One Aspect of Environmental Engineering – Modelling the Air Pollution Effects using Advection-Diffusion

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Abstract: This paper aims to contribute to the development of appropriate and sustainable solutions that enhance response readiness and facilitate the identification, processing, investigation and reporting of fire and explosion incidents. Additionally, it seeks to address the overall reduction and control of pollution levels. From this perspective, the elements and cases of pollutant emission factors are analysed concerning spatial distribution, mechanisms and elimination time. The concentration of air pollutants can be described by the advection-diffusion equation, a second-order partial differential equation (PDE). This approach exemplifies an interdisciplinary method, taking into account the atmospheric boundary layer, including wind limitations, daily temperature variations and the presence of eddies. To analyse the analytical and numerical solutions to the diffusion equation, a two-dimensional, time-independent case with a continuous terrestrial line source of pollutants was selected. The results, obtained using freely chosen parameters and appropriate boundary conditions determined according to literature sources, are presented in both code and graphical form. Modeling is recognized as an important complementary tool and can be applied to both short-term and long-term planning. In particular, this study investigates the potential of a numerical scheme for modeling advection, using the analytical solution as a reference within defined boundary conditions. This approach demonstrates its applicability in tracking diffusion processes caused by accidents or natural events, where air pollutants disperse from one area to another over time.

Keywords: air pollution; advection-diffusion; numerical solutions; environmental modeling

1 Introduction

The issues of air pollution, emissions diffusion and traceability continue to be research hotspots for scientists worldwide [1-5]. Air pollution refers to the presence of substances in the atmosphere at concentration levels that are harmful to human health and other living beings, may negatively impact plants and soil, or contribute to environmental degradation. These atmospheric substances with harmful effects are generally referred to as harmful substances or pollutants.

The main challenges and public focus include the emission of harmful substances from both fixed and mobile sources, the development of monitoring systems and the parallel advancement of normative, administrative and practical operations. These efforts aim to establish a framework and best practices for maintaining appropriate air quality levels [6-8]. Furthermore, monitoring, simulating and evaluating accidental and continuous pollution sources are crucial for building the capacity for timely and efficient responses.

This article aims to contribute to the development of appropriate and sustainable solutions that provide effective responses, facilitate the identification, processing, investigation and reporting of fire and explosion incidents and ultimately help reduce and control pollution levels. From this perspective, pollutant emission factors were analyzed concerning spatial distribution, mechanisms and elimination times. It is also important to consider the atmospheric processes that may influence the dispersion and removal of harmful substances (Figure 1).

Figure 1
Atmospheric processes concerning air pollution

The basic elements and processes related to sources, the atmosphere and receptors are crucial in the study of air pollution. For sources, it is important to consider their location, terrain configuration, emission time and duration, and other relevant characteristics. The atmospheric state also plays a critical role, as it influences the transport, direction, speed, dispersion and transformation of pollutants. On the receptor side, the way air pollutants are detected involves monitoring systems that must be carefully calibrated and positioned relative to the source location. This includes considering sensor sensitivity, as well as factors such as pollutant reduction, deposition and the presence of barriers. These aspects are essential for a comprehensive analysis and understanding of air pollution dynamics [9].

Air pollutants enter the atmosphere through natural processes or human activities. Natural sources of air pollution include vapors, wildfires, sandstorms and other natural events. However, industrial plants are among the most significant stationary artificial sources of atmospheric pollution [10-12]. Air pollutants can also be emitted from both mobile and stationary sources [13]. Artificial sources of pollutants include chimneys, ventilation outlets, landfills, waste and raw materials' storage facilities, vehicle exhaust systems and agricultural sprayers used for protective chemicals. In addition to these stationary and mobile sources, pollution sources in accidental situations must also be considered. Such incidents can cause a sudden increase in air pollution in specific areas, necessitating immediate corrective action.

Pollutants in the atmosphere can be transported by wind through advection, atmospheric diffusion, dry or wet deposition, re-suspension from soil after deposition, or chemical transformation. Due to these emissions and their atmospheric propagation, pollutants may be present in varying concentrations.

