QUANTIFICATION OF AIR POLLUTION SOURCES

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RESUMO – Quantificação de Poluição do Ar –
A atividade industrial é uma das principais causas da poluição do ar urbano. Várias técnicas são utilizadas para monitorar e analisar os agentes poluidores. A técnica de modelamento de receptor é uma delas. A aplicação de programação linear para a quantificação de fontes poluidoras do ar, utilizando o modelamento de receptor, é apresentada neste artigo. O estudo de caso apresentado quantifica as importantes fontes industriais responsáveis pela poluição atmosférica da Região Metropolitana de Vitória, localizada na região sudeste do Brasil.
Palavras-chaves: Programação Linear, Poluição do Ar, Modelamento de Receptor

ABSTRACT – Industrial activity is one of the major causes of urban air pollution. Several techniques are utilized to monitor and analyze polluting agents. The receptor modeling technique is one of them. The application of linear programming to the quantification of air pollution sources using receptor modeling is reported here. It consists of the quantification of important industrial contributions to the pollution of the atmospheric aerosols in the Metropolitan Region of Vitória (MRV), a geographic region with nearly a million inhabitants, located in the Southeast part of Brazil.
Keywords: Linear programming, Air Pollution, Receptor Modeling

1 INTRODUCTION

Industrial activity is one of the major causes of urban air pollution. Several techniques are utilized to monitor and analyze polluting agents. The receptor modeling technique is one of them. It is well rooted as a principle underlying the development of strategies for air pollution control. It offers a certain degree of operational efficiency, by using a simple but efficient assumption: the mass conservation during the atmospheric dispersion of particulate materials. Based on this assumption, it is possible to characterize almost completely the effects of polluting agents (sources) over specific geographical regions (receptors).

The total mass measured at a receptor is composed of a mixture of all the individual sources' contributions. Assuming that the principle of mass conservation holds, the concentration of individual chemical species at a receptor is related through a linear combination of concentrations of the same chemical species found at sources. If concentrations of a sufficient number of chemical species at a particular receptor and at all important industrial and natural sources are known, then the individual sources' contributions to the total mass, found at the receptor, can be determined by solving a set of linear equations called a receptor model.

The application of Linear Programming (LP) to the identification of air pollution sources using receptor modeling is presented here as well as the solution of a case study. It consists of the identification of important industrial contributions to the pollution of the atmospheric aerosols in the Metropolitan Region of Vitória (MRV), a geographic region with nearly a million inhabitants located in the Southeast part of Brazil.

This paper is divided in 5 sections. Section 2 presents the receptor modeling technique. Section 3 provides a formulation for receptor modeling using LP. Section 4 describes the MRV pollution problem, the case study presented in this paper. Section 5 shows the results of a LP used for quantification of individual sources' contributions to the total particulate matter in atmosphere at 2 (two) receptors located in the MRV.

2 RECEPTOR MODELING

Urban aerosols are complicated systems composed of materials from many different sources. Quantitative source impact assessment determines the sources' contributions, either based on dispersion models or via receptor modeling (Cooper and Watson, 1980).

Source-dispersion and receptor-oriented models have a common physical rule: both assume that the mass arriving at a receptor (sampling site) from a source j was transported with mass conservation during the atmospheric dispersion. As noted by (Thurston and Lioy, 1987), it is hypothesized that, if p sources exist, and if there is no source emission interaction causing mass removal or accretion, then the total mass (M) measured at a receptor is the sum of all the individual sources' contributions

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(Ms_j):

$$M = \sum_{j=1}^{p} Ms_j \quad (1)$$

The total mass at the receptor (M) has in its composition a predetermined number of chemical species, each one with a quantity m_i given by a linear combination of all individual sources' contributions (Ms_j) possessing property i:

$$m_i = \sum_{j=1}^{p} f_{ij} Ms_j \quad (2)$$

f_{ij} is the fraction of the i^{th} chemical species in emission from the j^{th} source.

Dividing both sides of equation 2 by the total deposited mass M, we get:

$$c_i = \sum_{j=1}^{p} f_{ij} s_j \quad (3)$$

c_i is the concentration of the i^{th} chemical species found at the receptor and s_j is the contribution of the j^{th} source to the total mass in the receptor (M).

The matrix version of equation 3 is:

$$\mathbf{c} = \mathbf{F}\mathbf{s}, \;\; \mathbf{c} \in \mathbb{R}^n, \;\; \mathbf{s} \in \mathbb{R}^p, \;\; \mathbf{F} \in \mathbb{R}^{n \times p} \quad (4)$$

$\mathbf{c}$ is a vector with the concentrations of the n chemical species found at the receptor. $\mathbf{s}$ is a vector with all the individual sources' contributions to the mass of the receptor, and $\mathbf{F}$ is a matrix containing all the fractions of the chemical species emitted by the sources. Every column of the matrix $\mathbf{F}$ is a source profile; it describes the concentrations of the n chemical species found at a particular source.

