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Chapter 1

The Problem – Air Pollution

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Abstract: An introduction is given about general aspects of air pollution. In addition, an overview is presented about the history of air pollution modeling.

Key words: Air pollution, Air pollution regulations, Air pollution modeling.

1 Our Natural Environment

Air pollution can be seen as the result of emissions of man-made, anthropogenic trace gases and particles into our environment.

The chemical composition of the current atmosphere differs considerably from the chemical composition of the natural atmosphere, as it existed in pre-industrial times. This means that, at the moment, nowhere on earth is there natural air, which could also be considered clean air. Our atmosphere is polluted everywhere, which means that the chemical composition differs from the pre-industrial situation.

The chemical composition of the natural atmosphere has shown gradual changes as long as the earth has existed. Life started on earth, in the oceans in fact, in an atmosphere that hardly contained any oxygen, only about 0.015% against the current level of about 21%. The atmosphere at that moment contained nearly 99% CO_2, some N_2, and only traces of H_2O and O_2. Because of the low oxygen level, no stratospheric ozone layer could have been formed. So, the surface of the earth received all the UV-B radiation that is captured these days by the ozone layer. This also explains why life had to start in the oceans, at about 10 m below sea level - a depth where the UV-B radiation was substantially lower.

At first, life on earth, which started about 3 billion years ago, was plant-like and with the aid of photosynthesis-produced oxygen. This way, the oxygen level slowly increased in the atmosphere. This increase in oxygen contributed to the development of a stratospheric ozone layer, making life on the surface of the earth possible, about 400 million years ago. Although fluctuations may have occurred, for example in the oxygen level, with possible maximum values up to 23%, the overall chemical composition of the natural atmosphere, as far as we know, has been relatively stable over the last 10 million years.

The chemical composition of the pre-industrial/natural global averaged atmosphere is shown in table 1:

Table 1. The chemical composition of the natural atmosphere.

	Gas	% by volume	ppm	ppm by the year 2000
Nitrogen	N_2	78.1		
Oxygen	O_2	20.9		
Argon	Ar	0.92		
Neon	Ne		18.2	
Helium	He		5.2	
Krypton	Kr		1.14	
Xenon	Xe		0.09	
Carbon dioxide	CO_2		280.0	360.0
Methane	CH_4		0.750	1.75
Nitrous oxide	N_2O		0.270	0.310

The composition given in table 1 is that of the dry atmosphere. H_2O-vapor has a concentration fluctuating between 40 ppm and 40,000 ppm (4%).

The ecosystem "life" created the chemical composition of the atmosphere in which this ecosystem can exist, i.e., a chemical composition in which life can sustain. The chemical composition with its high oxygen level is not in chemical equilibrium, but this non-equilibrium state can be maintained by life itself.

Based on this fact, James Lovelock developed the Gaia-theory (Gaia, the Greek goddess of the earth), [Lovelock (1972, 1979)]. In short, his theory states that the earth, including the atmosphere, is a 'living', homeostatic organism. In contrast, the surrounding planets where there is no life, Venus and Mars, have a completely different chemical composition, which is in chemical equilibrium (their atmosphere contains about 99% CO_2, some N_2, and nearly no O_2 and H_2O).

In other words, our atmosphere is a very special one, and we should handle it with care.

2 Air Pollution, Some Definitions

There are several conceivable approaches to define air pollution. For example, the change in the global, chemical composition of the pre-industrial atmosphere, as given in Table 1, and which is due to human influence, can be called air pollution; all man-made, anthropogenic emissions into the air can be considered air pollution. So air pollution - but at a very local scale, not detectable at a global scale - did not start until mankind started ‘to play with fire’.

The global increase in the concentrations of CO_2, CH_4 and N_2O (shown in Table 1), all greenhouse gases, could, and should be called 'air pollution' in the broad sense, even though these species are not toxic for human beings and the ecosystem.

Another approach is to distinguish between the emissions of safe, non-toxic, and harmful compounds, and only consider the last as air pollution. This distinction, however, has two clear drawbacks. About 1940 and even much later, manmade emissions of CFCs were considered safe because they are inert in the troposphere. However, the decrease of the stratospheric ozone layer has taught us differently. In the same way, CO_2 emissions are safe in the sense that they are not toxic, but their increase leads – most likely – to a climate change, which in turn will be harmful to large parts of the ecosystem.

