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Chapter 2

Air Pollution Modeling – An Overview

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Abstract: This chapter presents a brief review of air pollution modeling techniques, i.e., computer methods for the simulation of air quality processes. The review includes models developed or recommended by governmental agencies for regulatory applications. Both non-reactive (e.g., plume models) and reactive (e.g., photochemical models) are discussed. We also provide Web sites where the reader can download modeling software.

Key Words: Air pollution, Computer modeling, Eulerian and Lagrangian models, Gaussian models, puff models, photochemical models.

1 Introduction[1]

Air pollution modeling is a numerical tool used to describe the causal relationship between emissions, meteorology, atmospheric concentrations, deposition, and other factors. Air pollution measurements give important, quantitative information about ambient concentrations and deposition, but they can only describe air quality at specific locations and times, without giving clear guidance on the identification of the causes of the air quality problem. Air pollution modeling, instead, can give a more complete deterministic description of the air quality problem, including an analysis of factors and causes (emission sources, meteorological processes, and

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[1] Builtjes, P. (2003) The Problem – Air Pollution. Chapter 1 of AIR QUALITY MODELING – Theories, Methodologies, Computational Techniques, and Available Databases and Software. Vol I – Fundamentals (P. Zannetti, Editor). EnviroComp Institute (http://www.envirocomp.org/) and Air & Waste Management Association (http://www.awma.org/).

physical and chemical changes), and some guidance on the implementation of mitigation measures.

Air pollution models play an important role in science, because of their capability to assess the relative importance of the relevant processes. Air pollution models are the only method that quantifies the deterministic relationship between emissions and concentrations/depositions, including the consequences of past and future scenarios and the determination of the effectiveness of abatement strategies. This makes air pollution models indispensable in regulatory, research, and forensic applications.

The concentrations of substances in the atmosphere are determined by: 1) transport, 2) diffusion, 3) chemical transformation, and 4) ground deposition. Transport phenomena, characterized by the mean velocity of the fluid, have been measured and studied for centuries. For example, the average wind has been studies by man for sailing purposes. The study of diffusion (turbulent motion) is more recent. Among the first articles that mention turbulence in the atmosphere, are those by Taylor (1915, 1921).

2 Modeling of Point Sources

One of the first challenges in the history of air pollution modeling (e.g., Sutton, 1932, Bosanquet, 1936) was the understanding of the diffusion properties of plumes emitted from large industrial stacks. For this purpose, a very successful, yet simple model was developed – the Gaussian Plume Model. This model was applied for the main purpose of calculating the maximum ground level impact of plumes and the distance of maximum impact from the source.

The Gaussian plume model is illustrated in the figure below (Courtesy: Figure 19-5 of Boubel et al., 1994). The model was formulated by determining experimentally the horizontal and vertical spread of the plume, measured by the standard deviation of the plume's spatial concentration distribution.