Equation 4 is called a receptor model. In this simplified version, no fractionation of the concentrations of chemical elements from source to receptor is considered. It is assumed that all chemical species under consideration are lost or added in the atmosphere at a rate equal to that of the pollution mass as a whole. This simplification is valid only for short distances (e.g. within an urban space). There are also two other important concerns when using the receptor modeling technique:

1. all important sources of chemical species i must be included in the model. If one is not included, the other sources' contributions will be overestimated (Watson, 1979);
2. multicollinearities in the matrix $\mathbf{F}$ can greatly affect source contributions and should be avoided (Thurston and Lioy, 1987). If a source profile (a column of the matrix $\mathbf{F}$) is similar in nature to another (i.e. a strong tendency of linear dependence exists), it will be difficult to distinguish one from another, and their individual contributions may be biased in opposing directions, one being overestimated and the other underestimated.

If a particular receptor modeling problem complies with all these constraints, then it can easily be cast to a convex optimization problem and be efficiently solved.

Typically, matrix $\mathbf{F}$ and vector $\mathbf{c}$ are known and the objective is to estimate $\mathbf{s}$, in order to minimize the residual norm $\|\mathbf{F}\mathbf{s} - \mathbf{c}\|_g$. We use the notation

$$\begin{aligned} &\textit{minimize} \;\; \|\mathbf{F}\mathbf{s} - \mathbf{c}\|_g \\ &\textit{subject to} \;\; \mathbf{s} \in \mathbb{S} \end{aligned} \quad (5)$$

to describe a receptor modeling problem. $\mathbb{S}$ is a convex feasible set for $\mathbf{s}$ and it is introduced here to provide constraints to the solution of $\mathbf{s}$. For instance, the elements of $\mathbf{s}$ are the individual normalized mass contributions of each source to a specific receptor, and consequently, their sum must be equal to 1 (or 100 if expressed in percentage). Also, all the elements of $\mathbf{s}$ must be positive, since negative source contributions do not make any sense. Alternatively, depending on the problem, specific upper and lower bounds to each source contribution may also be included. All these constraints are represented by the feasible set $\mathbb{S}$.

3 LINEAR PROGRAMMING APPLIED TO RECEPTOR MODELING

The receptor modeling is a constrained norm minimization problem. This section provides a formulation for the receptor modeling problem using ℓ^1-norm residual.

Considering the receptor modeling problem defined in equation 5, for the ℓ^1-norm residual case, it can be rewritten as:

$$\begin{aligned} &\textit{minimize} \;\; \|\mathbf{F}\mathbf{s} - \mathbf{c}\|_1 \\ &\textit{subject to} \;\; \mathbf{1}^T\mathbf{s} = 1, \; \mathbf{s} \geq \mathbf{0} \end{aligned} \quad (6)$$

The minimization function and the constraints are convex functions of $\mathbf{s}$ and, therefore, equation 6 constitutes a convex optimization problem. Specifically, as noted by (Boyd and Vandenberghe, 1996), it can be cast to Linear Programming (LP) by introducing a new variable $\mathbf{v} \in \mathbb{R}^n$, and solving

$$\begin{aligned} &\textit{minimize} \;\; \mathbf{1}^T\mathbf{v} \\ &\textit{subject to} \;\; -\mathbf{v} \leq \mathbf{F}\mathbf{s} - \mathbf{c} \leq \mathbf{v}, \\ &\mathbf{1}^T\mathbf{s} = \mathbf{1}, \mathbf{s} \geq \mathbf{0} \end{aligned} \quad (7)$$

Note that $\mathbf{s}$ and $\mathbf{v}$ are feasible in equation 7 if and only if $v_i \geq \left|\mathbf{f}_i^T\mathbf{s} - c_i\right|$ for $i = 1, 2, \ldots, n$ and consequently by minimizing $\mathbf{1}^T\mathbf{v}$, $\|\mathbf{F}\mathbf{s} - \mathbf{c}\|_1$ is minimized.