The second drawback is that natural emissions can also be harmful, such as emissions of dioxine caused by a forest fire as a result of lightning.

One anthropogenic influence that has actually decreased “natural” emissions is the human intervention to prevent the widespread extent of wildland fires that used to exist prior to the 20th century (Barry, 2007). In the past century, substantial efforts were initiated, at least in the United States, to curtail the extent of natural fires due to the encroachment of human population in formerly remote areas. Recently, it has been realized that this human intervention has led to adverse effects such as the buildup of low-level brush that has led to more extensive fires that are harder to control. In addition, the benefits of wildland fires to maintain the ecosystem in its natural state have been compromised. One way to return closer to the level of natural wildfire emissions that existed in pre-industrial times is to conduct prescribed burning under controlled conditions to minimize the harmful effects of wildland fires while maximizing their benefits. Even so, the extent of “natural” emissions from pre-industrial fires will likely never be realized again because as population continues to encroach upon forested areas, there will be human intervention to restrict wildfires that would never have occurred in previous centuries.

Next to anthropogenic emissions, it is possible to distinguish between natural emissions and biogenic emissions.

Natural emissions should be defined as emissions caused by the non-living world, such as volcanic emissions, sea-salt emissions, and natural fires.

Biogenic emissions are emissions resulting from the ecosystem, like VOC-emissions from forests, and CH_4-emissions from swamps. In principle, natural and biogenic emissions lead to the chemical composition of the pre-industrial, natural atmosphere.

The philosophical question [whether manmade emissions should also be considered as biogenic, because man is part of the ecosystem] can be retorted by the distinction that mankind, by making fires, creates anthropogenic emissions.

Although the distinction in these three categories: anthropogenic, natural, and biogenic could be useful, quite a number of intermediate emissions exist. Examples are the NO-emissions by soil bacteria, which is a function of the earlier deposited nitrogen on the soil due to anthropogenic emissions of N-compounds or earlier deposited manure containing nitrogen. There is the question of whether or not VOC-emissions are due to planting or not planting of trees, and whether or not dust-emissions are the consequence of paving or not paving sandy roads. These are such intermediate emissions, biogenic or natural, but with a clear human influence.

Although anthropogenic emissions started when man learned to make fire, and the air quality, especially the concentrations of fine particles, surpassed air quality guidelines in and around the cave dwellings of the Neanderthal man, the impact of air pollution has been of a local character for a long time.

In Europe, elevation of concentration levels occurred for the first time in the middle ages, resulting in the first laws on air pollution that were often focused on odor nuisance around local factories. Also, burning coal for heating and cooking led to air pollution, until well into the last century. London for example, was 'famous' for its fog. Subsequently, the industrial revolution involved a tremendous increase in the use of fossil fuel for thermally-generated power to run factories and later to supply electrical power and as a consequence of industrial emissions from smelters, petrochemical plants, pulp mills, etc. Consequently, as from about 1850, a number of gases started to increase in concentration, like the gases mentioned in Table 1 - CO_2, CH_4 and N_2O – and in addition, for example, sulfate aerosols.

It should be emphasized here that air pollution in the strict sense (‘toxic’) and global (climate) change are interrelated phenomena. Directly, because they often have the same emission sources, and more indirectly because species like tropospheric ozone and aerosols play a role both in local and regional air quality, as well as in climate change.

3 Primary and Secondary Pollutants

The main, primary – i.e., directly emitted – gaseous pollutants are the following:

- Carbon compounds, e.g. CO_2, CO, CH_4, the VOC's (volatile organic compounds)
- Nitrogen compounds, e.g. N_2O, NO, NH_3
- Sulfur compounds, e.g. SO_2, H_2S
- Halogen compounds, e.g. chlorides, fluorides, bromides

The main, primary particle pollutants are the following:

- Particles smaller then 2.5 μm in diameter. Included are the Aitken nuclei, particles smaller than 0.1 μm in diameter, which grow rather fast by coagulation to larger particles. The chemical composition of these primary particles is, to a large extent, carbon but also heavy metals as iron, zinc, copper, etc., will also be contained in these particles.
- Particles with a diameter from 2.5 to 10 μm. These larger particles are often composed of sea salt and dust.

