Differential Equation Models For Atmospheric Pollutant Dispersion And Air Quality Dynamics

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Abstract
Atmospheric pollution is a major environmental and public-health problem, and mathematical models are essential for predicting the transport, dispersion, transformation, and removal of pollutants. This paper develops a differential-equation framework for assessing atmospheric pollutant dispersion and air-quality dynamics. The central model is the advection–diffusion–reaction equation, which describes the combined effects of wind-driven transport, turbulent diffusion, emissions, chemical transformation, and deposition. A simplified one-dimensional model is first developed and then extended to a two-dimensional urban setting. Analytical Gaussian-type solutions are used to interpret plume movement, while finite-difference discretization is proposed for time-dependent numerical simulation. The model is also extended to multiple pollutants through a coupled system of reaction equations. Stability, conservation, boundary conditions, and sensitivity to wind velocity, diffusion coefficient, emission rate, and reaction rate are discussed. An illustrative computational scenario demonstrates how stronger wind transports pollutants farther from a source while increased turbulent diffusivity broadens and lowers the concentration peak. The framework provides a mathematically transparent basis for air-quality forecasting, source assessment, environmental planning, and the design of monitoring and emission-control strategies.
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1. Introduction

Air pollution results from the release of gases and particulate matter from industrial facilities, transportation, power generation, domestic combustion, agriculture, and natural sources. Once emitted, pollutants are transported by atmospheric motion and redistributed by molecular and turbulent diffusion. They may also undergo chemical reactions, dry or wet deposition, and removal by precipitation. Because these processes interact over several spatial and temporal scales, direct measurement alone cannot describe pollutant behavior everywhere. Mathematical models provide a systematic means of estimating concentration fields from emission, meteorological, and chemical information.

The mathematical foundation of atmospheric dispersion modeling is the advection–diffusion equation. It is a partial differential equation expressing conservation of pollutant mass while accounting for transport by wind and spreading by turbulent diffusion. Stockie showed that the Gaussian plume model can be derived and interpreted through this equation and emphasized the mathematical connection between atmospheric transport, diffusion, and inverse source estimation [1]. Analytical methods such as the Generalized Integral Laplace Transform Technique (GILTT) have also been developed for time-dependent advection–diffusion problems in the planetary boundary layer [2].

For realistic air-quality applications, dispersion cannot always be treated independently of atmospheric chemistry. Modern chemical-transport systems include horizontal and vertical advection, diffusion, gas-phase reactions, photolysis, aerosol processes, cloud chemistry, and deposition [3]. Thus, differential-equation models range from simple single-pollutant equations to large coupled systems involving meteorology and chemical reaction mechanisms.

The objective of this research is to develop a compact differential-equation model that captures the principal processes controlling pollutant concentration. The study formulates governing equations, derives a simplified dispersion model, proposes a numerical solution procedure, analyzes qualitative stability and sensitivity, and discusses how the framework can be used for air-quality assessment. The model is intended to provide a bridge between elementary analytical models and more complex computational air-quality systems.

2. Literature Review

Atmospheric dispersion models have evolved from analytical plume equations to sophisticated three-dimensional chemical-transport models. Classical Gaussian plume models remain valuable because they provide simple estimates of steady concentration around continuous sources. Their

mathematical basis is the advection–diffusion equation, with assumptions such as steady wind, constant emission, and parameterized turbulent spreading [1].

Moreira et al. reviewed analytical solutions of the atmospheric advection–diffusion equation and described the GILTT approach for one- and two-dimensional time-dependent dispersion. Their work demonstrates how concentration can be expanded in eigenfunctions, producing a system of ordinary differential equations that can be solved analytically using integral-transform methods [2]. These methods are useful for understanding the influence of boundary-layer structure and turbulent diffusivity without the computational expense of a complete numerical atmospheric model.

For complex atmospheric chemistry, the governing system becomes a chemical-transport model. Byun and Schere described the CMAQ modeling framework, which combines meteorological fields, emission inventories, and chemistry-transport calculations. Its equations include horizontal and vertical advection, diffusion, gas-phase reactions, photolysis, aqueous reactions, aerosol dynamics, and deposition [3]. This illustrates that realistic air quality is inherently a coupled differential-equation problem.

Recent research continues to use the advection–diffusion equation for computational pollution assessment. Kaur and Shah used finite-difference techniques to simulate the spatiotemporal evolution of pollutant concentration from a continuous ground-level source, showing localization near the source followed by plume elongation in the wind direction and reduction of peak concentration as diffusion increases [4].

Reviews of air-pollution modeling also distinguish between process-based dispersion models, Lagrangian particle methods, Eulerian grid models, and hybrid approaches. Process-based models are particularly useful when pollutant chemistry is limited or when transport dominates the behavior of a species [5]. The literature therefore supports a hierarchy of models: simple differential equations for conceptual and local analysis, numerical advection–diffusion models for spatial prediction, and fully coupled chemical-transport models for regional air-quality assessment.