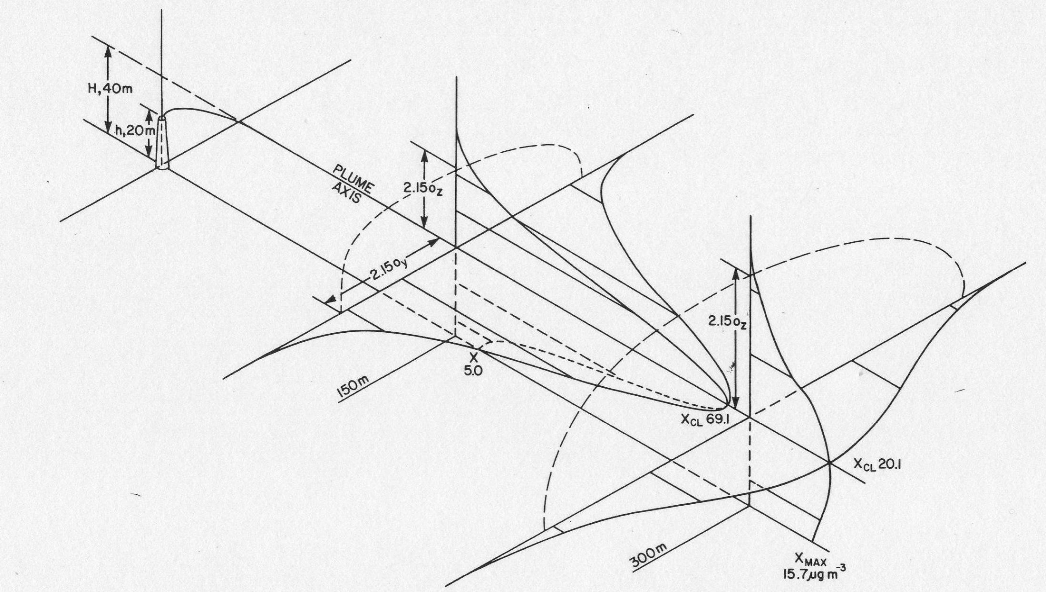

Fig. 19-5. Two cross sections through a Gaussian plume (total mass under curves conserved).

Experiments provided the geometrical description of the plume by plotting the standard deviation of its concentration distribution, in both the vertical and horizontal direction, as a function of the atmospheric stability and downwind distance from the source. The plotting is presented in the figure below (Courtesy: Figure 19-6 of Boubel et al., 1994).

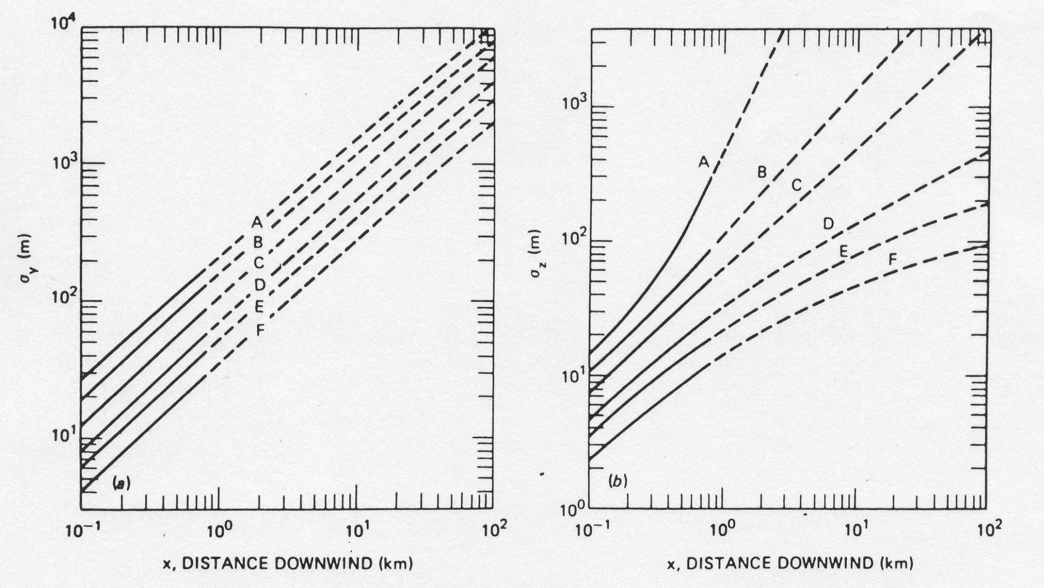

Fig. 19-6. Pasquill–Gifford σ_y (left) and σ_z (right). Source: From Gifford (12).

Atmospheric stability is a parameter that characterizes the turbulent status of the atmosphere. This parameter ranges from "very stable", class F, to "neutral", class D, up to "very unstable", class A.

The experimental sigma values discussed above are, in their functions with distance from the source, in reasonable agreement with the Taylor-theory. The differences are caused by the fact that the Taylor-theory holds for homogeneous turbulence, which is not the exact case in the atmosphere.

In the 1960s, the studies concerning dispersion from a point source continued and were broadening in scope. Major studies were performed by Högstrom (1964), Turner (1964), Briggs (1965) (the developer of the well-known plume-rise formulas), Moore (1967), Klug (1968). The use and application of the Gaussian plume model spread over the whole globe, and became a standard technique in every industrial country to calculate the stack height required for permits, see for example Beryland (1975) who published a standard work in Russian. The Gaussian plume model concept was soon applied also to line and area-sources. Gradually, the importance of the mixing height was realized (Holzworth, 1967, Deardorff, 1975) and its major influence on the magnitude of ground level concentrations. To include the effects of the mixing height, multiple reflections terms were added to the Gaussian Plume model (e.g., Yamartino, 1977).