Most air pollutants, except the halogen compounds, will be chemically transformed in the troposphere by the OH-radical. The OH-radical is formed in the troposphere by photo-dissociation of O_3, and subsequent reaction of oxygen with H_2O-vapor to OH (Levy, 1971). The OH-radical reacts not with N_2, O_2, H_2O, CO_2, but with other compounds as CO, CH_4, H_2, NO, NO_2, SO_2, NH_3. The OH-radical can be seen as the cleansing agent of the atmosphere, since it transforms primary air pollutants into secondary pollutants, which are subsequently removed from the atmosphere by dry and wet deposition. In this way the OH-radical determines the atmospheric residence time of most compounds in the atmosphere.

The main, secondary – i.e., formed in the atmosphere – gaseous pollutants are:

- NO_2 and HNO_3 formed from NO
- O_3 formed through photochemical reactions

The main, secondary particles are:

- Sulfate aerosols formed from $SO_{2,}$ and Nitrate aerosols formed from NO_2 followed by the reaction with NH_3 to form ammonium (bi) sulfate and ammonium nitrate.
- Organic aerosols formed from gaseous organic compounds.

These secondary particles consist mainly of small particles with a diameter less than 2.5 μm.

4 A Short History of Air Pollution Modeling

Air pollution modeling is an attempt to describe the causal relation between emissions, atmospheric concentrations, and deposition. Air pollution measurements give quantitative information about concentrations and deposition, but they can only give the levels at specific locations. In principle, air pollution modeling can give a more complete and consistent description, including an analysis of the causes - emissions sources, meteorological processes, physical and chemical transformations - that have led to these concentrations/deposition.

Air pollution models play an important role in science, because of their capability to assess the importance of the relevant processes. Air pollution models are the only method that quantifies the relationship between emissions and concentrations/depositions, including the consequences of future scenarios and the determination of the effectiveness of abatement strategies.

The concentrations of species in the atmosphere are determined by transport and diffusion. This means that in considering the history of air pollution modeling, some remarks should be made concerning transport and diffusion. Transport phenomena, characterized by the mean velocity of the fluid, have been measured and studied for centuries. For example, the average wind was studied for sailing purposes. The study of diffusion (turbulent motion) is more recent. Although turbulent motions have been observed from the moment people looked at rivers and streams, one could mention Reynolds' paper in 1895 as the scientific starting point for the formulation of the famous criterion for laminar-to-turbulent flow transition in pipes.

One of the first articles in which turbulence in the atmosphere is mentioned, was published by Taylor (1915). In later years, he developed the 'Taylor-theory of turbulent diffusion', Taylor (1921). In this theory, it is shown that the diffusion from a point source can only be described with a constant eddy diffusivity, K, for travel times, which are much larger than the turbulent integral time scale, the so-called diffusion limit. For smaller time-scales the effective turbulent diffusivity is proportional to the travel time.

Until about 1950, a number of studies were performed on the subject of diffusion in the atmosphere (Richardson and Proctor, 1925; Sutton, 1932; Bosanquet, 1936; Church, 1949; Thomas et al., 1949; Inoue, 1950; Batchelor, 1950). Already, the paper by Richardson considered long-range aspects; up to over 80 km. Bosanquet is one of the first who published about the impact of chimney plumes. A paper by Chamberlain (1953) already considered the deposition of aerosols.

4.1 Modeling of Point Sources

The study of the dispersion from low and high level point sources, especially experimental, was a major topic shortly after 1955. Papers on this subject appeared by Smith (1957), Gifford (1957 a, b), Hay and Pasquill (1957), Record and Cramer (1958) and Haugen (1959) both devoted to the Prairie grass experiment, Stewart et al. (1958), Monin (1955, 1959), Ogura (1959). Perhaps the first paper on this subject was by Roberts (1923).

The publication by Pasquill ‘Atmospheric Diffusion’, which appeared in 1962, was a major milestone in summarizing the work performed until that moment. It illustrates that air pollution modeling around the beginning of the sixties was focused on local dispersion phenomena, mainly from point sources with SO_2 as major component in the application studies.

The Gaussian plume model was formulated, in which the horizontal and vertical spread of the plume was determined experimentally. Tables appeared with the famous Pasquill-Gifford sigma-values in the horizontal and vertical direction, and as a function of the atmospheric stability ranging from very stable, class F, up to very unstable, class A. The experimental sigma values 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 case in the atmosphere.

In the sixties, 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 famous 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, 1970, 1972) and its major influence on the magnitude of ground level concentrations.