3. Research Work

3.1 Governing conservation equation

Let $C(x,y,z,t)$ denote pollutant concentration in mass per unit volume. The general conservation equation is

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathrm{u}C) = \nabla \cdot (\mathrm{K}\nabla C) + S - R(C) - D(C). \qquad -1$$

Here $u = (u,v,w)$ is the wind-velocity vector, K is the turbulent-diffusion tensor, S is the emission source term, $R(C)$ represents chemical removal or transformation, and $D(C)$ represents deposition or other loss mechanisms. For incompressible flow with approximately constant wind,

$$\frac{\partial C}{\partial t} + u \cdot \nabla C = \nabla \cdot (K\nabla C) + S - R(C) - D(C). \qquad -2$$

Equation (2) is the central differential equation of the proposed model.

3.2 One-dimensional model

For a pollutant transported along the x-direction with constant wind speed U and constant diffusivity D, with first-order removal rate k and source $S(x,t)$, the model becomes

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2}\right) + S(x,t) - kC. \qquad -3$$

The terms have clear physical meanings. $U\partial C/\partial x$ represents advection, $D\partial^2 C/\partial x^2$ represents turbulent spreading, S represents emission, and $-kC$ represents chemical or deposition loss.

For a continuous point-like source located at $x = 0$, the initial condition can be $C(x,0) = 0$ and the source can be represented by a Dirac delta function $S = Q\delta(x)$, where Q is the emission rate per unit cross-sectional scale. For transient studies, a Gaussian fundamental solution illustrates the competition between advection and diffusion:

$$C(x,t) \propto \left[\frac{1}{\sqrt{(4\pi Dt)}}\right] exp\left[\frac{-(x-Ut)^2}{(4Dt)}\right] exp(-kt). \qquad -4$$

The center of the plume moves approximately as $x = Ut$, while its standard deviation increases proportional to $\sqrt{(Dt)}$. The exponential factor $exp(-kt)$ represents first-order removal.

3.3 Two-dimensional urban model

For horizontal coordinates x and y, a simplified model is

$$\partial C/\partial t + U\partial C/\partial x + V\partial C/\partial y = K_x\partial^2 C/\partial x^2 + K_y\partial^2 C/\partial y^2 + S - kC. \quad -5$$

This model can represent pollutant transport around an urban area when vertical mixing has been parameterized or depth-averaged. Spatially varying wind and diffusivity can be included by replacing U,V,K_x,$K_y$with functions of position and time.

3.4 Chemical interaction model

For multiple pollutants $C_i, i = 1, \dots, N$, the general system is

$$\partial C_i/\partial t + u \cdot \nabla C_i = \nabla \cdot (K_i \nabla C_i) + S_i + \Sigma_j \nu_i j r_j(C_1, \dots, C_N). \quad -6$$

where $\nu_i j$is the stoichiometric coefficient and $r_j$is the rate of chemical reaction j. This structure can represent transformation of primary pollutants into secondary species such as ozone or secondary particulate matter. The coupled system is nonlinear when reaction rates depend nonlinearly on concentrations.

3.5 Boundary and initial conditions

An initial condition specifies $C(x, 0) = C_0(x)$. At an inflow boundary, concentration may be prescribed as $C = C_i$. At an impermeable boundary, zero normal flux can be imposed:

$$n \cdot (uC - K\nabla C) = 0. \quad -7$$

At an open outflow boundary, a convective or zero-gradient condition may be used. Correct boundary conditions are essential because artificial reflections or excessive pollutant loss can significantly affect computed concentrations.

3.6 Numerical method

For numerical simulation, the spatial domain is divided into a grid with spacing Δx and Δy. A finite-difference approximation of equation (5) can be written using central differences for diffusion. For example,

$$C_x x \approx \left(C_{i+1,j} - 2C_{i,j} + C_{i-1,j}\right)/\Delta x^2. \quad -8$$

Because advection can dominate diffusion, a stable upwind or flux-limited discretization is preferable for the advective terms. Explicit time stepping must satisfy a combined stability restriction involving the Courant number and diffusion number. An implicit or semi-implicit method can be used when diffusion is strong or when large time steps are required.

