Pi International Journal of Mathematical Sciences
© PIJMS | Volume 1 | Issue 1 | August 2025 | ISSN: 3107-9830 (Online)
Available online at: https://pijms.com/

Mathematical Modeling of Air Pollution Dispersion: A Comprehensive Review

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Received: 05 August 2025 | **Accepted:** 25 August 2025 | **Published:** 31 August 2025

Abstract

Air pollution is a pressing global concern affecting human health, ecosystems, and climate dynamics. Mathematical modeling serves as a critical tool for predicting pollutant behavior and designing mitigation strategies. This paper reviews major air pollution modeling techniques, including Gaussian and advection-diffusion models, Lagrangian particle tracking, Eulerian grid systems, and hybrid approaches, alongside emerging machine learning-based prediction models. Mathematical formulations such as the advection-diffusion equation, stochastic processes, and probabilistic frameworks are discussed in detail. Applications in complex terrains, street canyon environments, and health risk modeling are explored. The review concludes with future directions focusing on real-time hybrid modeling and integration with machine learning for sustainable environmental management.

Keywords: *Air pollution modeling, advection-diffusion equation, Lagrangian particle model, Gaussian plume model, stochastic modeling, machine learning, environmental health risk.*

1. Introduction

Mathematical modeling offers a valuable tool for understanding the dispersion of air pollutants arising from various sources and processes. It is employed when new pollution sources are introduced, emission levels change, or the need arises to corroborate ambient air quality measurements—thus serving a principal function in environmental monitoring and management. Predicting pollutant dispersion is crucial to maintain community health standards, and the development of mathematical models involves analyzing pollutant behavior under different conditions, identification of major influencing parameters, and applying the resulting equations to practical situations (Ulfah et al., 2015). Air pollution arises predominantly from human activities, resulting in direct environmental impacts and more profound consequences on the Earth's physical, chemical, and biological processes. Around 99% of urban inhabitants breathe air exceeding WHO guidelines at least once annually, with approximately 4 million premature deaths attributed to outdoor air pollution worldwide. Moreover, exposure to elevated pollutant levels is linked to adverse effects on numerous organs, including the respiratory, cardiovascular, and central nervous systems. Pollution sources are categorized as point (single, specific locations), line (distinct coordinates but with a linear extension), or area (distributed or multiple points over a large zone). Pollutants emitted directly from sources into the atmosphere and entering a chemical reaction immediately qualify as primary pollutants; those generated from the transformation of primary pollutants constitute secondary pollution. Mathematical modeling provides a computational description for simulating pollutant transportation and transformation, facilitating the systematic investigation of different mechanisms influencing environmental pollutants and, consequently, the examination of mitigation alternatives.

2. Overview of Air Pollution

Air pollution is the presence of substances in the atmosphere that have harmful effects for humans, plants, animals and the environment. These substances are also known as pollutants and they include gases, particulates and natural matter in forms and amounts which result in pollution of the atmosphere. Air pollution is presently a problem of global concern because it affects the health of the ecosystem and in particular human health. Air pollutants can be categorized as primary and secondary pollutants.

Primary pollutants are emitted directly from the source and include sulphur dioxide, oxides of nitrogen, carbon monoxide, carbon dioxide, hydrogen sulphide, ammonia, benzene, fluoride and lead. Secondary pollutants like ozone, acid rain, peroxyacetyl nitrate and smoke vine are formed in the atmosphere as the result of chemical reactions of primary pollutants. The effects of air pollution on human health are of great concern because exposures, particularly from carbon monoxide, particulate matter and lead, may lead to illness or premature death.

2.1. Types of Air Pollutants

Air pollution is the accumulation of one or more contaminant(s) in the atmosphere, to such an extent that they become injurious to health, biological life, property, and environment. Contaminants can be present in the air in the form of gaseous, liquids, or solids particles suspended in the atmosphere. Some of these contaminants occur naturally, whereas others originate from anthropogenic sources. The movement of pollutants in the atmosphere is controlled largely by atmospheric motions, or wind. Estimation of the consequences of release of pollutants can be achieved by wind tunnel studies, existing air pollution models, and mathematical models (Ulfah et al., 2015). When a mathematical model is used, one is estimating the health hazards and the environmental damage by making mathematical computations about the consequences of emissions.

2.2. Sources of Air Pollution

Basically, air pollution sources are discharge points of unclean air. The most noticeable, major source of polluted air is the combustion of fuel. Pollutants from fuel combustion come in many forms, gaseous and particulate, and are as diverse as the kinds of fuel (coal, oil, gasoline, diesel, natural gas, propellants, and all different kinds of “metals”) used as fuels and preservatives in these fuels. Most of the molten components of these fuels will be emitted as “particulate”, and the balance as gaseous emissions. Most air pollutants from combustion processes can be attributed to a "deficiency" in the process and hence can be reduced to trace levels, if the combustion process is perfect. In some processes, the burning of fuels can help to provide specific atmosphere for controlling process operations, as in boilers; in other processes, the burning process itself is the product, as in incinerators and crematoriums. Therefore, these sources of combustion-generated air pollutants given here will be primarily concentrated on the use of combustion from power plants, fossil fuel powered engines, coal furnaces, and home fireplaces (Ulfah et al., 2015).

