Mathematical Air Pollution Models: Eulerian Models

Chapter · January 2010

DOI: 10.1201/9781439847121-c5

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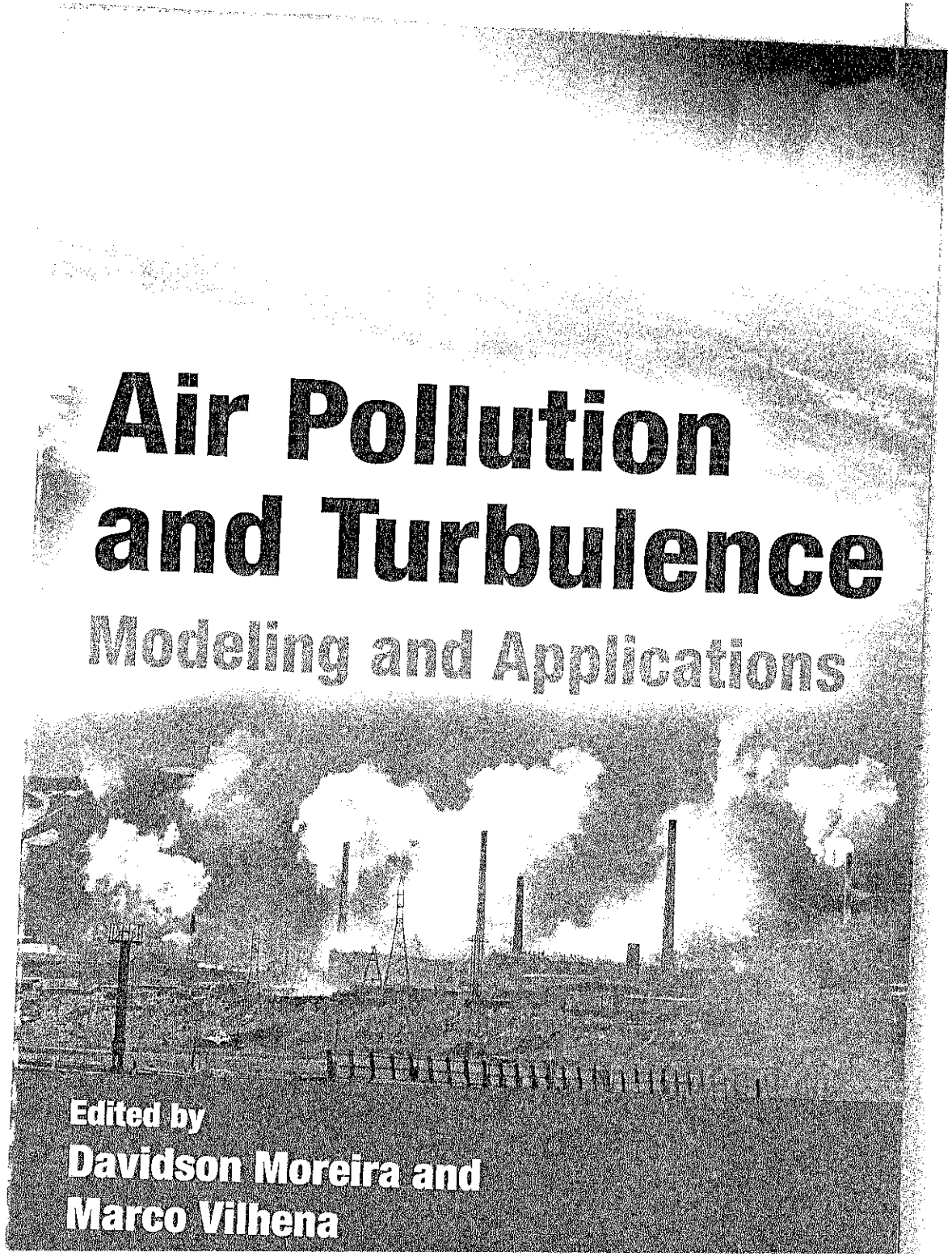

5 Mathematical Air Pollution Models: Eulerian Models

Tiziano Tirabassi

CONTENTS

5.1 INTRODUCTION

The management and safeguard of air quality presupposes a knowledge of the state of the environment. Such knowledge involves both cognitive and interpretative aspects. Monitoring networks and measurements in general, together with an inventory of emission sources, are of fundamental importance for the construction of the cognitive picture, but not for the interpretative one. In fact, air quality control requires

interpretative tools that are able to extrapolate in space and time the values measured by analytical instrumentation at field sites, while environmental improvement can only be obtained by means of a systematic planning of reduction of emissions, and, therefore, by employing instruments (such as mathematical models of atmospheric dispersion) capable of linking the causes (sources) of pollution with the respective effects (pollutant concentrations).

The processes governing the transport and diffusion of pollutants are numerous and of such complexity that it would be impossible to describe them without the use of mathematical models. Such models therefore constitute an indispensable technical instrument of air quality management. Mathematical models are in fact able to

- Describe and interpret experimental data
- Control air quality in either real or deferred time
- Monitor accidental emissions and assess risk areas
- Identify pollutant sources
- Evaluate the contribution of a single source to pollutant loading
- Assist in territorial management and planning

There exist innumerable, sometimes very diverse, mathematical models of atmospheric pollutant diffusion that may be utilized for the aforementioned purposes. In fact, the phenomenon of turbulent diffusion in the atmosphere has no single formulation, in the sense that no one approach has yet been proposed that is able to explain all of the observed phenomena.

5.2 OPERATIVE CHARACTERISTICS OF MATHEMATICAL MODELS

The choice of model is closely linked to the problem being confronted and to the meteoclimatic and orographic characteristics of the site under consideration. Available models can be subdivided on the basis of source characteristics:

- Point source
- Linear, area, and volume sources

or on the basis of orography:

- Flat terrain
- Complex terrain

They can also be classified on the basis of the size of the field they are describing:

- Short distance (distance from source less than 30–50 km)
- Mesoscale models (describing concentration fields of the order of hundreds of kilometers)
- Continental or planetary circulation models

Finally, models can be classified on the basis of the time resolution of the concentrations produced:

- Episodic models (temporal resolution of less than an hour)
- Short-time models (temporal resolutions greater than or equal to an hour, and less than or equal to 24 h)
- Climatological models (with resolution greater than 24 h, generally seasonal or annual)

5.3 THEORETICAL CHARACTERISTICS OF MATHEMATICAL MODELS

The theoretical approach to the problem essentially assumes four basic forms. In the K approach, diffusion is considered, at a fixed point in space, proportional to the local gradient of the concentration of the diffused material. Consequently, it is fundamentally Eulerian since it considers the motion of fluid within a spatially fixed system of reference. Such models are most suited to confronting complex problems, for example, the dispersion of pollutants over complex terrain or the diffusion of noninert pollutants. They are based on the numerical resolution, on a fixed spatial-temporal grid, of the equation of the mass conservation of the pollutant chemical species.