The basic concepts of predicting ground-level concentrations from stack emissions involved the variables listed below.

- Wind direction determines the trajectory of the emissions. Complications with this variable are that the wind direction varies with height and location, especially in stable conditions when the atmosphere is not well mixed. It is also well known that the validity of straight-line Gaussian plume models are limited to the degree of the wind persistence and other meteorological variables as a function of plume travel time.
- Wind speed affects both the plume rise of buoyant emissions (by affecting the rate of ambient air entrainment and source effects such as building and stack downwash) and the dilution of the emissions with ambient air. It is also well known that wind speeds generally increase with height due to frictional effects near the ground, but there can be challenges in simulating the vertical and horizontal changes of wind speed, similar to the wind direction challenges.

- The ambient temperature affects the rise of buoyant plumes in that the entrainment of ambient air into plumes will reduce their buoyancy with time. “Final” plume rise is considered to be reached when the vertical velocity associated with plume buoyancy is comparable to vertical wind fluctuations in the atmosphere.
- The stability of the atmosphere was, in the early era of Gaussian models, expressed as classes that ranged from 1 (very unstable) through 4 (neutral) and to 7 (very stable). The discrete stability classes were determined through several methods, including the Turner (1964) method based upon wind speed, solar elevation, and cloud cover, as well as alternative methods described in the United States Environmental Protection Agency (USEPA) document, Meteorological Monitoring Guidance for Regulatory Modeling Applications (2000). These alternative methods involve use of site-specific turbulence and wind data, as well as solar radiation, wind speed, and vertical temperature difference data. The specification of a stability class allowed Gaussian dispersion models to assign rates of plume dispersion in the vertical and horizontal, as well as to determine plume rise formulas.
- The mixing height is the height above the surface through which relatively vigorous mixing occurs. Early Gaussian dispersion models only considered limits to mixing in convective conditions, as defined by the height of a temperature inversion aloft. This variable was used in Gaussian models to determine a depth within which an emitted plume was trapped and into which it would eventually mix thoroughly after sufficient travel time. However, plumes emitted above the mixed layer height could be assumed not to be entrained within the mixed layer, and therefore not affect ground-level pollutant concentrations.

In addition to these plume modeling concepts, atmospheric scientists (e.g., Turner, 1969 and Pasquill, 1976) categorized six types of plume behavior visible under various conditions of stable and unstable conditions. The plume types were referred to as “looping”, “coning”, fanning”, “lofting”, “fumigation”, and “trapping”. Early Gaussian dispersion models were designed to simulate these effects through appropriate combinations of the variables described above as incorporated into dispersion modeling schemes. A review of the air pollution modeling papers published in the sixties and seventies indicates that these papers appear to be mainly written by meteorologists, specialized in boundary layer meteorology and atmospheric turbulence. These studies focused often on the effect of atmospheric stability on plume spread. During the next decade, besides research on local dispersion (for a good overview, see Nieuwstadt and van Dop, 1982), the spatial scale of air pollution modeling increased substantially.

In the period after 1980 to the present time (2009), additional enhancements were made to steady-state Gaussian models. Major developments in an improved understanding of the planetary boundary layer (PBL) began in the 1970s, as described by Venkatram (1978, 1980), Wyngaard (1988), Izumi (1971), Dyer

(1979), van Ulden and Holtslag (1985), Businger (1973), Panofsky et al. (1977, 1984), and Kaimal et al. (1976). One milestone involved numerical simulations by investigators Deardorff and Willis (see 1975, 1978, and 1981 papers), revealing the convective boundary layer's (CBL's) vertical structure and important turbulence scales. Insights into dispersion followed from laboratory experiments, numerical simulations, and field observations (Briggs 1973, 1984, and 1988; Lamb 1982; Weil 1988a,b). For the stable boundary layer (SBL), advancements occurred more slowly. However, a sound theoretical/experimental framework for surface layer dispersion and approaches for elevated sources existed by the mid-1980s (Briggs 1988; Venkatram 1988).

Advances in Gaussian models using stability classes were made in the USA with the Rough Terrain Diffusion Model (Paine and Egan, 1987), improvements in the Industrial Source Complex Model (USEPA, 1995a,b), and AUSPLUME in Australia (EPA Victoria, 2004).