Concentration measurements are typically taken at pre-established monitoring points and centers, where data is automatically collected. Based on the measured data, actions can be taken or plans developed with corrective measures to reduce pollutant concentrations [14]. Mathematical modeling can be employed for analysis and forecasting [15].

Modeling principles can be applied to facilities that emit pollutants during regular operations, as well as in the case of accidents that release significant quantities of pollutants into the atmosphere. However, regular monitoring and measurement systems may sometimes be nonfunctional or unable to provide real-time data on pollutant releases. This becomes particularly critical when information about pollutant concentrations is essential for enabling emergency actions to reduce emissions or to initiate other mechanisms and procedures to mitigate harmful effects on human health and the environment. Understanding the location of sources and the spatial distribution of pollutants is crucial from this perspective. Incorporating spatial data can significantly enhance overall awareness and risk assessment, leading to more effective and appropriate responses.

Assessing the spread of pollutants is a complex process due to the irregularity of pollutant transport and its dependence on terrain characteristics, obstacles and especially urban conditions. The application of air quality models in air pollution management remains challenging and has not been extensively reported [11, 13].

Furthermore, during facility construction, it is mandatory to conduct an analysis and assessment of environmental impact, including the effects of air pollution. This assessment involves evaluating all relevant aspects related to the application of mathematical models. Since some mathematical models for gradient transport of air pollutants do not have analytical solutions in completely general functional form for diffusivity and wind speeds, the paper discusses both analytical and corresponding numerical solutions for a selected case, including the boundary conditions required for numerical solutions.

In air pollution assessment, one of the primary goals is to obtain a spatial distribution of pollutant concentrations from various sources under specific meteorological and geographical conditions. To achieve this, it is necessary to gather data to understand the state and potential direction of pollutant dispersion. Depending on the conditions of the assessment, data can be collected or simulated by the model for a specific area and time. Through time, many scientists have researched possible solutions, following knowledge and computer power development. Mostly analyzing temporary stationary point sources by application of the Gaussian model. Since then, was recognized, the importance of modeling pollutant dispersion through line source [14]. The solution for a line source as discrete or continuous, has been challenged through time [14-16], as there is no general form of analytical solution, defining boundary conditions have to be used in relation of the case of interest. Almost the same situation exists with numerical solutions that require significant computer power in addition to the proper definition of boundary conditions [15-17].

Problem solving the basic gradient transport model analytically for completely general function forms for diffusivity K and wind speeds u, v and w might be overcome by numerical solutions [15]. The aim of our study was to demonstrate how numerical solutions can be used for a case chosen by the authors, followed by a discussion on the possible applications of modeling, including the selection of parameter values and boundary conditions. Additionally, the use of mathematical modeling for advection-dispersion of pollutants was presented as a valuable tool for assessing air pollution effects, emphasizing that mathematical models are essential for understanding the dynamics of air pollutant transmission.

A thorough analysis of air pollution phenomena often employs mathematical models that can be used for subsequent monitoring and prediction of pollution in specific areas. This aligns with growing concerns about air pollution and its effects on human health and the environment. The main contributions of the article are its interdisciplinary approach and its emphasis on practical modeling applications.

Based on previous research described by mathematical formalisms regarding the advection-dispersion of pollutants, the paper practically addresses a case involving a line source of pollutants. It analyzes both analytical and numerical solutions for this specific case, using parameters derived from relevant literature sources and the author's selection. Additionally, it examines the constraints that need to be defined for the numerical solution.

2 Modelling as a Tool for Monitoring, Assessment and Simulation

For air quality assessment, monitoring, simulation, or a combination of both can be used. Depending on various criteria, such as the expected level of model accuracy and complexity, additional data can be integrated and processed alongside the measured data.

Modeling is an essential complementary tool that aids in both short-term and long-term planning. The distribution of air pollutants is influenced by temporal and spatial data, including climate and other weather conditions, requiring multidisciplinary knowledge. This complexity is further compounded by the potential for cross-border influences. Modeling is also used to forecast air quality, offering predictive information that is valuable both during the planning process and in real-time situations when necessary.