Among the Eulerian models, box models constitute the most simple mathematical approach since they neglect the spatial structure of phenomena. They assume that the pollutants are uniformly distributed within a parallelepiped (box). From the theoretical viewpoint, this is equivalent to assuming infinite diffusion coefficients that provoke an instantaneous propagation of the pollutant within the considered box. The pollutant present in the box originates from internal sources or from external contributions transported by the wind or flows across the summit due to variations in the height of the box itself, which generally coincides with the height of the mixing layer.

Lagrangian models differ from Eulerian ones in adopting a system of reference that follows atmospheric motions. Initially, the term Lagrangian was used only to refer to the box or moving box models that followed the mean wind trajectory. Currently, this class includes all models that decompose the pollutant cloud into discrete "elements," such as segments, puffs, or computer particles. In particle models, pollutant dispersion is simulated through the motion of computer particles whose trajectories allow the calculation of the concentration field of the emitted substance. The underlying hypothesis is that the combination of the trajectories of such particles to simulate the paths of the air particles situated, at the initial moment, in the same position. The motion of the particles can be reproduced both in a deterministic and in a stochastic way. Gaussian models are theoretically based upon an exact, but not realistic, solution of the equation of transport and diffusion in the atmosphere, in cases where both wind and turbulent diffusion coefficients are constant with height. The solution is forced to represent real situations by means of empirical parameters, referred to as "sigmas." They can be either stationary (the time-independent plume models) or time-dependent (puff models). The name given to these models is derived from the fact that the pollutant distribution, both vertical and transverse to wind direction, is described by the famous curve discovered by the physicist-mathematician Gauss. The various versions of Gaussian models essentially differ in

the techniques utilized to calculate the "sigmas" as a function of atmospheric stability and the downwind distance from the emission source. Two basic techniques can be identified as serving this purpose: the first employs adimensional functions built on the basis of available measurements of turbulent intensity and the second adopts semiempirical functions for "sigmas" built for each stability class with which atmospheric turbulence has been schematized.

Analytic models can be considered an intermediate stage between K and Gaussian models. They conserve the simplicity of the latter, in that the concentration field is described by a simple formula, but, at the same time, they are also able to confront, in a theoretically correct way, situations in which the wind and turbulent diffusion coefficient vary with height.

5.3.1 Eulerian Approach: K Models

Eulerian models are the most suitable for tackling problems of greater complexity, for example, the dispersion of pollutants over complex terrain or the diffusion of noninert pollutants. They are based on the resolution, on a fixed spatial-temporal grid, of the equation of mass conservation of the pollutant chemical species, expressed in terms of concentration $c(x, y, z, t)$ (Zannetti, 1990):

$$\frac{\partial c}{\partial t} = -\mathbf{u}\cdot\nabla c + D\nabla^2 c + S \tag{5.1}$$

where

- $\mathbf{u}$ is the wind speed vector of the components u, v, w
- $D\nabla^2 c$ is the molecular diffusion term (generally neglected), with D the molecular diffusion coefficient
- S is the term referring to the source, measuring the emission intensity and representing the pollutant removal kinetic
- ∇ is the gradient operator
- ∇^2 is the Laplacian

In order to resolve Equation 5.1, it is necessary to know the wind field $\mathbf{u}$, something that is not possible since it is extremely variable in space and time, from the scale of centimeters to kilometers. Consequently, wind is divided into two parts:

$\bar{\mathbf{u}}$: The so-called ensemble average
$\mathbf{u}'$: The turbulent fluctuations of wind at mean nil

Thereupon the wind speed is expressed as the sum of the two components, mean and turbulent:

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}' \tag{5.2a}$$

The same considerations can be made for c. Therefore:

$$c = \bar{c} + c' \tag{5.2b}$$

The ensemble average refers to the mean value obtained by the repetition of many experiments in the same meteorological and emission conditions.

The new $\mathbf{u}$ and c are introduced into Equation 5.1; after several calculations and hypothesizing a wind with divergence nil, the following is obtained:

$$\frac{\partial \bar{c}}{\partial t} = -\bar{\mathbf{u}}\cdot\nabla\bar{c} - \nabla\cdot\overline{c'\mathbf{u}'} + D\nabla^2\bar{c} + \bar{S} \tag{5.3}$$

This equation includes some new variables (those with an apex) whose values are unknown. The appearance of new terms in equations for mean quantities leads to a number of unknowns greater than the number of equations. Thus, the system of equations is not closed and is therefore irresolvable. To close it, in fact, new equations of variance and covariance (second-order moments) would be required, but this would only shift the problem to a higher order since it would yield further unknown quantities that are third-order moments. Now, if it were decided to find equations for the third-order moments, this would yield unknowns of a higher order, that is, fourth-order moments, requiring the introduction of new equations. Iterating the procedure, the conclusion would be reached that the number of unknowns is always greater than the number of equations. A solution to this problem consists of utilizing only a finite number of equations, relative to a certain number of unknowns, parameterizing the remaining ones in terms of known quantities.

The most classic and widely used approach to obviate this problem is the parameterization of second-order moments, assuming a hypothetical analogy between molecular diffusion and the turbulent transfers. Such approach is referred to as the K-theory or flux-gradient theory, as it assumes that the flow of a given field is proportional to the gradient of an appropriate mean variable. This is a first-order closure of the set of equations under examination, since it conserves the equations relative to the first moments and parameterizes the second moments:

$$\overline{c'\mathbf{u}'} = -K\nabla\bar{c} \tag{5.4}$$

where K is the eddy diffusivity coefficient.

