonia (NH_3), nitrogen oxides (NOx) are the organic pollutants.

1.1. Composition and metal emission sources

According to Chow (1995), the following are the major compositions of PM mass:

- Geological matters (oxides of Al, Si, Ca, T, and Fe)
- Organic matter/carbon (OC – Consisting of hundreds of different compounds)
- Elemental Carbon (EC)
- Sulphates
- Nitrates
- Ammonium

Table 1. Degrada tion ra te *k* and conversion ra te of TiO_2 thin films deposi ted wi th di fferent dipping

Emission source	Ma rker elements
Soil	Al , Si , Sc, Ti, Fe, Sm, Ca
Road dus t	Ca , Al , Sc, Si , Ti , Fe, Sm
Sea salt	Na, Cl , Na^+, Cl^-, Br, I, Mg, Mg^{2+}
Oil burning	V, Ni , Mn, Fe, Cr, As , S, $SO4^{2-}$
Coal burning	Al , Sc, Se, Co, As , Ti, Th, S
Iron and steel indus tries	Mn, Cr, Fe, Zn, W, Rb
Non-ferrous metal industries	Zn, Cu, As , Sb, Pb, Al
Glass indus try	Sb, As Pb
Cement industry	Ca
Refuse incinera tion	K, Zn, Pb, Sb
Bi omass burning	K, C_{ele}, C_{org}, Br, Zn
Automobile gasoline	C_{ele}, Br, Ce, La , Pt, $SO4^{2-}$, NO_3^-
Secondary aerosol	SO_4^{2-}, NO_3^-, NH_4^+

Source: Guttikunda (2008). *Ma rker elements a re a rra nged by priori ty order.

In addition, liquid water absorbed by water-soluble species. Table 1 is source markers associated with various emission sources. Source markers are abundant in one source type but are minimally present in other source types. When a source has a chemical marker, it is easy to identify the dominant source, and receptor modelling helps to estimate the contribution of these sources based on factor analysis. Bellis et al. (2014) have categorized four main sources in Europe as:

(i) Traffic
(ii) Mineral/Crustal matter
(iii) Sea-salt, Sea-spray, and marine and
(iv) Regional-scale pollution and long-range transboundary anthropogenic pollution.

1.2. Apportionment of particulate pollution

In recent times, particulate pollution is being a big area of concern in the field of air pollution, and information is required on sources of pollution and their contribution to the ambient levels of pollution. To know how to reduce pollution in the environment, there is the need to conduct a source appointment study which will inform what the sources of pollution are and how much each source contributes to total pollution.

The two techniques (Figure 1) used to evaluate pollution sources are:

(i) Top-down or receptor-based modelling methods.
(ii) Bottom-up method or source-based modelling methods.

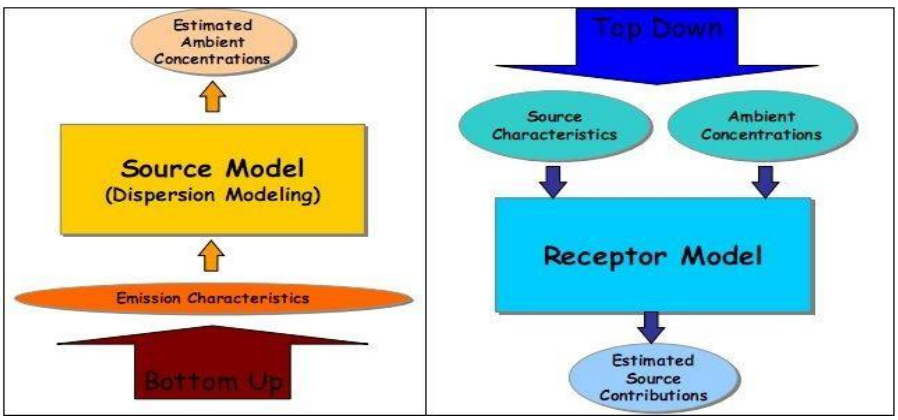

Figure 1. Bottom-up and top-down source apportionment [Source: Gu ttikunda (2011)]

1.3. Top-down modelling method

This method starts by monitoring the ambient pollution through the generation of data, thereafter utilizing models to relate measurements to specific sources of pollutants through chemical analysis of the samples. Top-down methods complement bottom-up methods. This method is applied for particulate pollution only. Figure 2 presents an outline of steps needed to use a source apportionment in a study area, especially urban area.