2.3. Health and Environmental Impacts

Air pollution results from the accumulation of diverse chemical species and sedimentary particles in the atmosphere, which in turn may adversely impact human health and the environment. Airborne pollutants, depending on their concentration, exposure route, and duration of exposure, can increase respiratory and cardiovascular diseases and may even lead to death. Some pollutants also cause acid rain and decreased agricultural yields (Bseibsu, 2016). Governments worldwide enact standards to protect human health and the environment by regulating the concentration of pollutants. Specific standards apply to certain pollutants; for example, the U.S. does not require regulation of carbon dioxide concentration unless it is part of an increase in greenhouse gases. Mathematical dispersion models link steady emission rates to outdoor concentrations and the deposition of air pollutants. Governments use these models in emission-control regulations, ambient air-quality planning, and permit evaluation (Ulfah et al., 2015).

3. Mathematical Modeling Fundamentals

Mathematical modeling is the art and science of developing and applying mathematical descriptions, concepts, and techniques to real-world phenomena. A model reproduces a system in terms of its constituent parts, their relationships and their interactions; it is a representation that enables analytical and experimental activities to be performed on the system (Ulfah et al., 2015). Mathematical modeling can be divided into several categories, one of which is a model based on physical phenomena (Tominaga & Stathopoulos, 2016). This category of model requires that the assumptions made and the specifications of the system are critical to and reflected in the mathematical formulation. The description of the physical phenomena being modeled forms the basis of these formulations and should be consistent with the system behavior. Analytical models, which are closed-form mathematical expressions of the system under certain assumptions, are ideal for this type of mathematical modeling. The mathematical formulation of dispersion is based on the mass conservation equation that describes convection, turbulent diffusion, and chemical reactions (P. Chernogorova and G. Vulkov, 2016). When new sources of air pollution arise or when the amount of pollutants emitted into the air changes, mathematical models are a useful tool for investigating the behavior and trends of pollutants. Mathematical formulations of transport and dispersion have been developed to identify relevant parameters. Air quality models have become integrated tools in environmental monitoring, management, and assessment of air pollution. An ideal model of air pollutant concentrations would allow researchers to forecast pollutant concentrations resulting from any specified set of pollutant emissions, at any location, and for any time period, for any specified meteorological conditions.

The main processes of dispersion of pollutants in the atmosphere are: convection, which transports pollutants by wind, and diffusion caused by turbulent air motion. The mathematical formulation of dispersion is based on the mass conservation equation that describes convection, turbulent diffusion, and chemical reactions. Atmospheric pollution modeling plays a vital role in developing the world's health perspective. With the growing number of models capable of addressing air quality problems, it is imperative to conduct an adequate evaluation process to help stakeholders, users, and decision makers choose the most appropriate modeling system for their specific needs.

3.1. Definition and Purpose

Mathematical modeling provides an essential complement to empirical and experimental studies for investigating air pollution dispersion. The purpose of air-quality models is to calculate the pollutant concentrations resulting from specified emissions and meteorological conditions and to deduce the corresponding spatial and temporal distribution. Conceptually the most straightforward depiction of the dispersion of pollutant in ambient air is to consider a volume of air containing one or more pollutants in a well-defined state, and to describe mathematically how this state changes with time. A state is commonly defined by the bulk thermodynamic quantities of pressure, temperature, and density of the gas and by the concentrations of pollutant involved. An air-quality modeling system is therefore a set of mathematical equations or algorithms capable of simulating the dynamics of specified pollutants on timescales varying from minutes to days and distances from a few tens of metres to several hundred kilometres (Ulfah et al., 2015). In general, one can distinguish two main classes of air quality models, based on whether or not transport phenomena — advection, diffusion, and deposition — are explicitly accounted for.

3.2. Types of Models

Air pollution models may be classified according to the source type, area, or purpose; the manner in which the model treats space, time, and the physical process; the treatment of atmospheric physics and chemistry; the mathematical solution; and the method of processing model results. One classification scheme is based on the mathematical approach used to simulate pollutant transport and transformation. Commonly applied models include Gaussian models, Lagrangian models, and Eulerian models.

Strengths and weaknesses of different model types influence the choice of a suitable model. Gaussian models rely on the Gaussian probability distribution and provide a standard means for computing pollutant concentrations from sources. Lagrangian models calculate dispersion by following pollutant ‘‘parcels’’ along their trajectories. Eulerian models divide the atmosphere into a fixed grid and solve the governing equations of transport and transformation in each grid cell.

3.3. Modeling Assumptions

Mathematical modeling involves constructing equations that describe physical systems or processes under investigation. Model types include integral, box, Gaussian, and cell models, each with specific assumptions about transport equations and input data. Critical assumptions often simplify complex processes; for example, chemical reactions may be neglected when transport and removal dominate pollutant behavior (Ulfah et al., 2015). Regarding flow dynamics, wind speed is commonly vectorized only in the horizontal plane, with vertical wind components assumed negligible on the scale of a few hundred meters. Plume dispersion models typically presume that the plume neither bends upward nor downward, remaining parallel to the ground. Eulerian models frequently assume flow incompressibility. Modeling pollutant dispersion within urban areas poses significant challenges due to the intricate geometry and spatial arrangement of streetcanyons and building obstacles. (Tominaga & Stathopoulos, 2016) emphasize the necessity of clearly defining the intended application and acceptable accuracy before method selection, given the complexity and practical constraints associated with comprehensive modeling approaches.

4. Dispersion Models

The mathematical description of air pollution dispersion involves three commonly used models (Ulfah et al., 2015).