The simplicity of the K-theory of turbulent diffusion has led to its widespread use as the mathematical basis for simulating urban, photochemical pollution. However, K-closure has its own limits. In contrast to molecular diffusion, turbulent diffusion is scale-dependent. This means that the rate of diffusion of a cloud of material generally depends on the cloud dimensions and the intensity of turbulence. As the cloud grows, larger eddies are incorporated in the expansion process, so that a progressively larger fraction of turbulent kinetic energy is available for the cloud expansion. However, eddies much larger than the cloud itself are relatively unimportant in its expansion. Thus, the gradient-transfer theory works well when the dimension of dispersed material is much larger than the size of turbulent eddies involved in the diffusion process, that is, for ground-level emissions and for large travel times. Strictly speaking, one should introduce a diffusion coefficient function not only of atmospheric stability and emission height but also of the travel time or distance from source. However, such time-dependence makes it difficult to treat the diffusion equation in a fixed-coordinate system where multiple sources have to be treated simultaneously. Otherwise, one should limit the application of the gradient theory to large travel times (Pasquill and Smith, 1983). A further problem

is that the down-gradient transport hypothesis is inconsistent with observed features of turbulent diffusion in the upper portion of the mixed layer (ML), where counter-gradient material fluxes are known to occur (Deardoff and Willis, 1975).

In addition, unlike molecular diffusion, turbulent diffusion is not a property of fluids, but of the turbulence itself or of flows, and it may vary greatly from one flow to another and from one region to another of the same flow. The above relations are essentially based only on a qualitative analogy between molecular and turbulent diffusion. For the first-order closure to be realistic, the mean concentration field must have a much larger timescale than that of turbulent transport.

Despite these well-known limits, the *K*-closure is widely used in several atmospheric conditions, because it describes the diffusive transport in an Eulerian framework, where almost all measurements are Eulerian in character. It produces results that agree with experimental data as well as any more complex model, and it is not as computationally expensive as higher-order closures.

The reliability of the *K*-approach strongly depends on the way the eddy diffusivity is determined on the basis of the turbulence structure of the PBL, and on the model's ability to reproduce experimental diffusion data. A great variety of formulations exist (Ulke, 2000). Most of them are based on similarity theory, and give different results for the same atmospheric stability, as well as discontinuities and jumps at the transition between different stability regimes of the PBL.

The tensor K (3×3) of turbulent diffusion, whose elements can be extrapolated from experimental measurements, is introduced in Equation 5.3. Then, by also applying the following approximations:

- The K tensor is diagonal.
- The molecular diffusion is negligible.
- c represents the concentration of a nonreactive pollutant (thus $\overline{S} = S$).

Equation 5.3 can be written in the form:

$$\frac{\partial \overline{c}}{\partial t} = -\overline{\mathbf{u}} \cdot \nabla \overline{c} + \nabla \cdot K \nabla \overline{c} + S \tag{5.5}$$

Equation 5.5 can be integrated (analytically or numerically) if input data for u, K, and S are provided, together with the initial and boundary conditions for $\overline{c}$.

Eulerian models and K models mainly differ in the functions utilized for the K coefficients and the techniques used for the integration of Equation 5.5.

Equation 5.5 can be resolved in two ways:

1. With analytic methods, obtaining exact solutions
2. With numerical methods, obtaining approximate solutions

5.3.2 Analytical Solutions

Analytical solutions of equations are of fundamental importance in understanding and describing physical phenomena. Analytical solutions (as opposed to numerical ones) explicitly take into account all the parameters of a problem, so that their influence can be reliably investigated, and it is easy to obtain the asymptotic behavior of the solution, which is usually difficult to generate through numerical calculations.

There are analytical solutions of the two-dimensional advection–diffusion equation (Tirabassi, 1989, 2003):

$$u\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) + S \tag{5.6}$$

where

u is mean velocity (the wind is assumed along x-axis, while z is the height)
C is the mean concentration
S is the source term
K_z is the vertical eddy exchange coefficient

Moreover, as usual, the along-wind diffusion was neglected because it was considered little in respect to the advection. Recently, a steady-state mathematical model for dispersion of contaminants in low winds was formulated by taking into account the longitudinal diffusion in the advection–diffusion equation (Moreira et al., 2005a).

Unfortunately, no general solution is known for equations describing the atmospheric transport and dispersion of air pollution. There are some specific solutions, the best-known being the so-called Gaussian solution, which does not, however, realistically describe the concentrations of pollutants in the air; in fact, the models based on it (so-called Gaussian models) use empirical parameters of dispersion in order to force the Gaussian solution to represent the actual concentration field. However, there are models based on non-Gaussian analytical solutions.

Roberts (1923) presented a bidimensional solution, for ground-level sources only, in cases where both the wind speed and vertical diffusion coefficients follow power laws as a function of height, that is,

$$u = u_1 (z/z_1)^{\alpha} \tag{5.7a}$$

$$K_z = K_1 (z/z_1)^{\beta} \tag{5.7b}$$

where z_1 is the height where u_1 and K_1 are evaluated.

Rounds (1955) obtained a bidimensional solution valid for elevated sources, but only for linear profiles of K_z. Smith (1957a) resolved the bidimensional equation of transport and diffusion with u and K_z power functions of height with the exponents of these functions following the conjugate law of Schmidt (i.e., "wind exponent" = 1 – "K_z exponent").

Smith (1957b) also presented a solution in the case of constant u, but K_z following:

$$K_z = K_0 z^a (H - z)^b \tag{5.8}$$

where K_0 is a constant and a and b can be

$a \geq 0$ and $b = 0$

$a = 0$ and $b > 0$ for $0 \leq z \leq H$

$a = 1$ and $b > 0$ for $0 \leq z \leq H$

$a = 1$ and $b = 0$ for $0 \leq z \leq H/2$; $a = 0$ and $b = 1$ for $H/2 \leq z \leq H$

where H is the height of the atmospheric boundary layer.

Scriven and Fisher (1975) proposed a solution with constant u and K_z as

$$K_z \equiv z \quad \text{for } 0 \leq z \leq z_s \tag{5.9a}$$

$$K_z = K_z(z_1) \quad \text{for } z_s < z \leq H \tag{5.9b}$$

where z_s is a predetermined height (generally, the height of the surface layer). This solution allows (as boundary conditions) a net flow of material toward the ground:

$$K_z \frac{\partial C}{\partial z} = V_g C \tag{5.10}$$

where V_g is the deposition velocity. The Scriven and Fisher solution has been used in the United Kingdom for long-range transport of pollutant. In Fisher (1975), the deposition of sulfur over the United Kingdom, Sweden, and the rest of Europe was compared, and it was found that the British contribution to deposition over rural Sweden was about one half of the Swedish contribution.

