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16.6 Environmental Modeling

Air Pollution Dispersion Modeling

Paolo Zannetti

To understand air pollution, it is mandatory, at any scale, to simulate correctly the dispersion characteristics of the emissions. Therefore, the role of meteorology is essential. Pollutants are typically transported by two types of flows: an "ordered" flow, which is characterized by average wind speed and direction, and a semirandom, turbulent flow, which is characterized by wind fluctuations. All dispersion models aim at simulating these two components. As further discussed below, dispersion modeling techniques can be categorized into four general classes: (1) Gaussian models; (2) Eulerian grid models; (3) Lagrangian box models; and (4) Lagrangian particle models.

Gaussian Models

All Gaussian models assume that the concentration of pollutants maintains a Gaussian distribution in space. The Gaussian distribution, as illustrated in Figure 16.6.1, is a symmetrical bell-shaped distribution which is described at any given point x by two parameters: the location of the peak (in this case, the centerline of the plume indicated by the segmented line) and the standard deviation (in this case, the spread of the plume mass about its center). Therefore, the dilution rate of the plume is fully characterized by the two standard deviations, σ_y and σ_z , expressed as a function of the downwind distance, x .

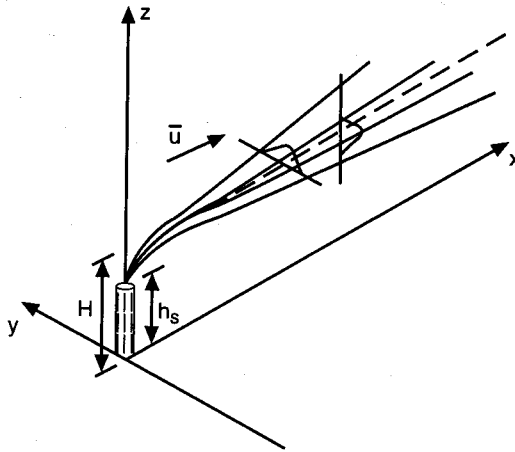


FIGURE 16.6.1 The Gaussian plume in a wind-oriented coordinate system (i.e., the wind is blowing toward the x axis). The plume is released from a source located at $(0, 0, h_s)$ and possesses an initial buoyancy. Therefore, the plume behaves as if it were originated from $(0, 0, H)$, where H is the effective emission height and $\delta h = H - h_s$ is the plume rise. The plume is advected by the average wind speed \bar{u} and expands in the horizontal and the vertical direction while maintaining a Gaussian distribution along both.

In mathematical notation, the Gaussian plume formula in Figure 16.6.1 can be written as

$$c = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{H-z}{\sigma_z}\right)^2\right] \quad (16.6.1)$$

where c is the concentration computed at the receptor (x, y, z) , Q is the emission rate, \bar{u} is the average horizontal wind speed, H is the effective emission height, and σ_y and σ_z are functions of the downwind

distance, x , with parameters that vary with the meteorological conditions (in fact, the stronger the turbulence intensity of the atmosphere, the larger the growth rate of σ_y and σ_z with x).

As can easily be seen, Equation (16.6.1) refers to a stationary state (i.e., c is not a function of time), uses meteorological parameters that must be considered homogeneous and stationary in the modeled area (i.e., between the source and the receptors at which concentrations are computed), and cannot work in calm conditions where the wind speed approaches zero (in general, the wind speed cannot be less than 1 m/sec when Equation (16.6.1) is applied). In spite of these limitations, the simplicity of the Gaussian approach, its relative ease of use, and, especially, the elevation of this methodology to the quantitative decision-controlling level in the United States (USEPA, 1978) have stimulated research aimed at removing some of the limitations of the Gaussian theory in modeling the real-world situations.

Equation (16.6.1) has been modified and expanded to incorporate, among others, the following factors: ground reflection, multiple reflections, hourly simulations, deposition and decay, chemical transformation, fumigation, complex terrain, gravitational settling, calm conditions, nonstationary and nonhomogeneous conditions, and long-term simulations. We summarize below some of these improvements.