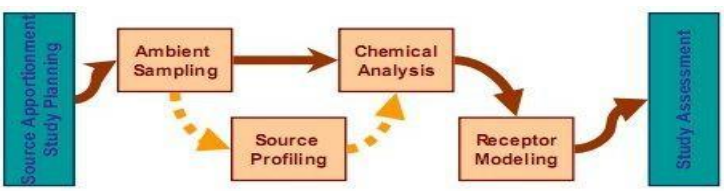

Figure 2. Top-down source apporti onment study [Source: Guttikunda (2011)]

Top-down analysis requires real-world measurement and knowledge of potential sources compared to bottom-up analysis which requires knowledge of source and source strengths as well as information on meteorology and local conditions.

1.4. Bottom-up modelling method

This modelling method utilizes sector–specific and technical emission factors in the construction of PM emission inventories. It must be noted that an accurate emission inventory is an important part of an air quality management system which can provide policymakers with reliable information on air pollution.

In air quality models, emission inventories are used as inputs which can be used to evaluate control strategies. It is paramount to quantify the accuracy and degree of representation of any inventory. There are no simple formulas when developing an emission inventory (Johnson et al., 2011).

Atmospheric models of dispersion, transport, and chemistry utilize information from emissions inventories to predict concentrations of air pollutants in the air. In doing so, it is necessary to resolve emission inventories in space and time and allocate emissions to specific locations. With this model, the PM pollution contributions from different sources can be quantified.

A bottom-up modeling method (Figure 3) quantifies pollution based on the distribution of pollution causing activities in a city. It is an important idea that if all cities establish an emission inventory baseline this would be useful for air pollution policy-related action plans (Guttikunda, 2011). A basic inventory can be developed using available information. According to Guttikunda (2011), various pollution-causing activities would be mapped out first, then each of the sources to quantify energy usage and emission would be zero.

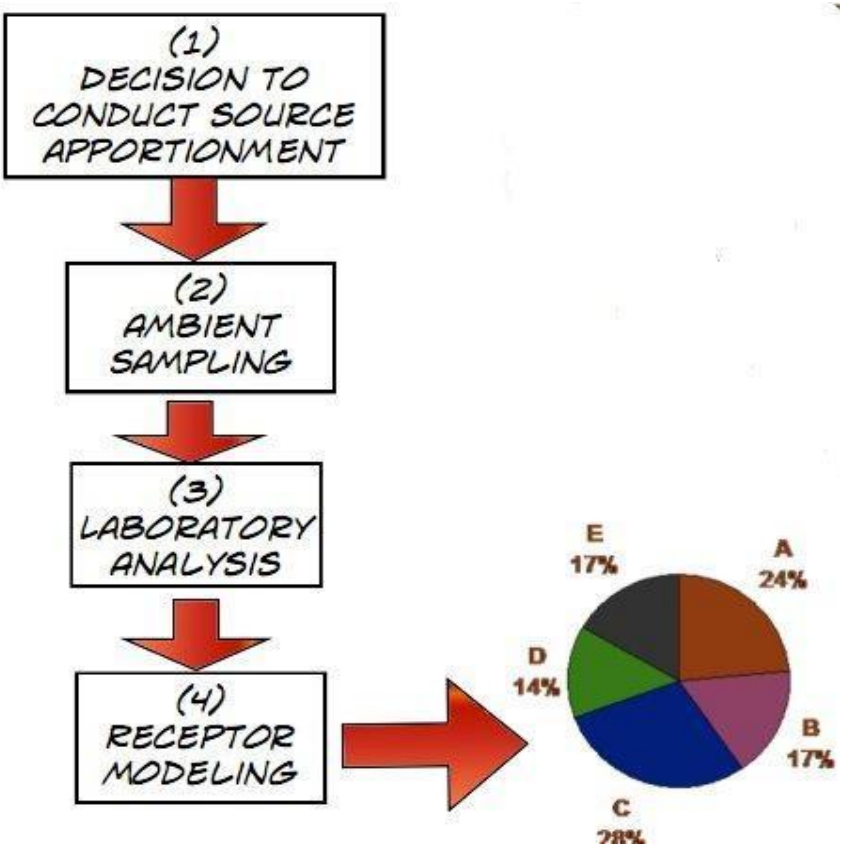

Figure 3. Bottom-up modeling meth od [Source: Guttikunda (2011)]

2. Emissions Inventory

An emission inventory is not directly utilized in a top-down analysis, which is essential for the quantification of source strengths and identification of source profile to assist in efficient and effective receptor modeling. Emission inventory will help in the determination of the area to locate receptors and also the determination of the area of possible hot spots.