Yeh and Huang (1975) and Berlyand (1975) published bidimensional solutions for elevated sources with u and K_z following power profiles, but for an unbound atmosphere, that is,

$$K_z \frac{\partial C}{\partial z} = 0 \quad \text{at } z = \infty \tag{5.11}$$

Demuth (1978) put forward a solution with the same conditions, but for a vertically limited boundary layer, that is,

$$K_z \frac{\partial C}{\partial z} = 0 \quad \text{at } z = H \tag{5.12}$$

The solutions of Yeh and Huang, Berlyand, and Demuth are used in KAPPAG air pollution model (Tagliazucca et al., 1985; Tirabassi et al., 1986; Tirabassi 1989).

By applying the Monin–Obukhov similarity theory to diffusion, van Ulden (1978) derived a solution for vertical diffusion from continuous sources near the ground only with the assumption that u and K_z follow power profiles. His results are similar to that of Roberts', but he provided a model for non–ground-level sources, but applicable to sources within the surface layer. SPM (Tirabassi and Rizza, 1995) is a model that utilizes the solution proposed by van Ulden.

Nieuwstadt (1980) presented a solution, which was a particular case of Smith's (1975b) solution noted above. Subsequently, Nieuwstadt and de Haan (1981) extended that solution to the case of a growing boundary layer height. Catalano (1982), in turn, extended the latter solution to the case of nonzero mean vertical wind profiles. Lin and Hildemann (1997) extended the solution of Demuth (1978) with boundary conditions suitable for simulating dry deposition to the ground.

Recently, Brown et al. (1997) derived equations for point source releases for the first four moments of the vertical concentration distribution and the magnitude and downwind location of the maximum ground concentration from the solution of Yeh and Huang (1975).

Finally, Moreira et al. (2005b) found a general two-dimensional steady-state solution for any profiles of wind and eddy coefficient diffusions.

5.3.3 Numerical Solutions

Among the techniques used to resolve Equation 5.5, the following should be mentioned:

- Finite difference method
- Finite elements method
- Finite volume method
- Spectral methods
- The method of confined elements

The finite difference method is the most simple technique and was the first to be used. The approximation of the finite differences of the advection term $\bar{\mathbf{u}} \cdot \nabla \bar{c}$, is, however, always associated with an error that artificially increases diffusion in the final results of the simulated concentrations. Several techniques have been developed with the aim of reducing this error, and notwithstanding the limitations posed by this model, it remains one of the most important and widely adopted methods of simulation.

Unlike analytic approaches, numerical techniques allow, from the theoretical viewpoint, the use of any function for K(x, y, z, t).

5.3.4 Eddy Diffusivity

The literature proposes several expressions for K_z, which is generally a function of height z (for instance, Pleim and Chang, 1992). For instance, an approach for estimating the eddy diffusivity K and dispersion parameters as functions of eddy scale size in the PBL and relative amount of turbulent energy has been recently proposed by Degrazia and Moraes (1992) and Degrazia et al. (1997, 2000). Making use of Taylor's statistical theory (Taylor, 1921), the Hay and Pasquill working approximation of the relationship between Lagrangian and Eulerian turbulence spectra (Hay and Pasquill, 1959), and a model for Eulerian spectra, such approach relates plume dispersion in a boundary layer mainly to the turbulent eddies acting in the different stability regimes of the boundary layer (Pasquill and Smith, 1983). Bearing the K-theory limitations in

mind, the main idea of the said approach is to obtain an eddy diffusivity scheme for practical applications in air pollution modeling, which reveals the essential features of turbulent diffusion, but which as far as possible preserves the simplicity and flexibility of the *K*-theory formulation. Degrazia et al. (1997, 2000) propose the vertical profiles of diffusion coefficients obtained by means of spectral techniques.

Several difficulties arise in the evaluation of the transversal turbulent diffusion. It is often, and not always correctly, hypothesized that,

$$K_h \cong K_y \tag{5.13}$$

where K_y is the transversal turbulent diffusion (supposing the wind is blowing in the direction of *x*-axis).

Another problem in the simulation of horizontal dispersion is the numerical error associated with the advection of the pollutant due to part of the mean wind. Such error is linked to the size of the spatial grid used to schematize the diffusion field, and can turn out to be greater than parameter K_h itself.

In the past, the most complex simulation techniques made widespread use of dynamic grid models, in particular with the application of the numerical method of finite differences and *K* closure. However, several major limitations of such applications have come to light:

1. The numerical approximation of the advection term often produces a fictitious diffusion.
2. *K* closure is a fundamentally incorrect approximation in strong turbulence conditions.
3. Since the concentrations are calculated as spatial means within three-dimensional cells of the grid, it is difficult to compare them with measurements carried out at single points in space.
4. It is difficult to link *K* eddy coefficients with experimental measurements in the atmosphere.
5. A correct application of *K* closure requires that the grid dimensions be smaller than those of the pollutant cloud, a condition that is difficult to satisfy the proximity to the source.

5.3.5 Box Models

Of the Eulerian models, box models constitute the most simple mathematical approach, since they ignore the spatial structure of phenomena. They assume that the pollutants are uniformly distributed within a parallelepiped. From a theoretical point of view, this is equivalent to assuming infinite diffusion coefficients, which provoke an instantaneous propagation of the pollutant introduced into the box under consideration. The pollutant present in the box originates from internal sources or from external contributions transported by wind or flows through the summit as a consequence of variations in height of the box itself, which generally coincides with the ML height.

In mathematical terms, the continuity equation that describes the aforementioned phenomenon is formulated as

$$X \cdot h \frac{\partial C}{\partial t} = X \cdot Q + h \cdot u(C_b - C) + X \frac{\partial h}{\partial t}(C_a - C) \tag{5.14}$$

where

Q is the time average emission flux of pollutants for unit area
t is time
C is the concentration at time t within the box
X is the length of the box along the wind direction
h is the depth of the box
u is the time averaged wind speed through the box
C_a is concentration at the box top boundary
C_b is concentration at the upwind boundary

In Equation 5.14, the last term is considered only if $\partial h/\partial t > 0$ (box height increasing); the box (Y) width does not appear because it multiplies all the terms of the equation. In Equation 5.14, the first member expresses the velocity at which the pollutant accumulates in the box.