3 Air Pollution Modeling at Urban and Larger Scales

Shortly after 1970, scientists began to realize that air pollution was not only a local phenomenon. It became clear - firstly in Europe - that the SO_2 and NO_x emissions from tall stacks could lead to acidification at large distances from the sources. It also became clear - firstly in the US - that ozone was a problem in urbanized and industrialized areas. And so it was obvious that these situations could not be tackled by simple Gaussian-plume type modeling.

Two different modeling approaches were followed, Lagrangian modeling and Eulerian modeling. In Lagrangian modeling, an air parcel (or “puff”) is followed along a trajectory, and is assumed to keep its identity during its path. In Eulerian modeling, the area under investigation is divided into grid cells, both in vertical and horizontal directions.

Lagrangian modeling, directed at the description of long-range transport of sulfur, began with studies by Rohde (1972, 1974), Eliassen (1975) and Fisher (1975). The work by Eliassen was the start for the well-known EMEP-trajectory model which has been used over the years to calculate trans-boundary air pollution of acidifying species and later, photo-oxidants. Lagrangian modeling is often used to cover longer periods of time, up to years.

Eulerian modeling began with studies by Reynolds (1973) for ozone in urbanized areas, with Shir and Shieh (1974) for SO_2 in urban areas, and Egan (1976) and Carmichael (1979) for regional scale sulfur. From the modeling studies by Reynolds on the Los Angeles basin, the well-known Urban Airshed Model-UAM originated for photochemical simulations. Eulerian modeling, in these years, was used only for specific episodes of a few days.

So in general, Lagrangian modeling was mostly performed in Europe, over large distances and longer time-periods, and focused primarily on SO_2. Eulerian grid modeling was predominantly applied in the US, over urban areas and restricted to episodic conditions, and focused primarily on O_3. Also hybrid approaches were studied, as well as particle-in-cell methods (Sklarew et al., 1971). Early papers on both Eulerian and Lagrangian modeling are by Friedlander and Seinfeld (1969), Eschenroeder and Martinez (1970) and Liu and Seinfeld (1974).

A comprehensive overview of long-range transport modeling in the seventies was presented by Johnson (1980).

The next, obvious step in scale is global modeling of earth's troposphere. The first global models were 2-D models, in which the global troposphere was averaged in the longitudinal direction (see Isaksen, 1978). The first, 3-D global models were developed by Peters (1979) (see also Zimmermann, 1988).

It can be stated that, since approximately 1980, the basic modeling concepts and tools were available to the scientific community. Developments after 1980 concerned the fine-tuning of these basic concepts.

4 Examples of Dispersion Models

We present below some discussion on specific air computer models that are particularly important and are used by a large community of scientists.

The US-EPA today recommends the following two computer packages for simulation of non-reactive chemicals (e.g., SO2):

- AERMOD: http://www.epa.gov/scram001/dispersion_prefrec.htm#aermod

  AERMOD is a steady-state Gaussian plume model. It uses a single wind field to transport emitted species. The wind field is derived from surface, upper-air, and onsite meteorological observations. AERMOD also combines geophysical data such as terrain elevations and land use with the meteorological data to derive boundary layer parameters such as Monin-Obukhov length, mixing height, stability class, turbulence, etc.

  AERMOD is today replacing the ISC models for most regulatory applications in the US.

- CALPUFF: http://www.epa.gov/scram001/dispersion_prefrec.htm#calpuff

CALPUFF is a non-steady state Lagrangian puff dispersion model. The advantage of this model over a Gaussian-based model is that is can realistically simulate the transport of substances in calm, stagnant conditions, complex terrain, and coastal regions with sea/land breezes.

CALPUFF is particularly recommended fro long-range simulations (e.g., more than 50 miles) and studies involving the assessment of the visual impact of plumes.

With the development of the VISTAS Version 6 model[2], CALPUFF can use sub-hourly meteorological data and run with sub-hourly time steps. This version of CALPUFF is appropriate for both long-range and short-range simulations.

5 Photochemical Modeling[3]

Photochemical air quality models have become widely recognized and routinely utilized tools for regulatory analysis and attainment demonstrations by assessing the effectiveness of control strategies. These photochemical models are large-scale air quality models that simulate the changes of pollutant concentrations in the atmosphere using a set of mathematical equations characterizing the chemical and physical processes in the atmosphere. These models are applied at multiple spatial scales from local, regional, national, and global.

