MATHEMATICAL MODELS FOR ATMOSPHERIC AND INDUSTRIAL POLLUTANT PREDICTION

G. Andria, A. Lay Ekuakille, M. Notarnicola

Dipartimento di Elettrotecnica ed Elettronica, Politecnico di Bari
Via E. Orabona 4, 70125 Bari, Italy

Abstract: As well known air quality changes can be predicted by mathematical models, like roll back models, empirical models, and dispersion models; or by physical models, like "wind tunnel" and analogous water models of simulation, or using "on situ" experiments with tracers. Mathematical models are more important in order to test and to predict pollutant effects in a given area. The aim of this work is to build effective models for atmospheric and industrial pollution to be predicted by using a Pair Comparison Technique (PCT). Experiments have been carrying out with laser-mode-switching equipment to make comparison with theoretical models.

Keywords: Air Monitoring, Pollutant Measurements, Prediction models, Air quality measurement, Pair comparison Technique.

1   INTRODUCTION

Potential effects of atmospheric and industrial pollution on air quality are determined by means of a suitable modeling. Models of air quality need input data that characterize emissions, meteorology, air chemistry in the considered area [1]. The adopted approach allows to establish *an impact scenario* as shown in Fig.1.
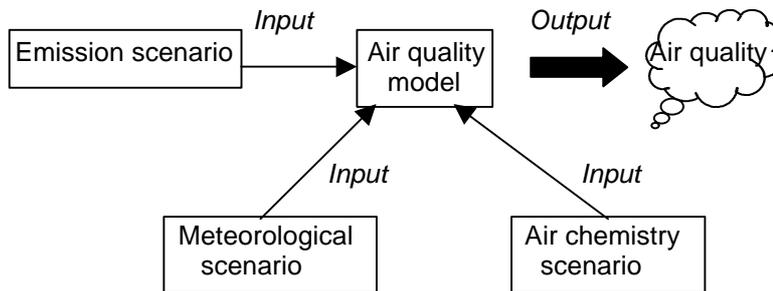

Figure 1. The modeling of Air quality

We define the impact scenario as a combination of emissions and atmospheric interactions (Meteorology and Air chemistry) that are simultaneously present to produce an impact on Air quality. Once build, impact scenarios supply requested information to identify appropriate input data for Air quality models. So we use mathematical models through statistical functions to predict the amount of air pollution from industrial uses. *Box models* are among the simplest ones; box model considers pollutants that are emitted in an air volume surrounded by virtual walls. It is not acceptable for quantitative analysis. *Roll back method* consists in an empirical model that supposes average environmental concentration in a given place is directly proportional to the amount of emission. Roll back method is only valid for preliminary analysis. *Empirical methods* use background and time - serie observations to produce a mathematical relationship between emission levels and air quality. The main disadvantage of empirical methods consists in the fact that they do not take into account successive behavior of atmospheric changes.

2   DATA PRE-PROCESSING

We suggest a new approach with *Gaussian, Lagrangian, Eulerian models* by using a Pair Comparison Technique (PCT). Gaussian, Lagrangian and Eulerian models are more complex than those described in the introduction.

A *Pair Comparison Technique* or *Pair Comparison File* (PCF) is a binary file that contains pairs of samples sorted by distance. It also includes either a copy of the original data file or a reference to it.

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We can work with more than 500,000 pairs on a Pentium Personal Computer without any problem.

The advantages of PCF are [2]:
a) calculating a measure of spatial continuity is fast with the help of a PCF since all pair distances have already been computed;
b) direct access to the pairs is granted. This allows the construction of *h-scatterplots* and *variogram clouds*.

PCF has been used to study the distribution of pollutant sources and to optimize the choice of these sources. This approach is practical because we are dealing with irregularly spaced data since all distances (for instance, between sources and evaluation points) can easily be derived from the grid layout.