The **advection-diffusion equation (ADE)** forms the basis of most air pollution models, describing the transport of a pollutant species in a moving fluid:

$$\frac{\partial C}{\partial t} + \vec{\mu}\nabla C = \nabla.(K.\nabla C) + S - R$$

Where:

- $C(x, y, z, t)$ = Concentration of pollutant (mass/volume)
- $\vec{\mu} = (u, v, w)$ = Wind velocity vector
- K = Turbulent diffusion coefficient tensor
- S= Source term (e.g., industrial emissions)
- R = removal term (e.g., chemical reactions, deposition)

This equation combines **advection** (transport by wind) and **diffusion** (turbulent mixing), forming the core of Gaussian, Eulerian, and Lagrangian models.

The Gaussian model uses solutions to the advection-diffusion equation. The Lagrangian model represents the fluid as a collection of particles that are advected by the mean wind and dispersed by turbulence. The Eulerian model uses the advection diffusion equation applied on a grid.

The Gaussian model assumes a homogeneous mean wind and diffusion coefficient, with turbulence represented by concentration distributions that are Gaussian in space and time. The Lagrangian model assumes a homogeneous mean wind and turbulence statistics, represented by parcels of fluid that are advected and dispersed by the turbulent velocity field. The Eulerian model does not assume a turbulent closure and solves the advection-diffusion model numerically.

4.1. Gaussian Dispersion Models

Gaussian plume models assume that atmospheric turbulence can be treated as a normally distributed diffusion process (A. Degrazia, 1998).

The general form of the GPM equation, used to calculate the concentration C at a point (x, y, z) downwind from a source, is given as:

$$C(x,y,z) = \frac{Q}{2\pi U\sigma_y\sigma_z} exp\left(-\frac{y^2}{2\sigma_y{}^2}\right)\left[exp\left(-\frac{(z-H)^2}{2\sigma_z{}^2}\right) + exp\left(-\frac{(z+H)^2}{2\sigma_z{}^2}\right)\right]$$

In this formulation, Q represents the source emission rate, U denotes the mean wind speed, and H is the effective stack height, which combines the physical stack height with the plume rise. The variables σ_y and σ_z are the primary dispersion coefficients, corresponding to the standard deviations of the Gaussian concentration distribution in the crosswind and vertical directions, respectively. These coefficients depend on the downwind distance x and, most importantly, on the atmospheric stability conditions.

The problem is governed by the same diffusion equation as steady-state molecular diffusion, but mixing parameters are empirically based on field experiments rather than molecular values. Specifically, the turbulent mixing coefficients are proportional to the distance transported, under the assumption of stationary, homogeneous turbulence. Neglecting the wind velocity gradient and considering a simple coordinate system, the dispersion of pollutants can be described with analytical expressions for concentrations downwind of the source. The assumptions of constant horizontal and vertical dispersion parameters and uniform wind speed lead to Gaussian distributions of pollutant concentration, enabling relatively straightforward computation of downwind concentration distributions.

4.2. Lagrangian Models

Several specific modelling approaches are available to simulate the dispersion of airborne contaminants. According to the dominant methodology, models can be classified as Gaussian, Lagrangian or Eulerian (Alessandrini & Ferrero, 2012).

Lagrangian models track pollutant particles as they move through turbulent airflows. Each particle's position is updated using stochastic differential equations:

$$dX = udt + \sqrt{2K}\, dW_t$$

Where:

- X = position vector of the particle
- u= deterministic wind component
- K= turbulent diffusion coefficient
- dW_t= Wiener process (random component representing turbulence)

This stochastic approach captures the randomness of turbulent flows and is especially effective for simulating street canyon environments and complex terrain.

Gaussian models use analytical solutions to the diffusion equation. Lagrangian and Eulerian models are two fundamental methods for solving the dispersion equation in wind fields

Lagrangian dispersion models describe air pollution dispersion by tracing the motion of 'fluid parcels' (fluid elements containing the pollutants of interest, pollutant molecules or modelling particles) through the atmosphere. Under typical dispersion conditions, fluid parcels move in the atmosphere subject to the effects of the mean wind (advection process), turbulence (diffusion process) and other forcing terms such as gravity or chemical reactions that might apply to the pollutants under consideration.

4.3. Eulerian Models

Eulerian models utilize spatially fixed Cartesian coordinates, characterizing the transportation and diffusion of air pollutants through air concentration fields within three-dimensional grid cells. These models are capable of simulating concentration levels of gaseous or particulate pollutants, covering extensive domains from local up to continental scales. The defining transport equation applied is the advection-diffusion equation, which has been employed to forecast concentration fields for various pollutants, including $SO_2, NOx, CO, CO_2,\ O_3$, and particulate matter. Generally developed for domains situated in flat terrain and extending over distances of a meter to approximately 200 kilometers, Eulerian models serve effectively to map air quality on regional or synoptic scales and to evaluate the influence of industrial and anthropogenic emissions (Ulfah et al., 2015).

5. Factors Influencing Air Pollution Dispersion

Meteorological factors affecting atmospheric dispersion include wind speed and direction, atmospheric turbulence, and terrain features. Wind direction influences the direction of pollutant dispersion. Wind speed affects the downwind distance pollutants travel and their dilution rate. Atmospheric turbulence enhances the vertical and horizontal dilution of pollutants, reducing ground-level concentrations. Terrain influences the development of wind and turbulence patterns, thereby affecting the ultimate dispersion of pollutants.

Wind velocity and direction span a large range over time and space and are therefore difficult to quantify. Consequently, the empirical Gaussian plume model handles these data by using simple additional inputs such as stability class and surface roughness, which approximate temporal variability. Topographical influence on dispersion is taken into account through a number of approximate methods (e.g., power law wind profile, the channeling or valley plume model). The model furthermore accounts for plume building downwash and complex terrain effects such as cavity formation and plume lofting.