Equation 7 can be expressed in standard LP form:

$$\begin{aligned} &\textit{minimize} \;\; \begin{bmatrix} \mathbf{0}^T & \mathbf{1}^T \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \mathbf{v} \end{bmatrix} \\ &\textit{subject to} \;\; \begin{bmatrix} \mathbf{F} & -\mathbf{I} \\ -\mathbf{F} & -\mathbf{I} \\ -\mathbf{1}^T & \mathbf{0}^T \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \mathbf{v} \end{bmatrix} \leq \begin{bmatrix} \mathbf{c} \\ -\mathbf{c} \\ \mathbf{0} \end{bmatrix}, \\ &\begin{bmatrix} \mathbf{1}^T & \mathbf{0}^T \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \mathbf{v} \end{bmatrix} = 1 \end{aligned} \quad (8)$$

The matrix $\mathbf{F}$ can be square, skinny (over-determined) or fat (under-determined). For all these cases there is an optimum solution for $\mathbf{s}$. Obviously, due to the constrained set $\mathbb{S}$, no guaranty of optimum zero residual exists even if $\mathbf{c}$ is in the range of $\mathbf{F}$.

4 THE MRV POLLUTION PROBLEM

The present study consists of the identification of the particulate matter in atmospheric aerosols in the Metropolitan Region of Vitória (MRV), Espírito Santo, Brazil. Góes satellite picture of the MRV is depicted in the figure 2. The MRV region covers an area of $1461\,\mathrm{km}^2$, consisting of the cities of Vitória, Vila Velha, Cariacica, Viana and Serra. This region has nearly a million inhabitants, and houses over 400 industries. The MRV is the main center of urban and industrial development of the state of Espírito Santo. The main sources of particulate matter and their emission characteristics within steel and iron ore processing industries have been studied to identify their contributions to the total amount of particulate air in MRV's atmosphere.

During the second half of the 80's, particulate matter concentration above $80\,\mu\mathrm{g\,m}^{-3}$ was recorded, coinciding with a period of low pluviometric precipitation and strong winds ($2\,\mathrm{m\,s}^{-1}$) coming from the north quadrant. Several electrostatic precipitators, filters, modern aspersion systems and others environmental equipment have since been installed by the local industries to reduce their contribution to the emission of dust to atmosphere.

The particulate matter in MRV's atmosphere is caused by 6 (six) main source groups:

group 1 (rich-iron content) – this group has more than 25% mass as iron. The main sources of this group are the blast-furnace, piles of ore, pellets, steel milling and sintering emissions;

group 2 (calcium-rich content) – this group contains sources with calcium as the main chemical element. It is represented by calcinating units and calcium-rich mineral piles stored at MRV;

group 3 (medium/high sulfur coal) – coal with medium/high sulfur content stored in MRV;

group 4 (natural calcium-bearing ore) – other calcium-rich minerals that are naturally emitted. Soil is the main source of such materials. Typical minerals of this group are calcite $CaCO_3$, and dolomite $CaMg(CO_3)_2$;

group 5 (titanium-rich ore) – black beach sand found in the state of Espírito Santo. This sand contains ilmenite TiO_2;

group 6 (low sulfur coal) – coal with low sulfur content stored in MRV.

Since all the air particulate sources in a specific group have chemical characteristics with strong linear dependence, it is impossible to distinguish their individual contributions to the total emission of particulate matter in atmosphere using receptor modeling.

Besides the air particulate sources, there are many filters installed in the MRV. Their objective is to measure the amount of particles in the air over specific geographic areas (receptors). Here, the data from two receptors will be considered, e.g. EAMES and Ilha do Boi. The sampling points were chosen considering the predominant wind direction (north) that flows from the industrial zone to Ilha do Boi and EAMES receptors (see last page picture). The sampling points are no more than 5 km far away from industrial sites. This distance can be considered convenient for the application of receptor modeling with reasonable results.

Table 1: Chemical characteristics of the 6 (six) main air particulate source groups in the Metropolitan Region of Vitória.

	Concentration (%) – Sources					
Elements	1	2	3	4	5	6
Fe	46.7	0.97	2.85	3.32	13.3	0.45
Al	0.54	0.42	1.90	1.99	0.50	1.35
Mg	2.13	34.8	0.13	3.2	0.76	0.27
Si	0.25	2.89	0.03	17.9	0.27	0.06
Ti	0.03	0	0	0	20.8	0.07

Table 2: Chemical characteristics of 2 (two) receptors located in the Metropolitan Region of Vitória.