3 AIR MODELING

3.1 Introduction

If we consider the pollutant contained in an atmospheric volume delimited by a closed surface, the temporal variation of pollutant amount will be equal to the sum of pollutant quantity produced in the same volume plus the net quantity of pollutant that flows through the contour surface. If C is the quantity of pollutant, V the current volume and S the contour surface, that is:

(*Temporal variation of C in V*) = (*Transportation of C through S*) + (*Production of C inside V*)

By developing analytically the above quantities , it is possible to get the following relationship:

$$\frac{\partial C}{\partial t} + u.\nabla C = -\nabla^2 q + E + R \tag{1}$$

where u represents the average wind velocity vector, and q is the flow of pollutant scattered point by point in any instant; E is the quantity of pollutant emitted instantaneously, R is the instantaneous net contribution resulting from chemical reactions triggered in the atmosphere, and the operator " " stands for *gradient*. Eq. 1 entirely describes pollutant dispersion, but its solution presents many difficulties and it is necessary to introduce a progressive series of approximations and reductions so that it is possible to make its resolution easy. The first step is the adoption of average concentrations instead of instantaneous ones. So we can get the same but easier formulation, where " ^{2}" is for *Laplacian*:

$$\frac{\partial C}{\partial t} + \overline{u}.\nabla \overline{C} = -\nabla^2 \overline{q} + \overline{E} + \overline{R} \tag{2}$$

Now it is possible to introduce some assumptions that lead to the widespread and easier formulation:
- the wind has a constant average direction along x-axis;
- the current pollutant is chemically inert so there are no chain reaction after its emission.
The interested atmospheric layer offers uniform conditions of turbulence, and so coefficients of turbulent scattering are constant and they are not zero in the directions (x,x), (y,y), (z,z). With these further assumptions it is possible to write again Eq. 2 in a compacted form:

$$\frac{\partial C}{\partial t} = \nabla(k.\nabla C) \quad \text{with } k \text{ as tensor of scattering coefficients} \tag{3}$$

In extended formulation Eq. 3 yields to:

$$\frac{dC}{dt} = \frac{\partial}{\partial x}\left(k_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial t}\left(k_z \frac{\partial C}{\partial z}\right) \tag{4}$$

where partial derivative with respect to time has been replaced by total derivative, by means of fluid system principle approximation.

3.2 Gaussian model

With other reductions and considerations Eq. 4 yields to gaussian model, that is

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$$C = \frac{Q}{2p\boldsymbol{s}_y \boldsymbol{s}_z \bar{u}} \exp\left[-\frac{1}{2}\left(\frac{y_r}{\boldsymbol{s}_y}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{h_e - z_r}{\boldsymbol{s}_z}\right)^2\right]$$ (5)

in which, u is the average horizontal wind speed, h_e is the effective emission height (i.e., $h_e = z_s + \boldsymbol{D}h$), and plume sigmas that depend upon Taylor's statistical theory of diffusion.

The Gaussian plume model is the most common air pollution model [3]. It is based on a simple formula that describes the tree-dimensional concentration field generated by a point source under stationary meteorological and emission conditions.

Concentrations computed by Eq. 5 depend strongly upon a correct calculation of $\boldsymbol{s}_y$ and $\boldsymbol{s}_z$, which is a major challenge for all Gaussian model applications and for this work. There are two general methods for computing $\boldsymbol{s}_y$ and $\boldsymbol{s}_z$. The first method, the preferred one, is based on the calculation of nondimensional functions and makes direct use of turbulence intensity measurements, when available. The second method relies on semiempirical calculations [4] in which the atmosphere is classified into "stability" classes and different σ functions are derived for each class [5].