This system is the basis of an important commercial air-quality modelling package (Lagrangian Particle Dispersion Model, LPDM-3E) that has been critically evaluated. Meteorological data from a regional weather forecasting model (WRF) allow the production of operational air quality forecasts with minimum data input from the user (Ulfah et al., 2015). Modelling studies of accidental releases normally link the prognostic meteorological model (situational forecasting) directly, or via the four-dimensional data assimilation (FDDA) system, to a long-range dispersion model such as MATCH-ADMS or MATCH-DEHM.

5.1. Meteorological Conditions

Dispersion of pollutants is mainly driven by advection via mean wind and turbulent diffusion. Gravitational settling also plays a crucial role. Therefore, meteorological conditions—both on large and local scales—substantially influence pollution distribution (Ulfah et al., 2015). Human comfort is directly affected by parameters such as temperature, humidity, rainfall, wind direction, and speed. Temperature is generally inversely proportional to height in the lower atmosphere and is influenced by factors like local topography, solar radiation, air mass history, soil properties, wind speed, and cloud cover (L. Palau et al., 2006). Under extreme radiation effects, the temperature profile may undergo inversion. Atmospheric pressure and relative humidity are also impacted by altitude, influencing pollutant diffusivity and concentration.

The atmospheric boundary layer represents the interface between the Earth's surface and the rest of the troposphere. Above this lies the free atmosphere, where turbulence is minimal, and pollutants can eventually become trapped during a temperature inversion. Atmospheric phenomena such as fog and clouds often form within this layer.

5.2. Topographical Effects

Topographic features influence air-pollutant dispersion by modifying flow fields and turbulence characteristics. Complex terrain distinguishes meteorological situations, breaking thermal stratification, thus altering dispersion conditions (Tomasi, 2017). When isothermal conditions over complex terrain are assumed, pollutant transport is affected by orographic flow and topographic shading effects, which depend on the orientation of dispersion with respect to the orography.

5.3. Urban Structures and Land Use

The clustering and shapes of building groups in a city govern air flow, pollution dispersion, and accumulation (Zhou et al., 2022). Air stagnation establishes under deep street canyons where vortices also strengthen the buildup of pollutants. Pollutant concentration and human exposure levels escalate sharply for building heights above about 40 m and at asymmetric aspect ratios. Urban morphology parameters, such as street canyon aspect ratio, building coverage, and building density, exhibit consistent and notable correlations with street-level air quality. Large-eddy simulation verified the expected impacts on the spatiotemporal variation of pollutant concentration. A small number of urban-layout parameters, augmented by a new index accounting for the orientation of building groups relative to prevailing wind, effectively identify street canyons highly affected by pollution. The prediction index provides effective guidance for the optimization of urban plans aimed at reducing air-quality problems.

6. Model Validation and Calibration

Data collection, statistical evaluation, and sensitivity analysis are critical for establishing confidence in dispersion model forecasts. Measurements from meteorological stations and air quality networks support the development of persistency and dispersion analyses. Although many available datasets only allow limited validation and calibration due to incomplete coverage or inadequate timespan, they still provide a means to assess a model's general performance for steady-state or synoptic conditions. Sensitivity studies are an important complementary approach to data-based validation techniques, enabling estimation of the effects of model assumptions, input uncertainty, and parameter values on predicted concentrations. Sensitivity analyses use physical insight and statistical evaluation to identify the most influential input variables, which facilitates development and narrows the focus of validation efforts.

Stationary air quality networks (e.g., the National Air Quality Routine Acoustic Monitoring Network) supply long-term pollution records. Combined with surface and upper-air meteorological data, these records provide the observational basis for persistency analyses. SEMS data from around the country are often employed to examine the applicability of model assumptions such as the use of mixing heights and National Weather Service (NWS) rawinsonde data. Video camera systems provide complementary records of dispersion patterns and visibility conditions during major events, and they serve to corroborate existing meteorological and air quality data (R. Goodin et al., 1976).

Continuous sampling techniques provide concentration data on the order of one sample every 5 to 10 min. Filter pack, canister, and cascade impactor results are typically available for several samples per day, offering long-term averages or wider pollutant coverage. Mobile reconnaissance measurements expand the spatial coverage considerably but require careful interpretation to maintain statistical significance. Particle volume, diameter, and count measurements characterize particulate distribution and serve to assess total suspended particulate (TSP) emissions, propagation, and deposition. Electron photomultiplier observations aid in model verification of point- and flaring-source predictions. Lastly, meteorological characterization and plume visualization through tracer studies generate comprehensive evaluations of dispersion models, including photographs.

6.1. Data Collection Methods

A comprehensive review of the development, validation and application of air pollution dispersion models is presented to illustrate how these models offer valuable tools for science and policy (Ulfah et al., 2015). Given the hazardous consequences of high concentrations of air pollution on human health and the environment, mathematical models that take into account the relevant physical and chemical processes of the atmosphere — the so-called dispersion models — have become increasingly important. The models describe the dispersion of air pollutants based on the similarity theory of turbulence, and are essential tools for pollution mitigation and management. Design and operational features of several near-field dispersion modeling techniques applied in the industrial and urban environment are described, and practical guidance on their use is provided (Tominaga & Stathopoulos, 2016).