Limited to stationary conditions ($\partial C/\partial t = \partial h/\partial t = 0$), and considering null the upwind concentration ($C_b = 0$), Equation 5.14 can be simplified as

$$C = \frac{Q \cdot X}{h \cdot u} \tag{5.15}$$

"Multibox" models also exist, in which the area of study comprises several contiguous communicating boxes. In each box, the concentration of the pollutant is uniformly distributed and the horizontal flow of exit from a box is the entry one of the contiguous box (Stern, 1976; Zannetti, 1990).

5.3.6 Gaussian Models

The Gaussian approach is widely used in air pollution studies to model the statistical properties of the concentration of contaminants emitted in the PBL.

The conditions under which the mean concentration of a pollutant species emitted from a point source can be assumed to have a Gaussian distribution are highly idealized, since they require stationary and homogeneous turbulence. In the PBL, the flow may be assumed to be quasi-stationary for suitably short periods of time (ca. 10 min to 1 h). However, due to the presence of the surface, there are variations with height of both the mean wind and turbulence that cannot always be disregarded.

Much effort has been devoted to the development of non-Gaussian models for handling the nonhomogeneous structures of PBL turbulence. However, they still result in excessively large computer runs, either for emergency response applications or for calculating concentration time series over a long time (e.g., a year). The latter is

especially important in the evaluation of violations of air pollution standards, which are often expressed in high percentiles.

Conversely, Gaussian models are fast, simple, do not require complex meteorological input, and describe the diffusive transport in an Eulerian framework, making the use of the Eulerian nature of measurements easy.

For these reasons, they are still widely employed for regulatory applications by environmental agencies all over the world. Nonetheless, because of their well-known intrinsic limits, the reliability of a Gaussian model strongly depends on the way the dispersion parameters are determined on the basis of the turbulence structure of the PBL and the model's ability to reproduce experimental diffusion data. A great variety of formulations exist (Hanna et al., 1977; Briggs, 1985; Berkowicz et al., 1986; Hanna, 1986; Bowen, 1994; Erbrink, 1995; Mohan and Siddiqui, 1997).

The Gaussian solution in a system of coordinates where x is along the direction of the wind, y is transversal to wind, z is the height, and source of intensity Q is located at $(0, 0, H)$, can be written as

$$C(x,y,z) = Q/(2\pi u\sigma_y\sigma_z)\exp(-y^2/(2\sigma_y^2))[\exp((z-H)^2/(2\sigma_z^2)) + \exp((z+H)^2/(2\sigma_z^2))] \tag{5.16}$$

where σ_y and σ_z are functions of the distance from the source and turbulent intensity, and are determined experimentally.

The physical phenomenon of diffusion of emitted material is therefore mathematically described by such models through the faster or slower "broadening" (expressed by an increase in the numerical value of the "sigmas") of a Gaussian curve (see Figure 5.1).

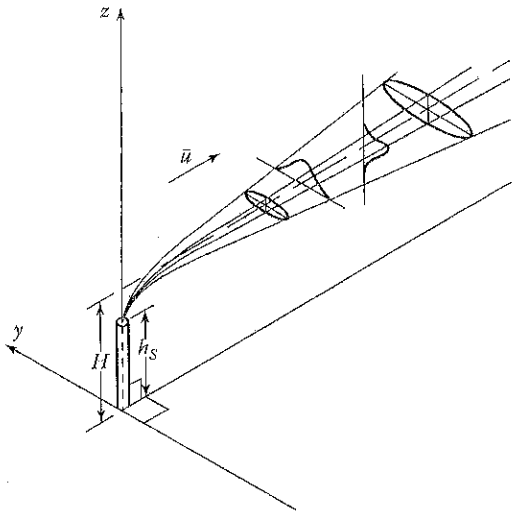

FIGURE 5.1 Gaussian distribution of a plume in a system of reference oriented in the direction of mean wind.

Gaussian models can simulate complex, area or volume sources, both by the spatial integration of the contribution of emissions (made possible because Gaussian models are linear to emissions), and, to obviate the difficulties of integration, by using special algorithms.

In practice, they can be relatively easy to use, and can be applied in numerous conditions (e.g., isolated sources, cities, road traffic, complex terrain). Moreover, bearing in mind that in practical applications, meteorological data are not generally available at both ground level and aloft at high temporal/spatial resolution, their performances are not poorer than those of other models. For these reasons, most operative models are based on the Gaussian approach.

The Gaussian model can be modified so as to extend its applicability to nonstationary and nonhomogeneous conditions, as well as to more complex orography. In particular, the breaking down of the plume into puffs has permitted the simulation of pollutant dispersion in pseudostationary conditions. Such models, illustrated below, decompose the plume into puffs, whose characteristics evolve in time and space together with the changing meteorological and emission conditions.

The various versions of Gaussian models essentially differ in the techniques utilized to calculate the "sigmas" as a function of atmospheric stability and the downwind distance from the emission source.

5.4 SEMIEMPIRICAL EXPRESSIONS OF THE σ

Several schemas exist for the calculation of σ_y and σ_z as functions of stability classes and of the downwind distance from the source.

Stability classes can in fact be calculated with semiempirical techniques using, for example, the method of Pasquill (Pasquill and Smith, 1983) based on simple meteorological observations (Tables 5.1 and 5.2) such as wind velocity, insolation,

TABLE 5.1
Stability Classification

		Wind Velocity at the Ground (m/s)				
Insolation/Cloud Cover		<2	≥2 and <3	≥3 and <5	≥5 and <6	≥6
Day	Strong insolation	A	A–B	B	C	C
	Moderate insolation	A–B	B	B–C	C–D	D
	Weak insolation	B	C	C	D	D
Day or night	Overcast	D	D	D	D	D
Night	Thin overcast or ≥0.5		E	D	D	D
	Thin overcast or ≤0.4		F	E	D	D

Source: Pasquill, F. and Smith, F.B., *Atmospheric Diffusion*, Halsted Press, John Wiley & Sons, New York, 1983.