To create emissions inventory, the activity data needed are the compilation of industrial energy consumption through audits and energy statistics, determine vehicle statistics from the transport census for vehicle miles traveled and also determine the domestic sector to obtain a sense of energy used at the household level. Later existing emission factors to calculate emissions by sector can then be used. At the end of gathering data input in energy used by sector, existing emission factor can then be used for the calculation.

$$\text{Emissions} = \text{Emission Factor} \times \text{Energy}$$

Emission factor unit of pollution released per unit of energy consumed.

If peradventure emission factor of the city is not available, the existing emission factor of the city from the literature can be employed in the calculation. The reason for this is that emission factors do not vary depending on the combustion technologies in use within the city. Figure 4 depicts the determination of an emissions inventory in a city.

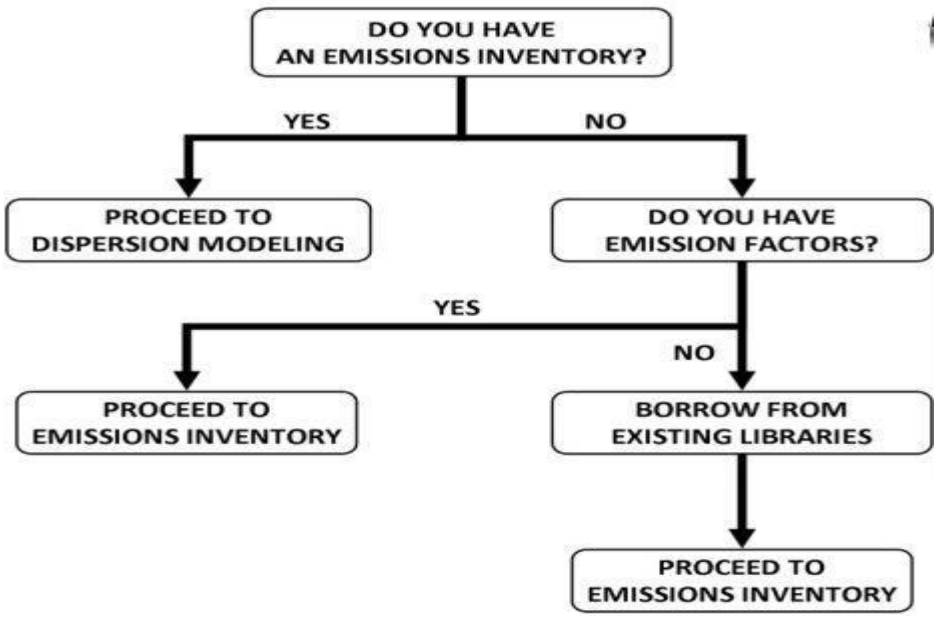

Figure 4. An emission inventory [Source: Guttikunda (2011)]

In emissions inventory, the particulate samples provide the contributions of various sources in percentage likewise the percentage contributions from the top-down method of analysis. The results obtained from the two methods are not alike, the results from emissions inventory provide the weight of pollution from various sources (mass/year), whereas the top-down methodology provides the source contributions to the ambient concentrations of mass per volume.

The results of emissions inventory and that of top-down study can be compared by converting the emissions into ambient concentration when a dispersion model is used.

It must be noted that the types of sources influence ambient concentrations. For example, a power plant releasing a lot of pollution contributions less to the immediate environment due to long-range

transport, while, for example, ground level emissions from vehicle exhaust, though a small percentage in the inventory has a disproportionately larger share in the local concentrating (Guttikunda, 2011).

2.1. Dispersion modelling

When using this dispersion model, it should be noted that physical and meteorological conditions have an important role to play. A pollutant emission rate and meteorological information are imputed to a mathematical model that disperses the emitted pollutant where the pollutants may also chemically transform, generating a prediction of the resulting pollutant concentration at a point in space and time (Chowdhury, Elizabeth, Cohen & Brauer, 2009). Topographical features and certain seasonal features can affect the air pollution concentrations, for example, in urban environments with the temperate and cold weather, there is the possibility to feel seasonality in their pollution patterns due to the increased fuel usage for their heating during the winter months.