Coefficients σ$_y$ and σ$_z$ are also called respectively *lateral and vertical dispersion coefficients*. Sigmas can be computed [6] as

$$\boldsymbol{s}_y = \boldsymbol{s}_q \, x(1 + 0{,}0308 \; x^{0{,}4548})^{-1} \quad \text{for} \quad x \leq 10.000$$ (6)

$$\boldsymbol{s}_z = \boldsymbol{s}_f \, x\left[1 + 0{,}945 \; (t/T_0)^{0{,}8}\right]^{-1} \quad \text{for} \quad z \geq 50 \text{ m}$$ (7)

in which

$$\boldsymbol{s}_q = b$$ (8)

with $b = 1{,}92 \pm 0{,}5$

$$\boldsymbol{s}_f = c$$ (9)

with c = 1,25 ± 0,03 and the diffusion time t. Elements σ$_\theta$ and σ$_\phi$ are called the *standard deviations of the crosswind and vertical wind vector components*.

4   SIMULATIONS AND RESULTS

Eq. 5 has been basically used in this work to overcome the hypothesis assumed by Draxler as indicated in [6] and [7]. The data used in this work are illustrated in Table 1.

Table 1. Database used for creating Gaussian Model

		Unit	Figure 2	Figure 3	Figure 4	Figure 5	Figure 6
Height	z	m	53	51	100	60	53
Real Height	h_e	m	50	50	50	50	50
Coefficient	b		1.92	1.97	1.97	1.97	1.92
Coefficient	c		1.28	1.28	1.28	1.28	0.3
Time	t	s	30	30	30	20	30
Reference time	T_0	s	50	50	50	60	50
Wind velocity	u	m/s	40	40	40	40	40

In any tri-dimensional figure, x-axis, y-axis and z-axis represent respectively Average Wind Velocity Vector u, Aperture and Concentration C.
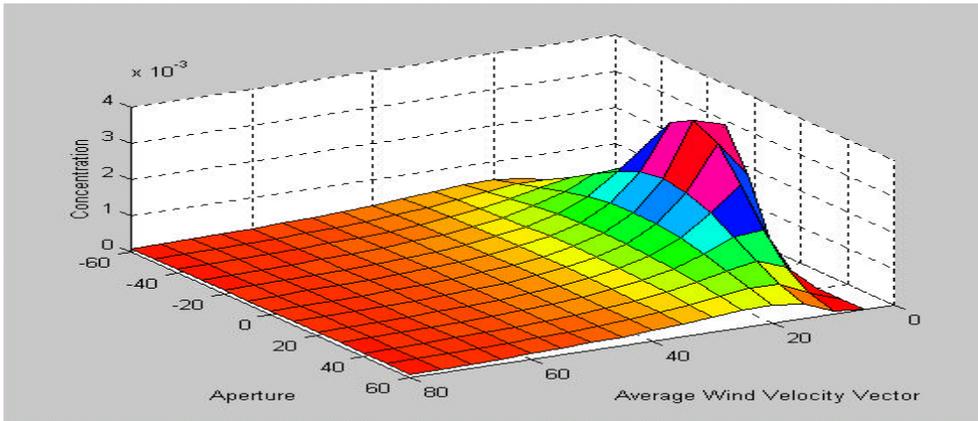
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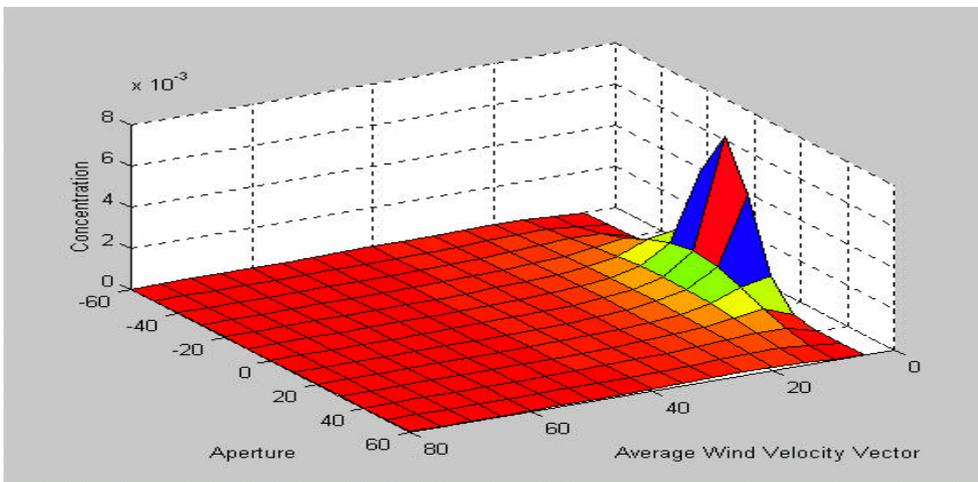**Figure 2.** Spatial distribution of concentration for z=53 m and b=1.92