The changes to the earlier straight-line Gaussian models brought about by application of the considerable research noted above were as follows, as described by Weil, 1985):

- Discrete stability classes were replaced by continuous functions of similarity scaling parameters such as the friction velocity (u_*), the convective velocity scale (w_*), and the Monin-Obukhov length (L).
- Variables such as wind direction and speed, temperature, and turbulence were scaled with height using available on-site measurements and enhanced with boundary-layer concepts.
- Mixing heights were generalized into both convective and mechanical (shear-induced) components.
- Source effects such as building downwash were improved with developments such as the PRIME model (Schulman et al., 2000).
- Plume interactions with terrain were advanced with the concept of the dividing streamline height in models such as CTDMPLUS (Perry et al., 1989; Perry, 1992).

Starting in the 1980s, researchers began to apply this information to applied dispersion models. These included eddy-diffusion techniques for surface releases, statistical theory and PBL scaling for dispersion parameter estimation, and a new probability density function (PDF) approach for the CBL. Much of this work was reviewed and promoted in workshops (Weil, 1985), revised texts (Pasquill and Smith, 1983), and in short courses and monographs (Nieuwstadt and van Dop, 1982; Venkatram and Wyngaard, 1988). By the mid- to late 1980s, new applied dispersion models had been developed, including the Power Plant Siting Program (PPSP) model (Weil and Brower, 1984), Second-Order Closure Integrated Puff (SCIPUFF) (Sykes et al., 1998), Operationelle Meteorologiske Luftkvalitetsmodeller (OML) (Berkowicz et al., 1986), Hybrid Plume Dispersion Model (HPDM) (Hanna and Paine, 1989), Multiple Source Dispersion Algorithm Using On-Site Turbulence Data (TUPOS) (Turner et al., 1986), and the Complex Terrain Dispersion Model Plus

Algorithms for Unstable Situations (CTDMPLUS) (Perry et al. 1989); later, the Advanced Dispersion Modeling System (ADMS), developed in the United Kingdom (Carruthers et al. 1992; CERC, 2004), was added as well.

In February 1991, the U.S. Environmental Protection Agency (USEPA) in conjunction with the American Meteorological Society (AMS) formed the AMS and EPA Regulatory Model (AERMOD) Improvement Committee (AERMIC), with the purpose of incorporating scientific advances from the 1970s and 1980s into a state-of-the-art Gaussian dispersion model for regulatory applications. AERMIC's early efforts are described by Weil (1992). To improve PBL parameterizations, other concerns such as plume interaction with terrain, surface releases, building downwash (PRIME model; Schulman et al., 2000), and urban dispersion were addressed. These efforts resulted in AERMOD (Cimorelli et al., 2005 and Perry et al., 2005), which was adopted as a recommended short-range dispersion model by the USEPA in late 2005.

4.2 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 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 and Saltbones (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.

The simulation of long-range transport as well as short-range transport in complex wind situations from individual sources was improved with the development of Lagrangian puff models such as CALPUFF (users guide - Scire et al., 2000) and the Second-Order Closure Integrated Puff (SCIPUFF) (Sykes et al., 1998; Santos et al., 2000). These models have a meteorological pre-processor as well as a dispersion module, and were specifically suited for the transport and dispersion of individual stack emissions for long distances. These models treat source emissions as being broken up into a series of puff releases. The puffs are advected throughout the modeling domain by the wind fields generated using the meteorological preprocessor (or supplied directly from mesoscale modeling output, such as MM5). Concentrations at user-specified receptors are computed by adding the contributions of all of the puffs currently in the modeling domain during each model time step (which can be a fraction of an hour). Puffs are grown and diluted using various dispersion formulas, and can be broken into smaller puffs if they become large and are subject to significant shears.

These models are useful for long-range transport issues as well as near-field impacts in special situations such as:

- Complex flows/dispersion effects
- Coastal zones
- Complex terrain
- Inhomogeneity in surface conditions/dispersion rates
- Plume fumigation, inversion breakup
- Calm and near-calm wind conditions.

Eulerian modeling began with studies by Reynolds et al. (1973) for ozone in urbanized areas, with Shir and Shieh (1974) for SO_2 in urban areas, and Egan et al. (1976) and Carmichael and Peters (1979) for regional scale sulfur. From the modeling studies by Reynolds on the Los Angeles basin, the well-known Urban Airshed Model-UAM originated. 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).