2.2. Advantages of bottom-up methods

- Locating pollution sources through the development of emission inventories.
- It is useful for the identification of potential sources of primary emissions.
- It can describe the relevant physical properties that affect the ambient levels (terrain, meteorological features).
- It makes understanding the chemical processes that influence local pollutant levels including the formation of secondary aerosols easy.
- It assists in documenting the potential for secondary aerosol formation.
- It identifies sources that would be most effective in controlling and affecting the ambient compliance level the most.
- It allows a direct estimate of the effect of changes in emissions on ambient pollutant concentrations, through emission control simulations.

Provision of spatial coverage of how sources impact air quality and exposure (Johnson et al., 2011).

2.3. Reconciling results

Top-down results can be used to correct the missing sources in the emissions inventory sources.

The dispersion modeling results can assist to identify the pollution hot spots in the city, where sampling for the top-down approach can be performed (Owoade et al., 2016).

Monitoring of data can assist in validating the results of dispersion modeling can be further expanded for evaluation of ‘what if’ emission scenarios.

Altogether, both methods provide a strong resource for developing a pollution central strategy.

3. Ambient Sampling

Selection of sampling sites, suitable sampler and size range and a filter is paramount. These depend on the chemical analyses one has in mind. When selecting sites, the topography, number of samples to collected areas, meteorological instrument, space, accessibility, power and security should be taken into consideration.

The choice of selecting a sampler will depend on the size range of particles and the method of chemical analyses. Examples of aerosol samplers are Hi -volume, medium-volume, low-volume dichotomous sampler, mini-volume samplers. They have different descriptions, particle sizes (□m) and flow rates (1/mm) (Khan et al., 2015). Commonly used filters matrices are pure quartz, coated quartz and Teflon, nylon, polycarbonate glass fiber and cellulose esters (Bellis et al., 2014). According to Bellis

et al. (2014), only quartz fiber filters are suitable for the determination of irons, elements and carbonaceous fractions.

3.1. Source profiling

A source profile identifies the quantities of specific air pollutants (elements and ions) released from individual sources (Fawole, Olofinjana & Owoade, 2016). Likewise, it provides important data used for source apportionment as these determine the next level of assessment and provide the basis for estimating. The more accurate source profile is more likely that quality results will follow. A source profile is a key to linking samples with sources.

Source profiles are likely to contain a wide range of element, ions, carbon fractions, organic compounds, isotopic abundances, particle size distributions and shapes. A source has a marker to be able to identify the dominant source, while receptor modeling assists to quantify the contributions of these sources based on factor analysis (Morales Betancourt & Nenes, 2014).

Organic marker compounds have become more useful as many toxic elements formally used as markers are removed from emission sources (Pb from gasoline engine exhaust).

Table 2. Elements and possible sources [Source: Johnson et al. (2011)

Elements	Source ma rker
Al, Si, Ca, Ti, Mn	Soils, dus t
S	Fossil fuels , anthropogeni c and biomass burning, oceans , soil erosion
Cl	CFC's , soil, sea salt and anthropogenic sources
K	Coal combustion, biomass burning, biomass fuels
C	Fuel oil and s teel fa ctories
Cr	Emissions from chemi cal plants , cement dust and crus tal sources .
Fe	Soils, smel ting indus try
Ni	Hea vy fuel oil combus tion
Cu	Indus tries and waste trea tment
Zn	Combus tion of coal and hea vy fuel oil
As	Solid mineral fuels , hea vy fuel oil, vol canoes ,s melti ng industry
Se	Hea vy fuel oil and glass production
Br	Gasoline, transporta ti on indus try
Rb	Crus tal sources
Pb	Paint indus try, leaded fuel use

Table 3. Elements, conic and carbon source markers Chow (1995), Johnson et al. (2011), Reid et al. (2013)