	Concentration (%) – Receptors	
Elements	EAMES	ILHA DO BOI
Fe	4.74	5.30
Al	1.48	1.47
Mg	1.58	1.69
Si	0.96	1.05
Ti	0.13	0.12

5 EXPERIMENTAL RESULTS

Tables 1 shows typical chemical characteristics of the 6 (six) main pollution source groups in the MRV. Table 2 displays the chemical characteristics of 2 (two) receptors in the MRV, Ilha do Boi and EAMES. They reflect the average concentration of chemical species found at sources and receptors during a 7-year period (from 1989 to 1996). The samples were collected taking into account the Brazilian regulations and meteorological conditions (de Souza *et alii*, 1996). The total suspended particles (dust having a diameter not greater than $100\,\mathrm{mm}$) and inhalant particles (dust having a diameter not greater than $10\,\mathrm{mm}$) were collected once a week during a 24-hour period.

According to Tables 1 and 2 and equation 8, the 2 (two) receptor models to be solved (Ilha do Boi and EAMES) have the following description:

$$\begin{aligned} \textit{minimize} \quad & \begin{bmatrix} \mathbf{0}^T & \mathbf{1}^T \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \mathbf{v} \end{bmatrix} \\ \textit{subject to} \quad & \begin{bmatrix} \mathbf{F} & -\mathbf{I} \\ -\mathbf{F} & -\mathbf{I} \\ -\mathbf{1}^T & \mathbf{0}^T \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \mathbf{v} \end{bmatrix} \leq (1-nc) \begin{bmatrix} \mathbf{c} \\ -\mathbf{c} \\ \mathbf{0} \end{bmatrix}, \\ & \begin{bmatrix} \mathbf{1}^T & \mathbf{0}^T \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \mathbf{v} \end{bmatrix} = (1-nc), \end{aligned} \tag{9}$$

$$\mathbf{F} = \begin{bmatrix} 46.74 & 0.97 & 2.85 & 3.32 & 1.33 & 0.45 \\ 0.54 & 0.42 & 1.9 & 1.99 & 0.5 & 1.35 \\ 2.13 & 34.84 & 0.13 & 3.2 & 0.76 & 0.27 \\ 0.25 & 2.89 & 0.03 & 17.9 & 0.27 & 0.06 \\ 0.03 & 0 & 0 & 0 & 20.8 & 0.07 \end{bmatrix}$$

For Ilha do Boi receptor, the values of $\mathbf{c}$ and nc are:

$$\mathbf{c} = \begin{bmatrix} 5.3 & 1.47 & 1.69 & 1.05 & 0.12 \end{bmatrix}^T$$
$$nc = 0.55\ (55\%)$$

For EAMES receptor, the values of $\mathbf{c}$ and nc are:

$$\mathbf{c} = \begin{bmatrix} 4.74 & 1.48 & 1.58 & 0.96 & 0.13 \end{bmatrix}^T$$
$$nc = 0.68\ (68\%).$$

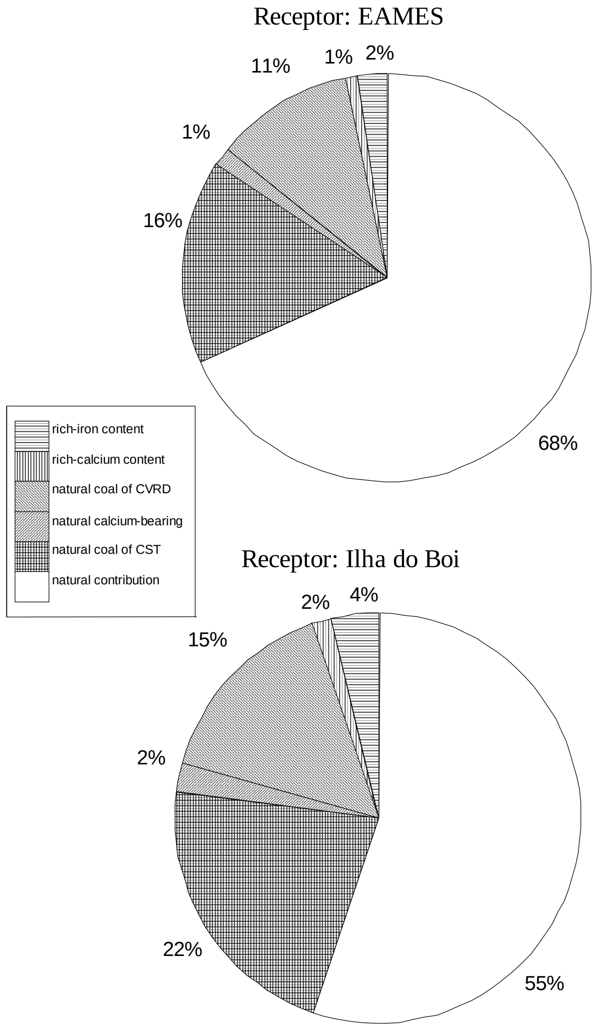

Figure 1: Industrial and natural contributions to the air pollution in 2 (two) receptors located in the Metropolitan Region of Vitória (MRV).