6.2. Statistical Validation Techniques

Model validation constitutes the final stage that ensures the generality and practical feasibility of a mathematical model, underpinning model reliability. In air pollution dispersion modeling, particular emphasis is placed on statistical tests owing to the availability of time series data, which are inherently dynamic and subject to uncertainties arising from diverse sources. Therefore, model evaluation critically involves testing for both stationary and non-stationary behavior. Stationary processes maintain time-invariant means and variances, rendering their statistical properties constant over time, whereas non-stationary processes exhibit time-variable statistical characteristics. Given that air pollution data typically manifest as non-stationary time series, specialized validation techniques that account for non-stationarity are imperative.

Accordingly, the validation methodology incorporates procedures capable of evaluating the accuracy of air pollution models across both stationary and non-stationary regimes (R. Goodin et al., 1976). The proposed approach employs testing requirements formulated separately to accommodate each regime, thereby enabling the comprehensive assessment of model performance. Consequently, the method addresses the dynamic nature of air pollution data and provides a quantitative basis for statistical comparisons in the context of model validation and calibration.

6.3. Sensitivity Analysis

Sensitivity analysis represents an essential component of air pollution dispersion modelling. It facilitates the recognition of those parameters that wield a dominant influence on model outputs, thereby assisting in model development, calibration, validation, and, ultimately—governed by appropriate ethical considerations—the design of effective pollution-mitigation strategies. Because industrial development frequently involves the manufacture of toxic or explosive substances, the large-scale production, storage, and transport of materials of this nature routinely entails the potential of catastrophic vapor-cloud dispersion. Such events can place relative constraints on each of the preceding processes. Accordingly, sensitivity analysis assumes considerable importance for the parametrization of source terms, the quantification of model uncertainties, the verification of scientific hypotheses, and the optimization of the degrees of system freedom. Parameters for which outputs exhibit only a weak or negligible dependence may be assigned nominal or mean values, so that the complexity of the problem can be reduced without any significant loss of accuracy (Pandya et al., 2008).

Because conventional air-quality models attempt to represent complex flow and dispersion phenomena within simplified postulated frameworks, they incorporate numerous empirically derived parameters that require specification. A comprehensive framework for addressing model and measurement uncertainties in environmental modelling has been developed and tested (Izarra-Garcia et al., 2008). An assessment of how uncertainties propagate through models has been conducted, along with an examination of the sensitivity of model results to uncertainties related to prescribed sub-models and initial or boundary conditions. In the context of a high-quality urban measurement dataset, global sensitivity methods are found to be superior to one-at-a-time approaches.

7. Case Studies

Air pollution models find application in a wide range of situations. Urban air pollution is a frequent cause for concern due to the general proximity of the public to the emissions and the potentially harmful compounds involved. Industrial air pollution is also of great interest, especially when accident releases or long-term exposure at low concentrations is involved. Modelling is also used to investigate long-range pollution where the prevailing winds carry pollutants far from the sources and several countries may be involved (Tomasi, 2017).

7.1. Urban Air Quality Modeling

Accumulation of pollutants in cities leads to air quality deterioration and ensuing negative health and environmental implications. A number of dispersion models are developed and applied to study the impact of individual sources as well as a group of urban pollution sources on city or regional scale. For example, a Gaussian puff model is applied to the Dubai Boat Show to quantify the emissions from high-speed boats in the creek surrounding the exhibition area. Dispersion of nitrogen oxides emitted by a thermal power plant at the south-eastern part of Ljubljana is simulated through a three-dimensional Eulerian model, while transport and dispersion of sulphur dioxide over the Iberian Peninsula is studied with three different Eulerian models during a stratospheric warming event capable of injecting tropospheric pollution into the stratosphere.

Modeling of primary and secondary pollutants associated with the formation of photochemical smog is also addressed. For example, estimates of pollutant concentrations during severe photochemical episodes in the Athens basin are obtained by the application of the UAM-IV model to a 20 × 20 grid with approximately 4 km of resolution, covering both the basin and the surrounding mountainous areas. The Lagrangian photochemical model MILLIPOL-MOSAIC is used to identify paths of long-range transport of secondary ozone and other pollutants. Furthermore, dispersion of traffic pollutants such as nitrogen oxides, carbon monoxide, benzene, 1,3-butadiene and benzopyrene in the Athens basin is investigated using a childhood asthma case in Fontana, CA, as an example. The model is used to evaluate exposure observationally estimated by distance from roadways.

7.2. Industrial Emission Studies

Dispersion models are often used along with other research tools to investigate many topics; some examples are a urban area study, industrial emission studies and long-range pollution dispersion models. Mathematical models are widely used in air pollution research and a broad variety of situations; the numerous existing models schematically follow, mainly due to different characteristics and applications. The siting of industrial plants and the environmental impact of their gaseous discharges are subjects, which have been widely examined in the last 20 years. Pollution dispersion codes are often used in this kind of studies and decision-making process. MEXDAM is an Eulerian model, which solves the pollutant concentration for a grid of points in the investigated domain and one dimension along the vertical direction. Industrial plants and major roads lanes can be introduced anywhere in the domain, while road traffic, meteorological and hourly emission data are read as input for each computational cell. The governing transport equations are solved using a finite element technique. A domain-decomposition approach allows the solution of the concentration field for the different emission sources. Model validation and calibration have been performed on an industrial site.

7.3. Long-Range Transport of Pollutants

Pollutants can be transported over considerable distances by upper atmospheric winds, exposing populations far from emission sources to hazardous substances. Such threats are illustrated by damage from radionuclides, hazardous chemicals, and suspended particles released from accidents; exposure of mid-continental populations to high levels of CO linked to intense vehicular activity; and crop failures possibly resulting from acidic fogs and rain in the Andes Mountains of Argentina. The time periods between the pollutant's emission and subsequent exposure at another location usually range from a few hours to days. At distances exceeding roughly 1000 km, longer meteorological and chemical time scales may substantially affect the concentrations and compositions of transported pollutants and must be considered.