Note: A, strongly unstable; B, unstable; C, weakly unstable; D, neutral; E, weakly stable; and F, stable.

TABLE 5.2
Classification of Atmospheric Stability

Stability Class	Stability Class of Pasquill	σ_θ (°)	Vertical Temperature Gradient (°C/m 10^{-2})	Richardson Number at 2 m	$\sigma_w/\bar{u}$
Very unstable	A	25.0	<–1.9	–0.9	>0.15
Moderately unstable	B	20.0	–1.9 to –1.7	–0.5	0.1 to 0.15
Slightly unstable	C	15.0	–1.7 to –1.5	–0.15	0.1 to 0.15
Neutral	D	10.0	–1.5 to –0.5	0	0.05 to 0.1
Slightly stable	E	5.0	–0.5 to 1.5	0.4	0 to 0.05
Moderately stable	F	2.5	1.5 to 4.0	0.8	0 to 0.05

Source: Zannetti, P., *Air Pollution Modelling*, Computational Mechanics Publications, Southampton, U.K. and Van Nostrand Reinhold, New York, 1990.

Note: σ_θ is the standard deviation of horizontal wind direction. $\bar{U}$ is the mean wind velocity. σ_w is the standard deviation of mean vertical wind velocity.

and, at night, cloud cover. Other techniques adopt measurements of the standard deviations of vertical wind velocity σ_w, horizontal wind direction σ_θ, the vertical gradient of temperature $\Delta T/\Delta z$, and the Richardson number, as illustrated in Table 5.2. Evaluations of stability classes through the standard deviation of wind velocity must be corrected in the nighttime, following Table 5.3, as proposed by Irwin (1980).

Once the stability classes have been evaluated, the "sigmas" are expressed as a function of distance downwind x, using one of the many formulae available in the literature, retrieved from experimental campaigns.

The Pasquill-Gifford sigmas (Gifford, 1961), presented in analytic form by Green et al. (1980) can be written as

$$\sigma_y(x) = \frac{k_1 x}{\left[1+\left(x/k_2\right)\right]^{k_3}} \tag{5.17a}$$

$$\sigma_z(x) = \frac{k_4 x}{\left[1+\left(x/k_2\right)\right]^{k_5}} \tag{5.17b}$$

where k_1, k_2, k_3, k_4, and k_5 are constants that vary according to atmospheric stability (see Zannetti, 1990).

TABLE 5.3
Correction of the Unstable Stability at Nighttime

Category Identified by σ_θ	Wind Velocity at 10 m (m/s)	Correct Nighttime Category
A	<2.9	F
	2.9–3.6	E
	>3.6	D
B	<2.4	F
	2.4–3.0	E
	>3.0	D
C	<2.4	E
	≥2.4	D

Source: Irwin, J.S., Estimating plume dispersion—A recommended generalized scheme, *Fourth AMS Symposium on Turbulence and Diffusion*, Reno, NV, 1980.

Note: Nighttime is considered to be from 1 h before sunset to 1 h after sunrise.

The Brookhaven sigmas (Smith, 1968), for which a power law is assumed (for both σ_y and σ_z), are written as

$$\sigma = ax^b \tag{5.18}$$

where the coefficients a and b vary according to the stability classes.

Briggs's sigmas (Briggs, 1973) distinguish between diffusion in the open country and urban environment (Table 5.4).

More recently, the "sigmas" have been expressed as functions of continuous variables of atmospheric turbulence. Most of them are based on the approach proposed by Pasquill (1971). He retained the essential features of Taylor's statistical theory, but evaluated the dispersion parameters in terms of the turbulence quantities and their related timescale using the following expressions:

$$\sigma_y = \sigma_v t S_y\left(t/T_L\right) \tag{5.19a}$$

$$\sigma_z = \sigma_w t S_z\left(t/T_L\right) \tag{5.19b}$$

where

σ_v and σ_w are the standard deviations of the transversal and vertical components of wind velocity

S_y and S_z are universal functions of the diffusion time t and Lagrangian timescale T_L

TABLE 5.4
Briggs's Sigma (1973) in the Open Country and Urban Environment

Pasquill	σ_y (m)	σ_z (m)
Urban dispersion parameters* (for distances between 100 and 10,000 m)		
A–B	$0.32x(1+0.0004x)^{-0.5}$	$0.24x(1+0.001x)^{0.5}$
C	$0.22x(1+0.0004x)^{-0.5}$	$0.20x$
D	$0.16x(1+0.0004x)^{-0.5}$	$0.14x(1+0.0003x)^{-0.5}$
E–F	$0.11x(1+0.0004x)^{-0.5}$	$0.08x(1+0.00015x)^{-0.5}$
Rural dispersion parameters (for distances between 100 and 10,000 m)		
A	$0.22x(1+0.0001x)^{-0.5}$	$0.20x$
B	$0.16x(1+0.0001x)^{-0.5}$	$0.12x$
C	$0.11x(1+0.0001x)^{-0.5}$	$0.08x(1+0.0002x)^{-0.5}$
D	$0.08x(1+0.0001x)^{-0.5}$	$0.06x(1+0.0015x)^{-0.5}$
E	$0.06x(1+0.0001x)^{-0.5}$	$0.03x(1+0.0003x)^{-1.0}$
F	$0.04x(1+0.0001x)^{-0.5}$	$0.016x(1+0.0003x)^{-1.0}$

Source: Briggs, G.A., Diffusion estimation for small emissions, in environmental research laboratories, air resources atmospheric turbulence and diffusion laboratory, Annual report, 1973. USAEC Report ATDL-106, National Oceanic and Atmospheric Administration, December 1974.

Reported below is a scheme based on the similarity theory and the micrometeorological variables proposed by Irwin (1983), which is included in several regulatory models:

$$\sigma_y = (\overline{v'^2})^{1/2} TF_y(T', T_{Lv}) \tag{5.20}$$

$$\sigma_z = (\overline{w'^2})^{1/2} TF_z(T, T_{Lw}) \tag{5.21}$$

with

$$F_y = \left[1 + 0.9(T/1000)^{1/2}\right]^{-1} \tag{5.22}$$

$$F_z = \left[1 + 0.9(T/500)^{1/2}\right]^{-1} \quad L < 0 \tag{5.23}$$

$$F_z = \left[1 + 0.945(T/100)^{0.806}\right]^{-1} \quad L > 0 \tag{5.24}$$

Modern expression of the "sigmas," in terms of wind variance and the Lagrangian integral timescale, on the basis of an atmospheric turbulence spectra model, are presented in Mangia et al. (1998).