The term nc was introduced in the constraint equations to take into account the contribution of natural sources. Studies have shown that in the MRV there is a large contribution of natural sources with significant concentration of the same chemical elements found at the 6 (six) main source groups (de Souza *et alii*, 1996). Since natural sources do not have well defined dimensions and also suffer industrial influences, it is extremely difficult to provide a precise quantification of their chemical concentrations.

The optimization problem defined in equation 9 was solved for both EAMES and Ilha do Boi Receptors. Figure 1 depicts the individual sources' contributions to the total particulate matter in atmosphere for these two sampling points (EAMES and Ilha do Boi receptors). Despite the large coal presence in airborne particles, there was no detectable ore presence. Since almost the same amount of ore and coal are handled in the MRV (9.10^5 ton/year), the distinct contributions are due to the different densities of these two materials, 1.38 g/cm^3 for coal and 3.88 g/cm^3 for ore. As expected, the largest industrial contribution to air pollution in the MRV is from natural coal.

6 CONCLUDING REMARKS

This paper presents the solution of a real receptor modeling problem via linear programming. It consists of the identification and quantification of important industrial contributions to the total suspended particulate matter in the Metropolitan Region of Vitória (MRV), Brazil.

The results of this case study illustrate that the utilization of linear programming and receptor modeling technique seems to be a promising way for quantification of the contributions of industrial sources to the pollution of urban aerosols.

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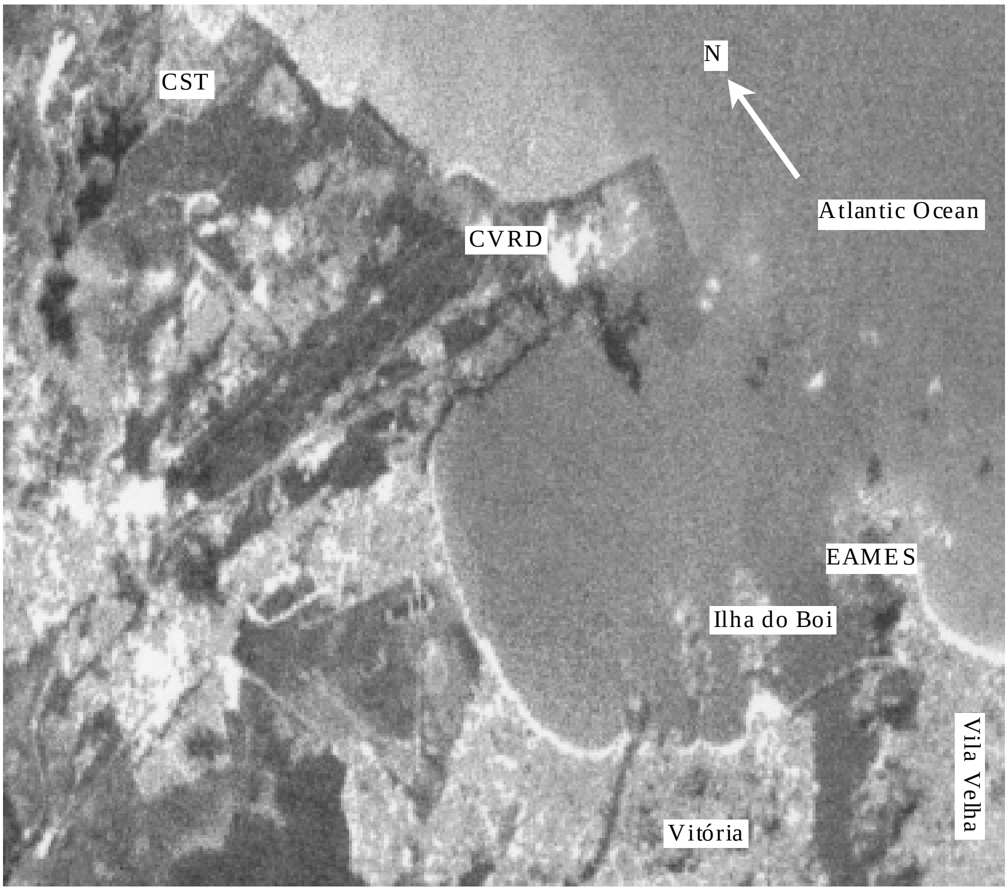

Figure 2: Góes satellite picture of the Metropolitan Region of Vitória (MRV).