Long-range transport models have been developed by incorporating puffs into grid, puff-on-cell, and reactive plume frameworks. These models, which explicitly consider wind shear, time variation of mean wind velocity, plume rise, and atmospheric chemical reactions, permit different characterization of cloud properties and mechanisms affecting chemical composition. Numerical simulations of particle motion in combined wave and turbulent fields provide insight into the influence of Stokes drift and turbulence on suspended material. Analogous models predict vertical dispersion, plume rise, and aerosol growth in a stratified boundary layer. Regional transport of atmospheric sulphates helps to explain observed sulphate maxima over Oceania. Dispersion of particles around individual power stations is modelled with three-dimensional cloud and trajectories formulations. Advection models forecast pollution within an urban heat island. Studies relevant to the Po basin illustrate the use of Lagrangian particle models in urban environments. Satellite data estimate emissions, which are then propagated across the North Sea by a regional atmospheric circulation model. Photochemical models undergo validation procedures. Statistical trajectory models simulate sulphur pollution in Europe and the Los Angeles basin (L. Drake, 1980) (Ulfah et al., 2015).

8. Recent Advances in Modeling Techniques

Mathematical air pollution models are employed for prediction of pollution concentrations based on given emissions. A perfect model would allow prediction of concentrations that would result from any combination of pollutant emissions, meteorological conditions, location, and time period, with total confidence in the prediction. Recent studies have explored advancements in modeling techniques, including the incorporation of machine learning and remote sensing data to enhance performance and predictive capability (Ulfah et al., 2015). Research on advection–diffusion models continues to underline their importance for understanding pollutant distribution, particularly under unstable atmospheric conditions. Pollution assessment over complex terrain benefits from the optimization of meteorological and pollutant transport modelling, although the application remains challenging and complex, even with sophisticated algorithms (Tomasi, 2017).

8.1. Machine Learning Applications

The extensive review illustrates the evolution of mathematical models used to describe the emission, dispersion, transformation, and deposition of pollutants in the Earth's atmosphere. A detailed classification of models based on the spatial scale of atmospheric phenomena, mathematical technique, geometry, size of flow disturbance, source configuration, and treatment of physical and chemical processes is provided. A synthesis of formal approaches adopted in the operational stage of model implementation shows the chicken–egg cycle linking model development, application, and evaluation. The validation problem and possible ways of addressing it constitute a matter of active research.

Urban neighborhood-scale pollution prediction represents a recent development. A machine learning technique is evaluated on its ability to predict the neighborhood-scale PM10 concentration in a compact city. The methodology involves developing separate ML prediction models for three different urban configurations; urban open spaces, street canyons, and subway platforms (Wai & K. N. Yu, 2023). Unix timestamps in the format of YYYYMMDD are applied to generate monthly, daily, and hourly features. Five different ML algorithms—random forest (RF), gradient-enhanced regression tree (GBRT), support vector regression (SVR), artificial neural network (ANN), and long short-term memory (LSTM)—are examined and compared with multiple linear regression and the persistence model using monitoring data. Among the ML models examined, LSTM and SVR show promising performances on both training and test data.

8.2. Integration with Remote Sensing Data

Worldwide, air pollution represents a major concern with overwhelming evidence on the harmful effects on health, ecosystems and economy, and improved, reliable estimates of pollution concentrations are crucial for monitoring compliance with regulatory standards and supporting epidemiological studies (Forlani et al., 2020). Recent advances geared towards improving the performance of the models include combination of modeling with machine learning approaches to maximize predictive capability, and integration with remote sensing data. A significant technical challenge is posed by the frequent discrepancy in spatial resolution between data sources, a problem widely known as change of support problem (COSP).

9. Policy Implications of Air Pollution Models

Mathematical modeling also informs air quality policies. Models have guided regulatory and public health policies in numerous countries, influencing urban transportation regulations and supporting the development of Vehicle Inspection and Maintenance programs (Ulfah et al., 2015). They facilitate the development of regulations and air quality standards, identify problems requiring attention, assess the effectiveness of control measures, and support emergency response management. The ability to rapidly estimate the impact of existing or proposed air pollution sources and their compliance with air quality standards offers a powerful tool to evaluate regulatory strategies and their implications.

D. N.C. Kavuri (2017) reviewed models employed to assess source contributions to particulate-type ambient air pollution in the urban steel city of Rourkela, India, analyzing historical data from 2010 to 2012 to forecast upper limit pollution levels. Source apportionment studies combined with forecasting provide a basis for policy decisions to address and remediate environmental pollution challenges (Chaitanya Kavuri, 2017).

9.1. Regulatory Frameworks

In recent decades, awareness of environmental pollution and its consequences has grown substantially, highlighting issues such as acid rain, ozone depletion, and the greenhouse effect. Accompanying these concerns are potential health challenges including respiratory diseases and fatigue, alongside the financial implications of pollution abatement. Air pollution studies often focus on emissions, transport, dispersion, and concentration over time, while recent research has shifted toward comprehensive control strategies. Degrees of pollutant dispersion and air quality are influenced by factors such as emission duration, emission quantity, transport, and the physical, chemical, and meteorological properties of the substances involved.