Some examples of photochemical models are the following:

- CMAQ: http://www.epa.gov/asmdnerl/CMAQ/index.html

  The primary goals for the Models-3/Community Multiscale Air Quality (CMAQ) modeling system are to improve 1) the environmental management community's ability to evaluate the impact of air quality management practices for multiple pollutants at multiple scales and 2) the scientist's ability to better probe, understand, and simulate chemical and physical interactions in the atmosphere. The newest Models-3/CMAQ version 4.5 is now available for download from the CMAS Website: http://www.cmascenter.org/download/release_calendar.cfm?temp_id=99999

- CAMX: http://www.camx.com/

  The Comprehensive Air quality Model with extensions is a publicly available open-source computer modeling system for the integrated assessment of gaseous and particulate air pollution. Built on today's

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[2] http://www.src.com/html/verio/download/download.htm

[3] http://www.epa.gov/scram001/photochemicalindex.htm

understanding that air quality issues are complex, interrelated, and reach beyond the urban scale, CAMx is designed to

- Simulate air quality over many geographic scales
- Treat a wide variety of inert and chemically active pollutants:
    - Ozone
    - Inorganic and organic PM2.5/PM10
    - Mercury and toxics
- Provide source-receptor, sensitivity, and process analyses
- Be computationally efficient and easy to use

The U.S. EPA has approved the use of CAMx for numerous ozone and PM State Implementation Plans throughout the U.S, and has used this model to evaluate regional mitigation strategies.

- UAM: http://uamv.saintl.com/

  The Urban Airshed Model® (UAM®) modeling system, developed and maintained by Systems Applications International (SAI), is the most widely used photochemical air quality model in the world today. Since SAI's pioneering efforts in photochemical air quality modeling in the early 1970s, the model has undergone nearly continuous cycles of application, performance evaluation, update, extension, and improvement. Other photochemical models have been developed during this long period, but no model today is more reliable or technically superior.

- CALGRID: http://www.arb.ca.gov/eos/soft.htm#calgrid

6 Other Models

Many additional models are available either for regulatory applications or for R&D studies. We provide a brief list below

6.1 Meteorological Models

- CALMET:
  http://www.src.com/html/calpuff/calpuff1.htm
  http://www.breeze-software.com/prod/brzSoftware.asp?P=CALMET

  CALMET is a meteorological diagnostic model that combines data from surface stations, upper-air stations, over-water stations, precipitation stations, with geophysical data like land use, terrain elevations, albedo, etc., to produce a fully 3-dimensional diagnostic gridded wind field for the duration of the CALPUFF simulation. This wind field is then passed into CALPUFF and is used to transport the emitted substances.

CALMET can link to prognostic meteorological models (i.e., MM5, ETA, RUC2, RAMS) and use their data to produce the gridded wind field.

- MM5: http://www.mmm.ucar.edu/mm5/

  The PSU/NCAR mesoscale model (known as MM5) is a limited-area, nonhydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale atmospheric circulation. The model is supported by several pre- and post-processing programs, which are referred to collectively as the MM5 modeling system. The MM5 modeling system software is mostly written in Fortran, and has been developed at Penn State and NCAR as a community mesoscale model with contributions from users worldwide.

  The MM5 modeling system software is freely provided and supported by the Mesoscale Prediction Group in the Mesoscale and Microscale Meteorology Division, NCAR.

- RAMS: http://rams.atmos.colostate.edu/rams-description.html

  RAMS, the Regional Atmospheric Modeling System, is a highly versatile numerical code developed by scientists at Colorado State University for simulating and forecasting meteorological phenomena, and for depicting the results. Its major components are:
  1. An atmospheric model which performs the actual simulations
  2. A data analysis package which prepares initial data for the atmospheric model from observed meteorological data
  3. A post-processing model visualization and analysis package, which interfaces atmospheric, model output with a variety of visualization software utilities.

6.2 Plume Rise Modules

Most air pollution models include a computational module for computing plume rise, i.e., the initial behavior of a hot plume injected vertically into a horizontal wind flow. In particular, AERMOD includes PRIME (Plume Rise Model Enhancements): http://www.epa.gov/scram001/7thconf/iscprime/tekpapr1.pdf

PRIME is an algorithm for simulating plume rise effects, including downwash as the plume travels over buildings.