Reflection terms can be added to Equation (16.6.1) to account for partial or total reflection of concentration at the ground. Similarly, reflection can be added at the top of the **planetary boundary layer, PBL** (typically, about 500 to 1000 m above the ground). If both reflections are implemented, the plume is trapped inside the PBL. Equation (16.6.1) is generally applied for periods of 1 hr. This allows the incorporation of time-varying emission and meteorological parameters. Chemistry and decay can be incorporated by introducing exponential decay terms (for example, it can be assumed that an emission of primary gaseous SO_2 is transformed into particulate matter SO_4^{2-} at a rate of 1% per hour). Gravitational settling will affect a plume of primary particulate matter. In this case, the plume centerline can be tilted to account for the settling velocity of the particles, which is a function of both particle size and density.

In addition to the Gaussian plume model, Gaussian segment and puff models can be used (Zannetti, 1986a). These models break up the plume into independent elements (plume segments or puffs) whose initial features and time dynamics are a function of time-varying emission and meteorological conditions encountered by the plume elements. These techniques allow us to account properly for nonhomogeneous, nonstationary conditions. Gaussian puff models, in particular, have the additional advantage of being able to simulate calm or low-wind conditions.

Complex terrain conditions affect the plume dynamics, both the motion of the centerline trajectory and the growth of σ_y and σ_z . Finally, the Gaussian plume model equation can be rewritten in a way to simulate long-term concentration averages (e.g., annual averages) by incorporating the joint frequency of occurrence of a predetermined set of emission and meteorological conditions.

Other Models

Eulerian grid models (Lamb [from Longhetto], 1980) simulate pollutant diffusion by superimposing a grid over the computational domain and numerically solving a mass-balance equation (typically, a partial differential equation, PDE, or a set of PDEs) in each grid cell at each time step. This is also called numerical integration. In general, the smaller the grid and time intervals, the more accurate the numerical solution.

Difficulties may be encountered in simulating atmospheric diffusion with the K-theory. In particular, the application of the K-theory to simulate vertical dispersion during daytime, unstable meteorological conditions is highly questionable. To improve the simulation ability of Eulerian grid models, equations of high-order moments of concentration, wind, and temperature fluctuations can be solved simultaneously. This approach is called high-order closure and requires the definition of more-complex, nonlinear relationships between the turbulent fluxes and the concentration fields.

Lagrangian box models are mostly used to perform fast simulations of photochemical smog. These models define a set of "boxes" (e.g., a column of boxes as illustrated in Figure 16.6.2) which are advected horizontally according to the local wind speed and direction. Each box encounters emissions along its trajectory. These emissions inject new pollutants inside the box. A full set of chemical reactions inside

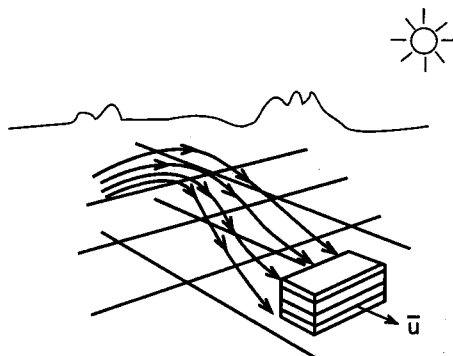


FIGURE 16.6.2 Lagrangian box modeling.

each box allows the simulation of the photochemical smog and the formation of secondary pollutants, such as ozone.

Lagrangian particle models provide a very interesting alternative method for simulating atmospheric diffusion. Particle motion can be produced by both deterministic velocities and semirandom pseudoveLOCITIES generated using Monte Carlo techniques. In the latter case, the trajectory of a single particle represents a realization from an infinite set of possible solutions, and, if enough particles are used, important characteristics can be inferred from the computation of particle **ensemble average** properties.

When using Lagrangian particle models to simulate air pollution, pollutant emissions (both gases and particulate matter) are represented by the injection of fictitious particles into the computational domain. Each particle represents a specified amount of pollution and is moved at each time step by a pseudoveLOCITY that is time and space dependent. Zannetti (1990) discusses alternative modeling approaches in more detail than is possible here.

Atmospheric Chemistry

Atmospheric chemistry deals essentially with four major issues (Seigneur, 1987): (1) photochemical smog in sunny, urban areas; (2) **aerosol** chemistry; (3) acidic deposition; and (4) air toxics. Chemical reactions can be simulated in two ways: (1) with simple first-order terms (e.g., a decay term) and (2) with a full chemical reaction scheme.