Mathematical models allow for the parameterization of important factors affecting atmospheric processes, enabling their analysis, assessment and prediction over the observed period. One of the advantages of mathematical modeling is its capacity to encompass a large number of sources over a wide area, utilize a vast amount of collected data and parameterize the characteristics of processes for detailed analysis. In considering pollutant emissions, the modeling process includes the categorization of sources, their physical characteristics, the mechanisms by which pollutants enter the atmosphere, and their dependence on meteorological conditions and soil characteristics. The models also account for the physical and chemical transformations of pollutants, dry and wet deposition, and the redistribution of pollutants caused by natural processes in the atmosphere.

Historically, air quality assessment has been based on observational data, as this approach best approximates reality. Although estimates based on modeling can often be uncertain, a combination of monitoring data and modeling estimates can be used to provide a more comprehensive and accurate assessment of air quality.

Modeling involves certain limitations, particularly concerning the preparation of a large amount of input data. This is especially challenging when incorporating real-time measured data, meteorological information, and their variations over time. These factors can establish baseline limitations in the modeling process. In practice, there are still relatively few sources equipped with systems for automatic emission monitoring. Challenges may include the lack of adequate meteorological data inputs, the adjustment of dispersion parameters to suit the conditions of the observed region and the characteristics of the local terrain. Additionally, models have a limited ability to accurately represent the real world in terms of spatial resolution and are dependent on the availability of data.

An efficient model requires expertise from multiple fields and professional users, aiming to adapt the model to best fit real-world situations [17-19].

2.1 Modelling of Air Pollutant Dispersion

The dispersion of pollutant substances in the atmosphere primarily occurs in the lower atmospheric layers, known as the atmospheric boundary layer. The height of this layer can vary significantly, ranging from a few tens of meters to several thousand meters. Within this layer, pollutants spread and mix with the surrounding air [20-22].

Extremely complex dispersion processes and interactions between pollutants and other atmospheric elements occur within the boundary layer. In studies of this area, one key issue is to achieve an accurate representation of these processes to understand their mechanisms and implications, which can have both short-term and long-term effects.

The dispersion processes occur mainly in the boundary layer, and the paper considers one aspect of these processes, including the movement and transfer of heat and mass [23]. These processes depend on a number of factors. Turbulent motion and turbulence add to the complexity of pollutant movement. Factors such as terrain configuration, heat transfer, cloud cover, humidity levels, heat reflection and absorption by the Earth's surface, the influence of the growing season, and other elements must be considered, as they can all impact the dispersion process.

Pollutants are transported by wind in the direction of its flow, spreading along this path. This spreading and expansion result from the chaotic movement of air, or turbulence. Turbulent movement is one of the most significant challenges in modeling the dispersion of pollutants in the air. Due to the turbulent nature of air movement, pollutants mix intensively with the surrounding air [24].

Modeling the dispersion of pollutants in the atmosphere is one of the most challenging scientific problems today, and seems likely to become even more significant in the future. It is crucial for determining pollutant concentrations, spatial distribution and the direction of movement.

Regarding the challenges in modeling atmospheric dispersion, the development of sophisticated software tools is crucial. These tools enable efficient numerical predictions based on initial parameters and defined boundary conditions [22].

Dispersion models are grounded in the principles of physical chemistry and atmospheric dynamics. These models are designed to predict the concentration of pollutants at specific points in time and space. The transport and transformation of pollutants in the atmosphere primarily occur through advection, along with turbulence and chemical reactions.

The development and application of these models require a comprehensive approach, involving collaboration among researchers from various fields [9]. This interdisciplinary interaction is essential for achieving accurate results and predicting pollutant concentrations in the atmospheric boundary layer in a timely manner.

The development of dispersion models has evolved over many years, resulting in a wide range of software tools, many of which are based on Gaussian-type mathematical models. Gaussian models are relatively straightforward to implement and have modest requirements for meteorological data. Advances in information technology and mathematical tools have enhanced the automation of measurements and data acquisition, enabling near-real-time simulations.

Stability categories used in these models, often based on Pasquill's stability classes, are traditionally derived from empirical procedures and subjective cloud observations. However, these can be replaced by more objective methods that use direct measurements of vertical air temperature gradients, global solar radiation and radiation balance to determine stability in real-time.