One significant issue in air pollution control centers on the presence of noxious gases emitted from industrial processes. The associated health risks necessitate monitoring and management of pollutant discharges. Air pollutants possess a variety of characteristics; for instance, some gases become denser than air, leading to phenomena such as ground hugging and other unexpected behaviors. The complexity of pollutant behavior is further compounded in urban regions due to large gas emissions, especially from industrial areas and heavy traffic, underscoring the need for mathematical modeling to predict their spread and behavior (Ulfah et al., 2015). In assessing alternatives for generators and combustion procedures, dispersion models play a vital role in economically and reliably evaluating air pollution impacts on a geographical scale (P. Chernogorova & G. Vulkov, 2016).

Air pollution is widely recognized as a critical policy and regulatory issue worldwide, influencing industrial operations and their locations. The impacts on public health and quality of life have necessitated the establishment of strict regulatory frameworks. To remain competitive, economically competitive, and compliant with governing regulations, industrially and municipally, every application must consider appropriate dispersion models to account for surrounding air concentrations during development phases (Ahmad Hussein Naser, 2019).

9.2. Public Health Policies

Public-health policies have been developed to diminish the population impact of urban air pollution. Partial restrictions on vehicular traffic reduce the total burnt fuel. The increase in doses of anti-allergic drugs between 1980 and 1995 was, with a few exceptions, negatively correlated with immobilization of vehicles (Ulfah et al., 2015).

Several epidemiological studies, performed first in the Los Angeles area and subsequently in Europe, detected associations between chronic exposure to ambient levels of air pollution and specific clinical outcomes as respiratory symptoms, reduced lung function, and low birth weight (Sally Liu et al., 2007). Additional European evidence has come from studies of such short-term effects (He et al., 2018).

10. Challenges and Limitations

The developed mathematical model offers a practical tool to analyze transport phenomena with new modeling techniques, suitable for diverse conditions and applicable to both gaseous and liquid pollutants released from various sources. Despite the range of available modeling approaches, a universally acceptable model remains elusive due to the inherent complexity of the subject. The perfect air pollutant concentration model would enable confident predictions for any specified set of pollutant emissions, meteorological conditions, location, and time period. Models grounded on basic physical laws are flexible enough to accommodate complex situations if comprehensive input data are available. Nevertheless, the growing complexity and number of parameters challenge effective management; in such scenarios, models calibrated with incomplete or uncertain input data tend to lose reliability.

10.1. Data Uncertainty

Uncertainty in air pollution data arises from incomplete understanding, inadequate measurements, and inaccurate emissions reporting in mathematical modeling of dispersion. Although some experimental uncertainty can be quantified (R. Goodin et al., 1976) , inaccuracies in pollutant emission inventories frequently cause outputs to deviate from field observations. Mathematical models assist in predicting pollutant behavior following new emission sources or changes in emission levels (Ulfah et al., 2015).

Transport and dispersion formulations facilitate the identification of parameters of interest. Integrated air quality models support environmental monitoring, management, and pollution assessment. The principal processes of pollutant dispersion are advection, which transports pollutants by wind, and diffusion, generated by turbulent air movement that transfers particles from areas of high to low concentration. Dispersion is mathematically formulated on the basis of mass conservation, incorporating advection, turbulent diffusion, and chemical reactions.

10.2. Modeling Complex Scenarios

Mathematical modeling facilitates the study of air pollutant behaviors following changes in sources or emission rates. Air quality models constitute integrated tools for environmental monitoring, management, and pollution assessment. A suitable concentration model predicts pollutant levels based on emission rates and meteorological conditions. Simulations elucidate the spread, extent, and intensity of pollution across an area. Atmospheric dispersion primarily comprises advection and diffusion. Advection transports pollutants via wind, represented by the horizontal wind speed vector $U = (u, v, w)$, while diffusion results from turbulent air motions causing particle movement from high to low concentrations. The mathematical formulation derives from mass conservation, incorporating advection, turbulent diffusion, and chemical reactions (Ulfah et al., 2015).

Outdoor air pollution remains a critical concern worldwide. Modeling near-field pollutant dispersion involves complex interactions between plumes and flow fields modified by building-induced turbulence. Approaches encompass field measurements, laboratory experiments, empirical models, and CFD simulations, each presenting distinct advantages and limitations. Near-field dispersion, occurring within a few hundred meters from emission sources, focuses on local emissions and interactions with built environments. Wind conditions, building aerodynamics, stack configurations, and topography represent key determinants of pollutant distribution (Tominaga & Stathopoulos, 2016).

11. Future Directions in Air Pollution Modeling

The previous section discussed the inherent limitations and uncertainties in air pollution models, particularly issues arising with sparse or uncertain meteorological and emission data. Future improvements are expected to focus on methodologies that effectively reduce these uncertainties and enhance predictive capabilities.

Artificial intelligence technologies such as neural networks offer significant potential for air quality modeling. Artificial neural networks trained with data from air monitoring stations and meteorological inputs have proven highly effective in modeling complex chemical transport processes (Chaitanya Kavuri, 2017). Coupling neural networks with physical models also enhances accuracy (Ulfah et al., 2015).

Datasets for training neural networks can be organized into three groups, reflecting the approach to model construction. When neural networks analyze all data prior to generating a model, the resulting dataset is considered homogeneous. Conversely, training networks using data subsets produces heterogeneous datasets. The third approach employs neural networks to examine data, discern underlying patterns, and then select the most relevant, thereby augmenting the data and its utility in training algorithms (Tomasi, 2017).