First-order terms for simulating atmospheric chemistry can be easily incorporated into any of the models previously discussed. For example, a radioactive pollutant with a specified decay rate (or half-life) can be simulated by introducing the following multiplicative term in any concentration equation

$$\exp(-t/T) \quad (16.6.2)$$

where t is the travel time and T is the time scale of the decay (easily related to the half-life of the chemical species). Similarly, chemical transformation from a primary to a secondary pollutant (e.g., from gaseous SO_2 to sulfate particulate matter, SO_4^{2-}) can be accomplished by introducing two exponential terms— $[\exp(-t/T)]$ and $[1 - \exp(-t/T)]$ —having the effect of simultaneously decreasing the SO_2 concentration and increasing the SO_4^{2-} concentration as time increases. First-order schemes, though relatively simple, may use parameters that are space and time dependent; for example, the SO_2 -to- SO_4^{2-} conversion rate may vary as a function of relative humidity and solar radiation.

Photochemical smog, which in the past only affected large cities at low latitudes, such as Los Angeles, has become today the most important and common air pollution problem in urban areas throughout the world. Overall, the photochemical smog reactions can be summarized as



where ROG are primary reactive organic gases and NO_x include primary NO and mostly secondary NO_2 . This smog includes carbon monoxide (CO), ozone (O_3), formaldehyde (HCHO), peroxyacetyl nitrate (PAN), nitric acid (HNO_3), particulate matter (PM; especially secondary particles, such as nitrates and organic particles), and other products.

A full chemical reaction scheme is required to simulate complex phenomena, such as the photochemical smog described above, and can be incorporated today only inside Eulerian grids or Lagrangian box models. A typical reaction set, applied in each grid cell at each time step, can be written in terms of linear combinations:

$$\sum_{m=1}^M r_{nm} C_m \rightarrow \sum_{m=1}^M p_{nm} C_m \quad n = 1, 2, \dots, N \quad (16.6.4)$$

where M species participate in N reaction steps, c_m is the concentration of the m th species, and r_{nm} and p_{nm} are numerical constants. Each reaction rate is generally expressed as a product of the concentrations of the species involved, with a temperature-dependent rate constant.

The main difficulty in using Equation (16.6.4) to simulate the photochemical smog is the treatment of **organic compounds**. In fact, due to the very large number, organic species cannot all be included explicitly. Three different types of gas-phase chemical mechanisms are generally used: (1) surrogate mechanisms, which use the chemistry of one or two compounds in each class of organics to represent the chemistry of all species in that class; (2) lumped mechanisms, in which the grouping of chemical compounds is done on the bases of their similar structure and reactivity; and (3) the carbon bond approach, which splits each organic molecule into functional groups using the assumption that the reactivity of the molecule is dominated by the chemistry of each functional group. Each classification technique necessarily introduces a simplification and, therefore, a potential simulation error.

Some key reactions involve the **photolysis** of such species as NO_2 , HCHO, and nitrous acid (HONO). These one-specie reactions require the calculation of the photolysis rate constant which is a function of, among other things, of solar elevation and temperature.

Aerosol chemistry is particularly difficult to simulate and computationally expensive. However, inclusion of aerosol dynamics within air quality models is of primary importance because of the health effects associated with fine particles in the atmosphere, visibility impairment, and the acid deposition problem. Simple first-order reaction terms can be used to simulate the transformation of SO_2 into sulfates and NO_x into nitrates. These terms can be included in any model. However, a comprehensive simulation of aerosol processes can only be performed within an Eulerian grid or a Lagrangian box model and must include the following fundamental equation of aerosol dynamics (Milford and Russell, 1993) which describes aerosol transport, growth, coagulation, and sedimentation

$$\frac{\delta n}{\delta t} + \nabla \cdot \bar{\mathbf{u}}n + \frac{\delta I}{\delta v} = \frac{1}{2} \int_0^v \beta(\bar{\mathbf{v}}, \mathbf{v} - \bar{\mathbf{v}}) n(\bar{\mathbf{v}}) n(\mathbf{v} - \bar{\mathbf{v}}) d\bar{\mathbf{v}} - \int_0^\infty \beta(\bar{\mathbf{v}}, \mathbf{v}) n(\bar{\mathbf{v}}) n(\mathbf{v}) d\bar{\mathbf{v}} - \nabla \cdot \mathbf{C}n \quad (16.6.5)$$

where n is the particle size distribution function, $\bar{\mathbf{u}}$ is the wind velocity, I is the droplet current that describes particle growth and nucleation due to gas-to-particle conversion, v is the particle volume, β is the rate of particle coagulation, and \mathbf{C} is the sedimentation velocity.