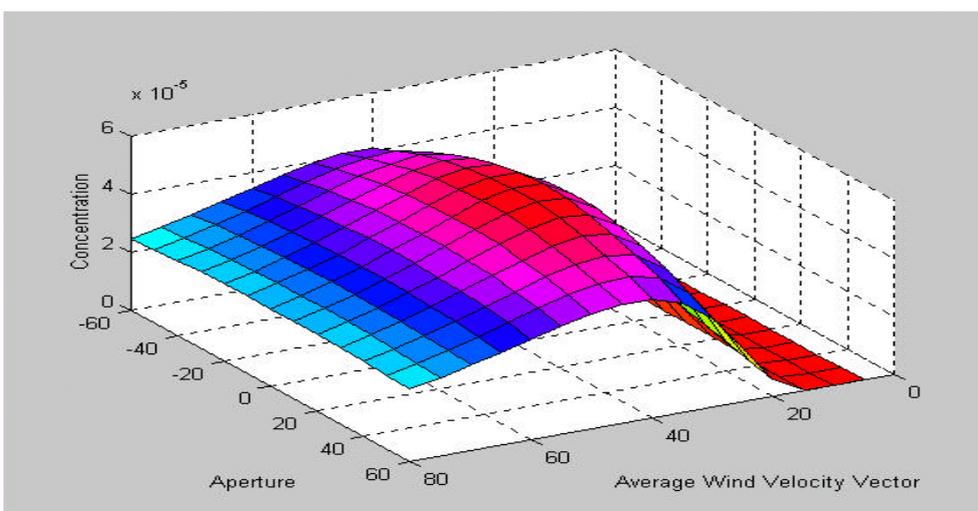**Figure 3.** Spatial distribution of concentration for z=51m and b=1.92+0.5

Figure 4. Spatial distribution of concentration for z=100 m and b=1.92+0.5

Returning to Table 1, it is possible to make some important comments; all figures agree to Gaussian Models with particular characteristics to be explained. Fig. 2 is a more recurrent case study, while the other figures show singular situation. First of all, we see that it can be possible to get the same results as illustrated in Fig. 3, Fig. 5 and figure 6 by managing on standard deviations. In Fig. 6 we have assigned c=0.3, out of the range requested by common experiments (see Eq. 9). When the difference between h_e and z decreases, the aperture along y-axis decreases and the concentration suddenly falls; that is, the surface trend goes to a conic surface with vertex that coincides with the maximum of concentration. It is necessary to notice it. In terms of plume, Fig. 4 describes a case of strong lapse condition that is commonly called *looping*.
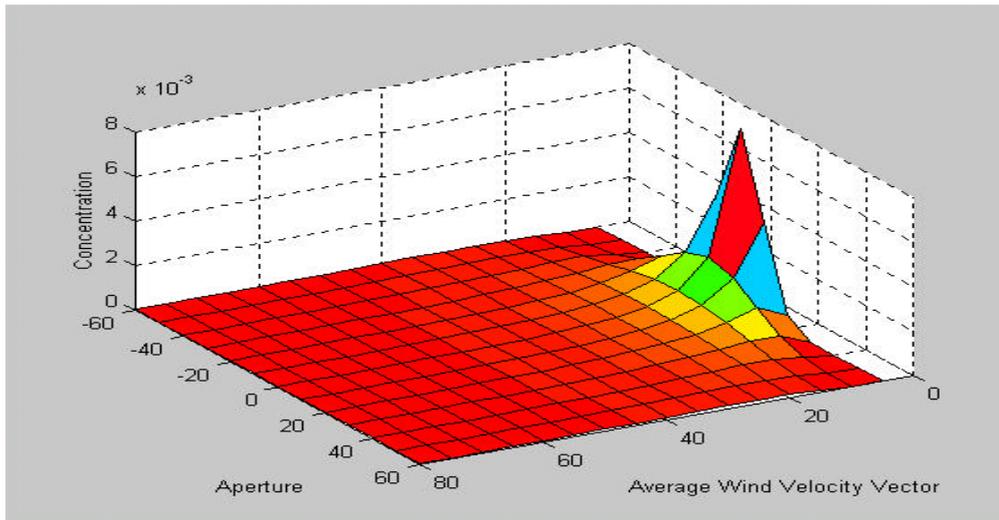