Remote sensing and machine-learning methodologies hold promise due to the high volume of available observations, especially from satellite databases. Numerous satellite products reliably constrain aerosol emissions. Integrating additional input variables with land-use information supports further exploration of the multifaceted determinants of aerosol concentrations. The inclusion of auxiliary variables enriches comprehensive air quality forecasting and facilitates the development of real-time monitoring systems and historical climatologies for environmental applications.

11.1. Emerging Technologies

Article presents a comprehensive review of mathematical modeling of air pollution dispersion, intended to complement the textbook Overview of Air Pollution and serve as a reference that surveys emerging modeling techniques and analyzes applications in urban, industrial, and long-range transport contexts. In the Introduction, modeling of air pollution dispersion is introduced and modeled dispersion is linked to the Overview of Air Pollution, emphasizing modeling formulation and techniques rather than a broad review of pollution sources or effects. Section 1: Introduction discusses modeling air pollution dispersion and links the topic to the Overview of Air Pollution (to appear). Section 2: Overview of Air Pollution summarizes pollutant types, sources, and key characteristics, emphasizing impacts and distinction from greenhouse gases. Section 3: Fundamental Mathematical Modeling describes mathematical modeling concepts, benefits, types, and underlying assumptions. Section 4: Dispersion Models explains the mathematical bases of Gaussian, Lagrangian, and Eulerian formulations, including assumptions and structural differences. Section 5: Factors Influencing Air Pollution Dispersion examines the meteorological, topographical, and urban topographic conditions affecting dispersion. Section 6: Model Validation and Calibration covers data collection procedures, statistical methods, and sensitivity analyses employed for model evaluation. Section 7: Case Studies presents modeling applications to selected urban, industrial, and long-range transport scenarios. Section 8: Recent Advances in Modelling Techniques encompasses developments involving machine learning and remote sensing from air quality data. Section 9: Policy Implications of Air Pollution Models explores regulatory and public health considerations. Section 10: Challenges and Limitations addresses primary unresolved issues in air pollution modeling. Section 11: Emerging Technologies highlights recent technological trends and interdisciplinary techniques critical for future modeling directions. Section 12: Conclusions draws together the main elements of the review and discusses future developments.

11.2. Interdisciplinary Approaches

Mathematical modeling in air-pollution dispersion draws on the expertise of a number of disciplines—the physical, chemical, economic, political, social, mathematical, and numerical sciences (Ulfah et al., 2015). A comprehensive inventory should therefore both recognise the value of this interdisciplinary approach and acknowledge the extensive mathematical repertoire that is woven into it. "Dispersion" models fall cleanly into this category. They come in a range of formats—most notably Gaussian plume or puff, Lagrangian particle, and Eulerian grid models—but all interpret an air-pollution event as the solution to a quantitatively specified mathematical problem. Since the issue of differential equations is always involved, their remit is clearly disciplined, in that the problem of pollution dispersion must be described in terms of quantities and equations that the mathematical sciences can supply (Tominaga & Stathopoulos, 2016). By contrast, the economic, political or social dimensions currently remain peripheral to the modeller's concern. This implies in turn that the scientific contributions do not encompass the full fat of an interdisciplinary framework, since there is effectively a mathematical embargo on the specification of any issue that lies outside the discipline's immediate remit.

12. Conclusion

Mathematical models for air pollution provide a systematic representation of the physical, chemical and biological processes determining the emission, dispersion, chemical reaction, and removal of pollutants. The ability of these models to predict pollution concentrations at locations in time and space is invaluable for regulatory, planning, and exposure assessment purposes. Accurate predictions at levels of current interest for air quality standards require mathematical formulations that represent the physical processes governing pollutant concentrations.

Environmental professionals rely on models for screening and detailed analyses. Because every model has assumptions and is developed for specific applications and environments, it is important to understand the appropriateness of a particular model for a given application. Model formulations range from simple empirical relations to complete three-dimensional, time-dependent photochemical grid models. Model selection depends on the questions posed, pollutant types and characteristics involved, processes included, spatial and temporal scales, receptor locations, and data availability for application and evaluation.

Dispersion models characterize the distribution of pollutant material from an emission source. The concentration at any location is determined from initial emissions, ambient conditions, transport, and removal mechanisms. The rate of momentum, heat, mass, and moisture exchange between the lower air and Earth's surface controls flow near the surface and the character of pollutant dispersion.

The concentrations adjacent to a source arise from primary emissions of chemical compounds and from chemical transformations of the emitted pollutants that generate secondary pollutants. Primary pollutants such as carbon monoxide, sulfur dioxide, and particulate matter are emitted directly. Secondary pollutants such as ozone, peroxyacetylnitrate, and sulfate result from atmospheric chemical reactions involving other gases. Computer simulation models have the inherent capability to address the complexity of multiphase chemistry within the atmosphere. Sophisticated dispersion models incorporate chemical transformations by simulating the atmospheric reaction mechanisms.

The inadvertent situations of pollutants released to the atmosphere emonstrate the usefulness, flexibility, and timeliness of mathematical models for operational forecasts for emergency preparedness and response. thai air pollution is from transport of contaminants within and through the atmosphere from emission sources or receptors located in remote geography locations. In almost all air-poil group or contaminant dispersion situations, mathematical models provide the only practical method for accurately estimating the concentration distribution or fallout (Ulfah et al., 2015).

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Cite this Article:

Manisha Halder, Manish Sharma, " Mathematical Modeling of Air Pollution Dispersion: A Comprehensive Review", *Pi International Journal of Mathematical Sciences,* ***ISSN:*** *3107-9830 (Online), Volume 1, Issue 1, pp. 07-25, August 2025.*

Journal URL: *https://pijms.com/*