The simulation of heterogeneous and aqueous-phase chemistry is of key importance for regional-scale acid deposition and **stratospheric** ozone models, but is usually neglected in urban photochemical applications where the main goal is the simulation of **tropospheric** ozone.

Deposition

Chemical species are removed from the atmosphere by two mechanisms: reaction and deposition. While chemical reactions may produce new pollutants, deposition is the real process in which the atmosphere cleans itself. Some pollutants are highly reactive and, consequently, have short lifetimes. For example,

ozone has a typical lifetime of 2 min and, therefore, its concentration will drop unless it is continuously regenerated. Other pollutants have longer lifetimes. For example, SO₂ has a typical lifetime of 13 days. Therefore, under certain circumstances, it can easily accumulate during multiday episodes (e.g., the "London" smog). Finally, there are pollutants with very large lifetimes. Because of their low reactivity, they do not cause adverse effects on human health but, nevertheless, can diffuse on a global scale and affect the thermal balance of the Earth. Methane and carbon dioxide are a good example, both with a typical lifetime of 7 years.

Deposition terms can be introduced in any model discussed above. For example, dry deposition can be described by the following formula

$$F_i = V_d c_i \quad (16.6.6)$$

where F_i is the flux of a species i to the ground, c_i is the concentration of the species i at some reference height (e.g., 1 m), and V_d is the deposition velocity. The term V_d has been measured under various meteorological conditions and for a number of surface types (Wesley et al., 1985). Therefore, the calculation of F_i is straightforward.

Wet deposition (i.e., precipitation scavenging) depends upon the intensity and size of raindrops. Fog and cloud droplets can also absorb gases, capture particles, and accelerate chemical reactions. Wet deposition is quantified by computing the wet flux of pollution to the surface. This calculation requires the estimate of the washout coefficient, which can be inferred (Scott, 1982) as a function of storm type and precipitation amounts.

Because of dry and wet deposition, acidic components such as sulfuric acid particles, particulate nitrate, and nitric acid gas are transferred from the atmosphere to the Earth. Areas which are tens and hundreds of kilometers downwind of large SO₂ and NO_x sources (e.g., power plants and smelters) suffer the greatest impact.

Statistical Models

Statistical models are often used in air pollution studies. They include frequency distribution studies, time series analysis, Kalman filters, receptor-modeling techniques, and others. A general distinction between statistical and deterministic approaches is that air pollution deterministic models initiate their calculations at the pollution sources and aim at the establishment of cause/effect relationships, while statistical models are characterized by their direct use of air quality measurements to infer semiempirical relationships. Although very useful, especially for real-time short-term forecasting, statistical models are generally unable to provide cause/effect relationships, with the exception of receptor modeling.

The basic concept of the receptor-modeling approach is the apportionment of the contribution of each source, or group of sources, to the measured concentrations without reconstructing the dispersion pattern and trajectory of the pollutants. Typically, receptor models start with *observed* ambient aerosol concentrations measured at a receptor and seek to apportion the concentrations among several source types (e.g., industrial, transportation, soil, etc.), based on the known chemical composition (i.e., the chemical fractions) of source and receptor materials.

In mathematical notation, the concentration c_{ik} of the species i in the k th sample at a certain monitoring station can be written as

$$c_{ik} = \sum_{j=1}^p a_{ij} D_{jk} E_{jk} \quad (16.6.7)$$

where p sources (or groups of sources) are assumed to contribute to c_{ik} , a_{ij} is the fractional amount of the component i in the emission from the j th source, D_{jk} is the atmospheric dispersion term, and E_{jk} is the emission rate (i.e., $D_{jk} E_{jk} = S_{jk}$ is the total contribution of the source j to the k th sample at the receptor location). Dispersion models assume a_{ij} , D_{jk} , and E_{jk} to be known (or obtainable from emission and