2.2 Mathematical Modelling of Air Pollutant Dispersion

One perspective is that air pollution processes can be modeled either through implemented through physical modeling in laboratories or through mathematical modeling using a series of analytical and numerical algorithms that describe the physical and chemical aspects [25]. Physical models provide a basis for validating mathematical models. However, since physical models are not widely available, this paper will focus on mathematical models.

Mathematical models can be classified into deterministic and statistical categories. Deterministic models are based on mathematical descriptions of atmospheric processes where the emission of substances affects air pollution [24, 26]. To determine the meteorological parameters influencing the characteristics and movement of pollutants, it is essential to have measured meteorological data. These models account for factors such as dry and wet deposition, re-suspension of pollutants by wind, and the physical and chemical properties of the pollutants. Given that the atmosphere is the quickest route for environmental contamination, the application of these models is crucial for timely prediction and response.

Modeling atmospheric dispersion involves mathematically describing the transport of pollutants in the atmosphere [21, 25]. In this context, dispersion refers to the processes of diffusion (due to turbulence) and advection (due to wind) near the Earth's surface. The most common mathematical models for atmospheric dispersion are based on parameterizing meteorological and environmental conditions and solving systems of differential equations numerically [27].

The advancement of digitalization and software tools continues to enhance the importance of mathematical models in atmospheric dispersion. Although these models are rarely developed purely on theoretical grounds, they rely on practical experience and complement measurements from nature and physical models when available.

The concentration of air pollutants can be described by the advection-diffusion equation, a second-order partial differential equation. This represents an interdisciplinary application of mathematics with direct industry relevance [28-30]. Models consider the atmospheric boundary layer, usually extending up to about one kilometer above the Earth's surface, and account for factors such as wind influence, daily temperature variations and eddies. Most models focus on the lower layers of the atmosphere and often exclude emissions from aircraft and large-scale accidents.

Key factors to consider in these models include the direction and strength of the wind, temperature and its variations, and parameters related to turbulence [15, 31]. Fick's first law describes the rate of diffusion, stating that the mass flux of pollutants is proportional to the concentration gradient. The second Fick's law defines the change in concentration over time.

$$J = \frac{\partial C}{\partial t} = -D\frac{\partial^2 C}{\partial x^2} \quad , \tag{1}$$

where C - concentration [kg/m^3], J - diffusion flux [kg/m^{2}s], x - distance [m] and D - diffusion coefficient of the component that depends on other components in the mixture [m^2/s], t - time [s].

A basic gradient transport model might be represented by equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = S + \frac{\partial}{\partial x}K_x\frac{\partial C}{\partial x} + \frac{\partial}{\partial y}K_y\frac{\partial C}{\partial y} + \frac{\partial}{\partial z}K_z\frac{\partial C}{\partial z} \quad , \tag{2}$$

in equation (2) the mixed element is omitted, as it is $\frac{\partial}{\partial x}K_{xy}\frac{\partial C}{\partial y}$, as they usually not significant [14]. It is important to note that the diffusion equation implicitly incorporates both time and spatial reference. The average values of wind components (u, v and w) and pollutant concentration (C) represent the mean values over time and spatial distribution. Turbulence effects are implicitly accounted for through the K coefficients, which represent the diffusion coefficients.

Equation (2) cannot be solved analytically in general and a generalized functional form for diffusivity K and wind speeds u, v and w. Therefore, finding a solution involves certain limitations, such as specifying the particular forms of K and u.

2.3 One Gradient Conveying and Model

To analyze both analytical and numerical solutions of the diffusion equation, a two-dimensional, time-independent case is selected. This involves variable values for u and K for a terrestrial continuous line source of pollutants. The diffusion from an infinite linear source with a crosswind represents a simplification of equation (2) and is expressed as:

$$u\frac{\partial C}{\partial x} = \frac{\partial\left(K_z\frac{\partial C}{\partial z}\right)}{\partial z} \quad , \tag{3}$$

with boundary conditions:

$C \to 0, \text{as } x, y \to \infty;$

$C \to \infty, \text{as } x = z \to 0;$

$K_z \frac{\partial C}{\partial z} \to 0 \text{ as } z \to 0 \text{ and } x > 0; \text{ and}$

$\int_0^\infty uCdz = Q_l, x > 0;$

where Q_l (mass per unit length per time) represents the strength of the continuous line source.