3.7 Air-quality indicator

For an assessment period T, a time-averaged concentration can be defined as

$$C_a vg(x, y) = 1/T \int_0^T C(x, y, t)dt. \quad -9$$

A normalized exposure indicator may then be defined by

$$E(x, y) = C_a vg/C_r ef, \quad -10$$

TABLE I: Air Quality Dispersion Simulation Parameters

Parameter	Symbol	Value	Unit
Effective Stack Height	H_s	45.0	m
Emission Rate	Q	120.5	g/s
Mean Wind Speed (at 10m)	u_{10}	4.2	m/s
Eddy Diffusivity (y-axis)	K_y	15.2	m^2/s
Eddy Diffusivity (z-axis)	K_z	3.8	m^2/s
Mixing Layer Height	H_i	850.0	m
Surface Deposition Velocity	v_d	0.01	m/s

where $C_r ef$is a selected air-quality guideline or reference concentration. Values above unity indicate locations where modeled average concentration exceeds the selected reference level. The indicator is useful for mapping relative pollution burden, although regulatory assessment must use the applicable pollutant-specific standard and averaging period.

4. Stability and Model Analysis

4.1 Qualitative stability

Consider the homogeneous one-dimensional equation

$$\partial C/\partial t + U\partial C/\partial x = D\partial^2 C/\partial x^2 - kC. \quad -11$$

Using a Fourier mode $C = e^{i\xi x+\lambda t}$, substitution gives

$\lambda = -D\xi^2 - k - iU\xi.$ -12

Therefore,

$Re(\lambda) = -D\xi^2 - k \leq 0.$ -13

For $D > 0$or $k > 0$, all nonzero spatial modes decay with time. The imaginary component $-U\xi$ represents transport of the disturbance without changing its amplitude. This result establishes the basic mathematical stability of the linear advection–diffusion–decay model: diffusion and removal damp concentration perturbations, while pure advection transports them.

4.2 Conservation

Integrating equation (3) over a closed domain gives a total-mass balance. In the absence of source, boundary flux, and removal, total pollutant mass is conserved. With first-order removal, total mass decreases at a rate proportional to the integrated concentration. This provides a useful numerical verification test: a computational scheme should reproduce the expected mass balance within discretization error.

4.3 Sensitivity to parameters

Wind speed U primarily controls the travel time and downwind displacement of the plume. Increasing U generally moves a pollutant cloud more rapidly and, under a continuous-source steady approximation, can reduce concentration near the source because the same emission is distributed through a greater advective flux.

The diffusion coefficient D controls plume width. Larger D causes faster spatial spreading and lower peak concentration, while smaller D produces a narrower plume with greater local concentration gradients. The removal coefficient k determines the temporal and spatial persistence of a pollutant. Larger k causes faster decay and reduces downwind concentrations.

The source strength Q directly increases concentration in a linear nonreactive model. Therefore, uncertainty in emission inventories can translate almost proportionally into uncertainty in predicted concentration. This makes source estimation and inverse modeling important applications of differential-equation models. Stockie demonstrated how concentration measurements can be used to formulate an inverse source-identification problem using least squares [1].

4.4 Illustrative scenario

Consider a continuous source releasing a nonreactive pollutant into a uniform wind field. At the beginning of the simulation, concentration is concentrated near the source. As time increases, the plume center moves downwind approximately according to $x = Ut$, while its width increases approximately according to $\sqrt{(Dt)}$. Consequently, the peak concentration decreases as the pollutant spreads.

If wind velocity is increased while diffusivity remains fixed, the plume reaches downwind receptors more quickly and becomes more elongated in the transport direction. If diffusivity is increased, the concentration field becomes broader and smoother. If a first-order removal process is included, concentrations decline more rapidly with time and distance. These qualitative behaviors agree with analytical advection–diffusion theory and recent finite-difference simulations [1,4].

The framework can therefore support scenario studies in which emission controls, meteorological conditions, or chemical removal rates are varied. For example, a 30% reduction in the source term in a linear model produces approximately a 30% reduction in concentration under identical meteorological and chemical conditions. This does not necessarily imply the same reduction in health risk because exposure depends on population distribution, toxicity, time averaging, and pollutant interactions.

5. Conclusion

This paper developed a differential-equation framework for assessing atmospheric pollutant dispersion and air-quality dynamics. The central advection–diffusion–reaction equation provides a unified mathematical representation of wind transport, turbulent diffusion, emissions, chemical transformation, and deposition. Simplified one- and two-dimensional forms were presented together with Gaussian-type analytical behavior and a finite-difference numerical solution strategy.

The stability analysis demonstrates that diffusion and first-order removal generate damping of concentration perturbations, while advection mainly transports disturbances. The analysis also shows that wind speed controls plume travel, turbulent diffusivity controls spatial spreading, emission strength controls concentration magnitude, and chemical-removal rates determine persistence.

The proposed framework is intentionally compact and can be extended to spatially variable meteorology, multiple pollutants, nonlinear chemistry, atmospheric boundary-layer structure, and three-dimensional numerical models. It can also be coupled with monitoring data for parameter estimation and inverse source identification. Future work should integrate real-time meteorological observations, satellite or ground-based concentration measurements, uncertainty quantification, and machine-learning-assisted parameter estimation. Such hybrid approaches can improve air-quality forecasting while retaining the physical interpretability of differential-equation models.

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