Source type	Dominant pa rti cle size	<0.1%	0.1%–1%	1%–10%	>10%
Pa ved road	Coa rse (2.5–10 μm)	Cr, Sr, Pb, Zr	$S0_4^{2-}$, Na^+, K^+, P, S, Cl , Mn, Ba, Ti	Ec, Al , K, Ca , Fe	Oc, Si
Unpa ved road dust	Coa rse	NO^-_3, NH^+_4, P, Zn, Sr, Ba	SO^{2-}_4, Na^+, K^+, P, S, Cl , Mn, Ba, Ti	Oc, Al , K, Ca , Fe	Si
Cons truction	Coa rse	Cr, Mn, Zn, Sr, Ba	SO_4^{2-}, Na^+, K^+, S	Oc, Al , K, Ca , Fe	Si
Agri cul ture soil	Coa rse	NO_3^-, NH_4^+, Cr, Zn, Sr	SO_4^{2-}, Na^+, K^+, S, Cl, Mn, Ba , Ti	Oc, Al , K, Ca , Fe	Si
Na tural soil	Coa rse	Cr, Mn, Sr, Zn, Ba	Cl^-, Na^+, Ec, P, S, Cl, Ti	Oc, Al, Mg, K, Ca, Fe	Si
Lake bed	Coa rse	Mn, Sr, Ba	K^+, Ti	SO_4^{2-}, Na^+, Al, S, Cl, K, Ca , Oc, Se	Si

Motor vehicle	Fine (V-2.5 μm)	Cr, Ni Y, Sr, Ba	Si, Cl, Al, Si, P, Ca, Mn, Fe, Zn, Br, Pb	Cl , NO_3^-, SO_4^{2-}, NH_4^+, S	Oc, Ec
Vegetative burning	Fine	Ca, Mn, Fe, Zn, Br, Rb, Pb	NO_3^-, SO_4^{2-}, NH_4^+, Na^+, S	Cl^-, K^+, Cl , K	Oc, Ec
Residual oil combustion	Fine	K^+, Oc, Cl, Ti, Cr, Co, Cr, Se	NH_4+, Na^+, Zn, Fe, Si	V, Oc, Ec, Ni	S, SO_4^{2-}
Incinerator	Fine	V, Mn, Cu, Ag, Sn	K^+, Al , Ti , Zn, Hg	NO_3^-, Na^+, Ec, Si , S, Ca , Fe, Br, La , Pb	SO_4^{2-}, NH_4^+, Oc, Cl
Coal -fired boiler	Fine	Cl, Cr, Mn, Ga, As, Se, Br, Rb, Zr	NH_4^+, P, K, Ti, V, Ni, Zn, Sr, Ba, Pb	SO_4^{2-}, Oc, Ec, Al , S, Ca , Fe	Si
Oil fired power plant	Fine	V, Mn, Sb, Cr, Br, Ba	Al , Si , P, K, Zn	NH_4^+, Oc, Ec, Na, Ca, Pb	S, SO_4^{2-}
Smelters	Fine	V, Mn, Sb, Cr, Ti	Cd, Zn, Mg, Na , Ca , K, Se	Fe, Cu, As, Pb	S
Marine	Fine and coarse	Ti , V, Ni, Sr, Zr, Pb, Ag, Sn, Sb, Pb	Al, Si, K, Ca, Fe, Cu, Zn, Ba , La	NO_3^-, SO_4^{2-}, Oc, Ec	Cl^-, Na^+, Na, Cl

Of the source that emits primarily carbonaceous particles, then the use of organic compounds markers would be necessary. Table 4 depict the elements ions, carbon and possible sources.

3.2. Analytical technique for ambient and source samples

The common methods of analysis used in top-down source apportionment are shown in Table 4.

Table 4. Methods of analysis utilized in the top-down source apportionment [Source: Chow (1995) and Xu et al. (2013)

Parameters measured	Methods of analysis
Particle mass	Gravimetric analysis, β-gauge monitoring
Ions (F^-, Cl^- NO_2^-, PO_4^{3-} $BrSO_4^{2-}$ NO_3^-, K^+, NH_4^+)	Ion chromatography or automated colorimetric analysis .
Elements (Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, As, Se, Br, Rb, Y, Sr, Zr, Mo, Pd, Ag, Cd, In, Sn, Sb, Ba, La , Au, Hg, Ti , Pb, and U)	XRF, PIXE, INAA, ICP, Emission spectroscopy, AAS
Individual organic compounds	Solvent extraction method, gas chromatography-mass spectrometer (GC-MS), high performance liquid chromatography (HPLC).
Total carbon, elemental carbon, organic carbon, carbonate carbon, thermal carbon fractions	Thermal manganese oxidation method , thermal optical resistance of thermal optical transmission method
Total carbon	Thermal combustion method
Absorbance (lighta bsorbing carbon)	Optical absorption transmission densitometry, integrating plate or integrating sphere method

INAA: inductive neutron activation analysis; ICP: inductively coupled plasma; AAS: atomic absorption spectrophotometer; XRF: X-ray fluorescence; PIXE: proton induced X-ray emissions.

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