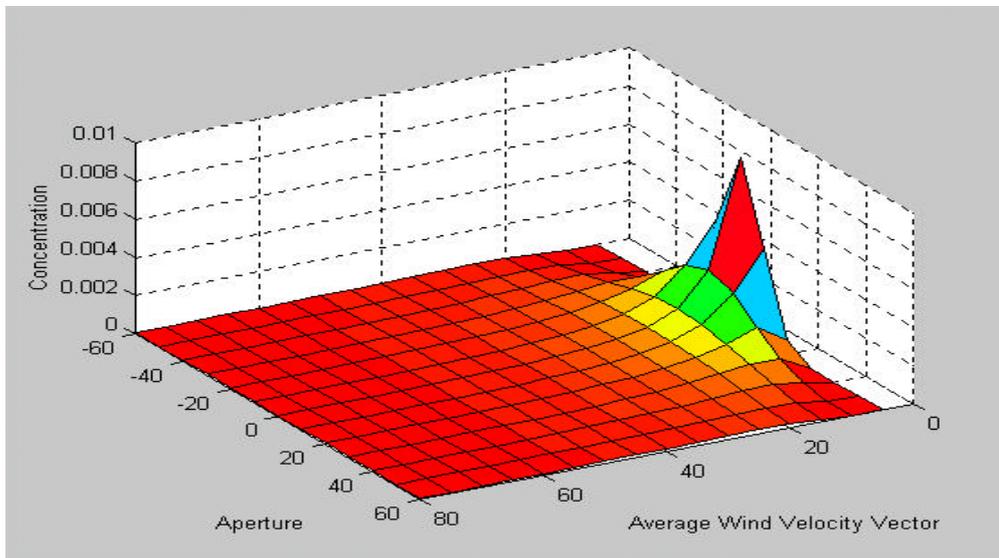**Figure 5.** Spatial distribution of concentration for z=60 m, T_0=60 s and t=20 s

Figure 6. Spatial distribution of concentration for z=53 m, b=1.92 and c=0.3

According to the data analysis and the trend of the above surfaces, we can say that attention must be paid in locating instrumentations for monitoring air pollutants; for instance at x=40 m, only in Fig. 4 we can get meaningful values. That is the reason for which it is suitable and compulsory to insert measured data into in a model. We have used real and concrete data concerning an existing situation in order to compare simulated results from actual ones.

5   CONCLUSIONS

We have presented a variation of Gaussian Model by using different standard deviations from those which are commonly used.   This work has shown the possibilities of getting good results with Gaussian Models. We have used Pair Comparison Technique in order to process data from different point sources. We know that with restrictive hypothesis it is possible to get bad results. However simulations have demonstrated the validity of instrumental data. Gaussian model, in this work, has allowed us to reach reliable values. We can still improve the reliability by using climatological models that compute concentrations for long observation period.

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AUTHOR(S): Aimé LAY EKUAKILLE - Dipartimento di Elettrotecnica ed Elettronica , Politecnico di Bari, Via E. Orabona 4, 70125 Bari - Italy , Phone ++0039 80 596.3317, Fax ++039 80 596.3410 , E-mail: alekuakille@iol.it