5.5 GAUSSIAN MODEL EXTENSIONS

As mentioned above, the Gaussian model can be modified to allow the simulation of dispersion in certain cases:

- Linear, area, and volumetric sources of emission
- Complex terrains (valleys, cities, and coastal areas)
- Particular meteorological conditions, such as those leading to the phenomena of fumigation or confinement of pollutants
- Diffusion of heavy or reactive pollutants

There also so-called climatological models, in which each concentration value calculated by an equation similar to Equation 5.10 is attributed a weight, depending on the frequency of occurrence of the meteorological conditions corresponding to the given concentration value (Tirabassi et al., 1989; Zannetti, 1990).

To extend the range of applicability of the Gaussian method also to nonhomogeneous and nonstationary conditions, puff models have been developed. Here, the plume emitted is subdivided into a series of independent elements, which evolve as a function of the variation of meteorological conditions in space and time (Zanetti, 1990).

5.5.1 Gaussian Puff Models

Puff models were introduced to simulate the behavior of pollutants in nonhomogeneous and nonstationary meteorological and emission conditions (Zannetti, 1990). The emission is discretized in a temporal succession of puffs, each of which shifts into the area of calculus thanks to a three-dimensional wind field that is time variable.

Gaussian puff models assume that each emission of pollutants in a time interval Δt releases into the atmosphere a mass of pollutants $\Delta M = Q\Delta t$, where Q is the emission rate, which is variable in time.

Each puff contains the mass ΔM, and its baricenter is transported by the wind, which may vary in space and time.

If at time t the center of a puff is localized at $\mathbf{p}(t) = (x_p, y_p, z_p)$, then the contribution of this puff to the calculated concentration in the receptor place at $\mathbf{r} = (x_r, y_r, z_r)$ is given by the following relation:

$$\Delta c = \frac{\Delta M}{(2\pi)^{3/2}\sigma_h^2\sigma_z} \exp\left[-\frac{1}{2}\left(\frac{x_p - x_r}{\sigma_h}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{y_p - y_r}{\sigma_h}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{z_p - z_r}{\sigma_z}\right)^2\right] \tag{5.25}$$

which is Gauss's distribution for the concentration field of a single puff. Equation 5.25 requires the evaluation of σ_z and σ_h for every single puff. The total concentration of

a pollutant retrieved by a receptor is calculated by summing the contributions Δc of all the puffs emitted by all the sources present.

A crucial difference between expressions (5.16) and (5.25) should be noted: in the latter a different diffusion term replaces the advection term, with the resulting disappearance of the mean wind velocity u from the expression. This means that in a puff model the wind velocity influences the calculation of the concentration only in the density of puffs in the region of diffusion (the lower the wind velocity, the closer the puffs emitted by a source). For this reason, puff models, unlike the Gaussian model described in Equation 5.16 (the concentration tends to the infinity for u tending toward zero), can be used to simulate diffusion in calm wind conditions.

Puff models are also suitable for the simulation of diffusion over complex orographies: in this case a three-dimensional wind field must be reconstructed from orographic characteristics and available anemometric measurements.

5.6 SPECIAL ALGORITHMS UTILIZED IN GAUSSIAN AND ANALYTIC MODELS

Gaussian and analytic models generally make use of algorithms based on empirical considerations to describe complex real situations. The various models presented in the literature are differentiated according to the algorithms adopted. Listed below are some phenomena relative to such situations.

5.6.1 Plume Rise

Once emitted into the atmosphere, plume tends to continue to rise due to is initial momentum. If hot, the rise is also caused by Archimede's force. In fact, warm fumes are less dense and therefore lighter than the surrounding air. Different formulae are presented in the literature to describe this phenomenon. The most commonly used are those developed by Briggs (Briggs, 1975).

5.6.2 Downwash

This phenomenon arises from the perturbation of the wide field and turbulence caused by structures present in the area of pollutant emission. There are two types of downwash: stack downwash and building downwash. Stack downwash refers to the lowering of the plume due to the perturbation of the wind field caused by the source itself. It is evaluated through an artificial decrease in the emission source height.

Building downwash is a distortion of the plume caused by buildings situated in proximity of the source. The distortion is also evaluated through an empirical modification of the "sigmas."

5.6.3 Plume Trapping

It consists of the entrapment of pollutants in a layer of the atmosphere close to the ground due to a thermal inversion at a level higher than that of fume emission. Mathematically, the situation is described by Gaussian models as a multiple reflection of pollutants between the terrain and the base of the inversion.

5.6.4 Ground Deposition

Ground deposition of the diffuse material is evaluated by means of various algorithms. Listed below are those most commonly utilized.

- The decrease of material in the air is expressed by an exponential decrease on the basis of a value of the average life of the pollutant.
- The decrease of material in the air is expressed by a fictitious decrease of the emission flux as a function of the distance from the source.
- A lowering of the plume axis height is introduced as a function of the distance from the source to describe the fall due to the gravitational force of the diffuse material.
- The ground deposition flux is expressed as the concentration at the ground for an assigned constant deposition rate.
- Ground deposition due to meteoric precipitation is parameterized by an exponential decrease linked to the precipitation intensity.

5.6.5 Chemical Reactions

The mathematical description of the chemical transformation of the pollutants dispersed in the atmosphere is a highly complex field of study that remains far from any satisfactory solutions. On the one hand, basic problems exist in the knowledge and quantification of the chemical reactions occurring in the atmosphere, while on the other, there are considerable difficulties in representing reactions higher than the first order (particularly, with constant fast reactions). Generally speaking, semiempirical models empirically describe the impoverishment of a reactive pollutant by means of an exponential decrease on the basis of an assigned value of average lifetime of the pollutant. The K models prove to be theoretically most correct in representing the diffusion of chemically reacting material. However, they are limited by the fact that their characteristic time of transport and dispersion is not shorter than that of chemical reactions, which at times make description of dispersion with chemical reactions problematic, even using numerical models (Seinfeld and Pandis, 1997).