6.3 Particle Models

Particle models are based on Lagrangian methods for simulating atmospheric diffusion. In these models, plumes are represented by thousands (even hundreds of thousands) of “fictitious” particles, which often move with semi-random trajectories in order to recreate the random components of atmospheric turbulence. These high-resolution models are particularly useful for simulating short-term releases from sources with highly variable emission rates in complex dispersion scenarios. Particle models are capable of simulating very short-term concentrations (e.g., 1-minute averages). Examples are listed below:

- Kinematic Simulation Particle (KSP) Model in CALPUFF
  http://www.src.com/html/verio/download/CALPUFF_UsersGuide.pdf
- MONTECARLO (Zannetti and Sire, 1999)

6.4 Deposition Modules

Many air pollution models include a computational module for computing the fraction of the plume deposited at the ground as a consequence of dry and wet deposition phenomena.

6.5 Odor Modeling[4]

The mechanisms of dispersion of odorous chemicals (e.g., mercaptans) in the atmosphere are the same as the dispersion of other pollutants. However, when multiple pollutants are emitted, masking and enhancing effects may occur. In this case, the relationship between concentrations of individual chemicals and odor is not well defined and odor must be characterized in terms of an odor detection threshold value for the entire mixture of odorous chemicals in the air. This is why, in odor modeling applications, it is often preferred to express the emission in "odor units".

Odor models must include algorithms to simulate instantaneous or semi-instantaneous concentrations, since odors are instantaneous human sensations.

6.6 Statistical Models

Statistical models are techniques based essentially on statistical data analysis of measured ambient concentrations. These models are not deterministic, in the sense that they do not establish nor simulate a cause-effect, physical relationship between emissions and ambient concentrations. Two main types of statistical models exists:

- Air Quality Forecast and Alarm Systems:

  Statistical techniques (e.g., time series analysis, spectrazl analysis, Kalman filters) have been used to forecast air pollution trends a few hours in advance for the purpose of alerting the population or, for example, blocking automobile traffic. For a review of these techniques, see Finzi and Nunnari (2005).

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[4] http://www.weblakes.com/Newsletter/July002006.html
http://www.nywea.org/Clearwaters/pre02fall/302140.html

- Receptor Modeling[5]:

  Receptor models are mathematical or statistical procedures for identifying and quantifying the sources of air pollutants at a receptor location. Unlike photochemical and dispersion air quality models, receptor models do not use pollutant emissions, meteorological data and chemical transformation mechanisms to estimate the contribution of sources to receptor concentrations. Instead, receptor models use the chemical and physical characteristics of gases and particles measured at source and receptor to both identify the presence of and to quantify source contributions to receptor concentrations.

  One of the most common receptor models is the Chemical Mass Balance (CMB) Model EPA-CMBv8.2. This model[6] is one of several receptor models that have been applied to air quality problems over the last two decades. Based on an effective-variance least squares method (EVLS), EPA has supported CMB as a regulatory planning tool through its approval of numerous State Implementation Plans (SIPs), which have a source apportionment component. CMB requires speciated profiles of potentially contributing sources and the corresponding ambient data from analyzed samples collected at a single receptor site. CMB is ideal for localized nonattainment problems and has proven to be a useful tool in applications where steady-state Gaussian plume models are inappropriate, as well as for confirming or adjusting emissions inventories.

6.7 Modeling of Adverse Effects

Special models or mathematical techniques are available to calculate the adverse effects of air pollution. These models include:

- Health effects (e.g., cancer risk)
  http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=116283
- Visibility impairment
  http://vista.cira.colostate.edu/IMPROVE/Publications/Principle/EPA_Report/chapter5.pdf
- Global effects, such as climate change
  http://www.epa.gov/appcdwww/apb/globalchange/
- Damage to materials
- Ecological damages

7 Further Reading

We encourage the reader to examine the book series "AIR QUALITY MODELING": www.envirocomp.org/aqm

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[5] http://www.epa.gov/scram001/receptorindex.htm

[6] http://www.epa.gov/scram001/receptor_cmb.htm

This books series represents the most comprehensive effort to review all aspects of technical issues related to air pollution modeling. New volumes in the series will expand and complement the scope of effort. The book series is also published in electronic format with Internet pointers and visualizations.

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