Recent advances in “whole atmosphere models” have produced state-of-the-art photochemical models capable of simulating ozone, regional haze, and fine particulate impacts of thousands of sources distributed over large regions. These models include CMAQ (Byun and Ching, 1999), CAMx (Morris et al., 2004), and TAPM (Hurley, 2005). Similar to the Lagrangian models mentioned above, these models employ a meteorological pre-processor. They also require extensive emissions preprocessing in order to appropriately characterize the numerous chemical constituents used in the model. The models employ advanced gas phase chemistry mechanisms in its computations. They also generally have sophisticated post-processors and graphical user interfaces to facilitate display and interpretation of the modeling results.

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 and Rohde, 1978). The first, 3-D, global models were developed by Peters and Jouvanis (1979) (see also Zimmermann, 1988).

In the period after 2000, operational weather prediction models were linked with integrated models such as HYSPLIT (ARL, 2009). As noted by the model documentation, the HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory) model is a complete system for computing simple air parcel trajectories to complex dispersion and deposition simulations. The dispersion of a pollutant is calculated by assuming either puff or particle dispersion. The model's default configuration assumes a puff distribution in the horizontal and particle dispersion in the vertical direction. In this way, the greater accuracy of the vertical dispersion parameterization of the particle model is combined with the advantage of having an ever-expanding number of particles represent the pollutant distribution.

In general, Lagrangian particle models are like Lagrangian puff models except that they treat emissions as numerous particles that are moved in time by a mean wind and a random (Monte Carlo) turbulent component. The concentration in a model grid box is determined by counting the number of particles that are in the box at any given time.

There are other modeling approaches used for specialized applications. A partial list is provided below.

- Dispersion models suitable for heavy gas releases are needed to account for near-field slumping and spreading of accidental releases of a heavy gas. The alternative model area at USEPA's web site at www.epa.gov/scram001 lists some of these models.
- Computational fluid dynamics (CFD) models incorporate complex wind flow models with very small grid sizes (on the order of 1 m) and small times steps (on the order of 1 s) so that small-scale turbulence effects can be resolved by the model. They are useful for complex flows with complicated structures that are not readily accommodated by larger-scale routine models. The models are highly computer intensive and are generally limited to case studies rather than extensive time simulations.
- Wind tunnel models are also useful for studying complex geometries that are not amenable to conventional modeling approaches. Although many controlled experiments can be conducted by this technique, it is difficult to simulation stable or unstable boundary layers in a wind tunnel. In addition, artificial boundary conditions are required due to the finite size of the wind tunnel.

5 Air Pollution Modeling Guidelines

Many countries have their unique ambient standards and have issued guidelines for approved modeling procedures. These standards and modeling guidelines are subject to change. The bulleted items below provide selected web sites for information as of early 2010.

- World Bank International Finance Corporation environmental guidelines are available at: http://www.ifc.org/ifcext/sustainability.nsf/Content/EnvironmentalGuidelines.
- United States modeling guidance: www.epa.gov/scram001. This site also has a link to individual state websites. It also lists alternative models, some of which were developed in other countries.
- United States national ambient air quality standards: http://www.epa.gov/ttn/naaqs/
- Canadian air quality standards are available at http://www.hc-sc.gc.ca/ewh-semt/air/out-ext/reg-eng.php. Modeling guidance is issued by individual provinces (e.g., Ontario, Alberta, and British Columbia).
- Mexican air quality standards are compared to USA standards at http://www.epa.gov/ttncatc1/cica/airq_e.html.
- European air quality standards are provided at http://ec.europa.eu/environment/air/quality/standards.htm. Databases on European emissions and monitoring are available through http://www.eea.europa.eu/themes/air.
- Various European countries use different dispersion modeling approaches. However, "Guidance on the use of models for the European air quality Directive" issued by the Forum for Air Quality Modelling in Europe (FAIRMODE) is meant to "provide a harmonised focus for modelling activities that are relevant to the Air Quality Directive". This document is available at: http://fairmode.ew.eea.europa.eu/fol404948/Model_guidance_document_v5_1a.pdf/download.
- Australia's air quality and emission standards are available at http://www.environment.gov.au/atmosphere/airquality/standards.html. Individual Australian states have established their own modeling procedures, which are available on their respective web sites.
- New Zealand has a guideline for atmospheric dispersion modeling available at http://www.mfe.govt.nz/publications/air/atmospheric-dispersion-modelling-jun04/html/page11.html.

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