The third boundary condition ensures that there are no changes at the contact of the materials with the lower boundary, nor with the ground. According to the literature, many authors have explored obtaining an analytical solution to equation (3) in a specific functional form that defines K_z and u. This solution is applicable only to ground-based sources where the size of an eddy is smaller than the plume size. Roberts (1923) provided the correct solution for these conditions:

$$K_z = K_1 \left(\frac{z}{z_1}\right)^n , \tag{4}$$

$$u = u_1 \left(\frac{z}{z_1}\right)^m , \tag{5}$$

with a comprehensive solution that provides:

$$C(x, y) = \frac{Q_l z_1^m (m-n+2)}{2u_1 \Gamma(s)} \left[\frac{u_1}{(m-n+2)^2 z_1^{m-n} K_1 x}\right]^s \times exp\left[\frac{u_1 z^{(m-n+2)}}{(m-n+2)^2 z_1^{m-n} K_1 x}\right] , \tag{6}$$

where $s = (m + 1) / (m-n + 2)$ and Γ is a gamma function, for which the values used in modelling [14] are given in Table 1.

Table 1

Gamma function values for typical values of stability class[1]

m	***n***	***s***	***Γ (s)***
0.9	0.1	0.679	1.33
0.8	0.2	0.692	1.31
0.7	0.3	0.708	1.29
0.6	0.4	0.727	1.26
0.5	0.5	0.750	1.23
0.4	0.6	0.778	1.19
0.3	0.7	0.813	1.15
0.2	0.8	0.857	1.11
0.1	0.9	0.917	1.06
0	0	0.5	1.77

[1] Assumption m = 1-n; for the last row and assumption for the last row is that K and u are constants

The assumption used in Table 1, for the values of stability classes, is $m = 1\text{-}n$, which is derived from the relationship within the surface boundary layer

$$U_*^2 = K\frac{\partial u}{\partial z} \ . \tag{7}$$

Since u_*^2 is constant in the surface boundary layer, it follows that $m = n\text{-}1$, where K is related to z^n and u is related to z^m. By simplification-specifically, in the case where u and K are constant (i.e. $m = n = 0$, as shown in the last row of Table 1), a Gaussian solution is obtained.

$$C = \frac{Q_l}{1{,}23u_1}\left[\frac{u_1}{4K_1x}\right]^{\frac{1}{2}} \times exp\left[\frac{u_1z^2}{4K_1x}\right] \ . \tag{8}$$

The Gaussian model assumes an idealized scenario with a stationary source under constant meteorological conditions over long distances. It presupposes idealized plume geometry, flat terrain, a complete mass balance, and dispersion that follows a Gaussian distribution.

3 One Case of the Dispersion Model - Continuous Line Source

In order to develop a solution sample for the selected gradient transport models, a demo software tool - Mathematics was used, which by design, can solve complex mathematical problems. In addition to the possibility of solving basic and complex mathematical functions, relatively simple numerical solution of differential equations and visualization of solutions are also possible.

For making a presentation of the analytical solution (6), the code with specific parameters defined was developed as well as a graphical representation of the solutions given in Figure 2. Strength of the source (*Q1*), stability conditions according to Pasquill's classification, values according to the assumption of a low vegetation layer in the environment, initial *K* and *u,* values calculated according to the Roberts function are used as parameters.

To generate a sample numerical solution for differential equation (3), the sample code with defined parameters and constraints (boundary conditions) was provided in Figure 3. This code illustrates the functions that determine the values of the diffusion parameters *K* and *u*. The initial parameters, corresponding to stability classes, are based on values given in Table 1 and literature sources.