5.7 NEW OPERATIVE MODELS

As mentioned above, most operative models for estimating gas and particle dispersion in the atmospheric boundary layer are based on the Gaussian approach. Such models are founded on the hypothesis that the pollutant is dispersed in a homogeneous turbulence. However, due to the presence of terrain, turbulence is generally not homogeneous along the vertical direction. In addition, the inputs of Gaussian models often refer to simple turbulence schemes.

Over the past 20 years, following the works of Holtslag and van Ulden (1983), Weil and Brower (1984), van Ulden and Holtslag (1985), Trombetti et al. (1986),

TABLE 5.5
Values of *a* and *b* in Equation 5.26

Stability Class	*a*	*b*
A	−0.0875	−0.1029
B	−0.03849	−0.1714
C	−0.00807	−0.3049
D	0.0	0.0
E	0.00807	−0.3049
F	0.03849	−0.1714

and Beljaars and Holtslag (1990), it has been possible to evaluate the fundamental parameters for the description of the characteristics of the surface and atmospheric boundary layers using measurements close to the ground. This has allowed the development of models that describe pollutant diffusion using as input ground-based meteorological data (which can be acquired by automated networks), but which are able to evaluate directly atmospheric turbulence, through the value of the Monin-Obukhov length and the attrition velocity, rather than empirical classes, like those of Pasquill-Gifford.

A relation between the old stability classes and the new parameterization has been proposed by Golder (1972), through an experimental relation between L and stability classes (see also Trombetti et al., 1986). Algebraically, it is expressed by

$$1/L = a\, z_0^b \tag{5.26}$$

where

z_0 is the ground roughness
a and b are expressed as in Table 5.5

Among the new-generation models, of particular note are the Danish model OML (Berkowicz et al., 1986) and British model ADMS (Carruthers et al., 1992); the American model HPDM (Hanna and Paine, 1989), and new model AERMOD, proposed by the U.S. EPA. Among the puff models are CALPUFF (Scire et al., 1999), M4PUFF (Tirabassi and Rizza, 1997), and SPM (Tirabassi and Rizza, 1995).

5.8 EVALUATION OF MODEL PERFORMANCES AND RELIABILITY

A correct use of atmospheric transport and diffusion models must be based on a study of their capacity to represent real situations correctly. When possible, it is advisable to test the reliability of the model adopted using the data of topographic and meteorological scenarios characteristic of the areas where they are deployed. Models are evaluated by

- Assessing the soundness of process descriptions
- Examining the computer code for errors
- Examining the reasonableness of the results
- Calculating the sensitivity of model results to change in inputs
- Comparing evaluated concentrations from different air pollution models
- Comparing simulated and observed concentrations

Usually, an air quality measurement network, whether in an urban or industrial site, is designed according to specific criteria, so that it alone cannot provide all the information necessary for the validation of a model: the number of points and typology of measurements, whether of chemical or meteorological parameters, are generally insufficient to provide an overall coverage of the territory, or to guarantee a complete range of information against which to test the model. This is perfectly understandable, since in designing a network that must function stably over an area the tendency is to minimize the number of measurement points, which are normally fixed, in order to give greater evidence to the time evolution of concentrations rather than their spatial distribution.

In general, a monitoring network can contribute to model validation, when it is suitably integrated with other sensors during intensive measurement campaigns specially organized for this purpose.

It must be borne in mind, when using models, that, while they are rather sophisticated instruments that ultimately reflect the current state of knowledge on turbulent transport in the atmosphere, the results they provide are subject to a considerable margin of error. This is due to various factors, in particular the uncertainty of the intrinsic variability of the atmosphere.

Models, in fact, provide values expressed as an average, that is, a mean value obtained by the repeated performance of many experiments, while the measured concentrations are a single value of the sample to which the ensemble average provided by models refer. This is a general characteristic of the theory of atmospheric turbulence and is a consequence of the statistical approach used in attempting to parameterize the chaotic character of the measured data. At the same time, the uncertainty linked to the stochastic character of the parameterization of the atmosphere depends on turbulence intensity and is a function of the mean sampling time. Atmospheric diffusion models ultimately present errors that can be reduced as an uncertainty inherent in the phenomenon they describe. The reducible errors originate from the use of an incorrect or insufficient set of input data and/or from the intrinsic inadequacies of the particular model. As previously noted, irreducible errors are due to the statistical nature of the parameterization of the turbulent fluxes responsible for the dispersion of the material emitted into the atmosphere. However, studies of model performance validation indicate errors in input data (both of emission and meteorology) to be the factor responsible for the greater contribution of the total uncertainty of models. Irwin et al. (1987), using Monte Carlo techniques to simulate to propagation of errors from those of input data, showed that the interval of error of the concentration maximum and of its distance from the source may be double the interval of error of the input data. A model is generally deemed acceptable if the estimated values are within a factor of two of the observed data.

A considerable amount of work has been done, especially in the United States, on the quantitative assessment of model performances. The adopted approach varies according to whether the validation refers to the scientific validity of the model or to the usefulness of the model in environmental management. In validations for management purposes, less importance is attributed to deterministic processes (processes of cause and effect), while attention is focused on the correspondence between observed and predicted values. For such analyses to be objective, it is necessary to utilize different data from those adopted for the parameterization of the model itself. Particular attention is paid, on the whole, to the comparison of concentration maxima both with and without temporal and/or spatial simultaneity.

Generally, the attempt is made to objectivize the validation of model performances by adopting statistical indices that describe their capacity to represent observed data. Among them, the most widely used are (Hanna, 1988):

nmse (normalized mean square) = $\overline{(C_o - C_p)^2} / \overline{C_o C_p}$

cor (correlation) = $\overline{(C_o - \overline{C}_o)(C_p - \overline{C}_p)}/\sigma_o\sigma_p$

fa2 = percentage of data for which $\mathbf{0.5 \le C_o/C_p \le 2}$

fb (fractional bias) = $(\overline{C}_o - \overline{C}_p)/(0.5(\overline{C}_o + \overline{C}_p))$

fs (fractional standard deviation) = $(\sigma_o - \sigma_p)/0.5(\sigma_o + \sigma_p)$

where the suffixes o and p respectively refer to observed and predicted concentrations, and the bar indicates the mathematical mean.

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