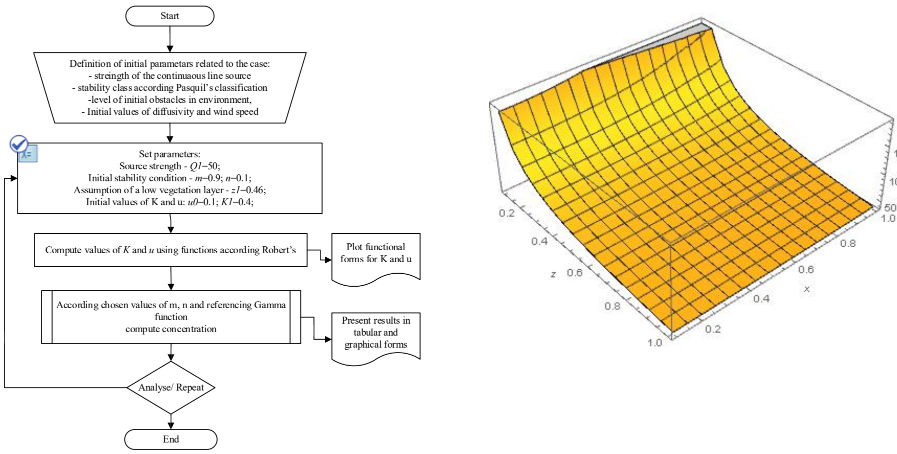


Figure 2

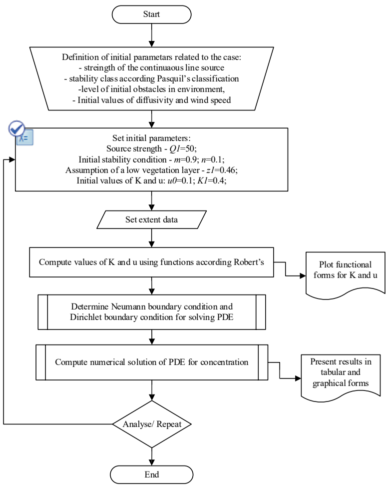
Overview of the analytical solution under specified boundary conditions

The parameter related to the strength of the source is defined with the assumption of a low vegetation layer surrounding the source. The values of K and u were determined according to Roberts' findings [15, 33], with initial coefficients K_1 and z_1 derived from the literature. Figure 3 shows the solution obtained for the parameters corresponding to the first type in Table 1, while Figure 4 illustrates the representation for modified parameters related to stability classes (penultimate type in Table 1).

Only the numerical solution for the initial parameters, as shown in Figure 3, and the result after changing the parameters for the stability class, depicted in Figure 4, are considered. These solutions provide an overview of the advantages and possibilities of parameterizing the model according to modified values, which can correspond to various cases of pollutant dispersion.

A special case of the pollutant dispersion scenario is the Gaussian model, where stability class values are equal to zero. The model corresponding to this case is illustrated in Figure 5.

The model, based on its foundational setup, has identified several limitations. Parameterization was conducted under specific conditions and model elements, which are subject to variability. These models can be compared with real-world situations [31-35]. In subsequent iterations, adjustments can be made to refine and validate the models against existing data and varying conditions. The primary advantage of developing numerical solutions lies in their versatility and the ability to analyze the obtained results. Continuous improvements and adjustments can be implemented to enhance stability and reliability, providing a robust basis for further examination and application.



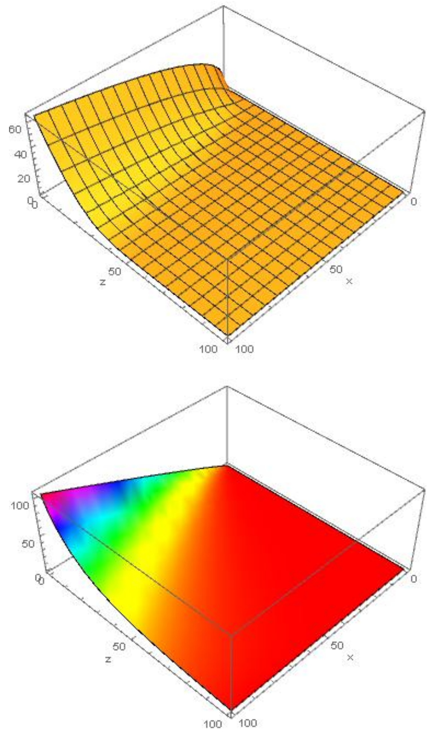


Figure 3
Representation of a numerical solution for the initial parameters of stability classes (m = 0.9; n = 0.1)

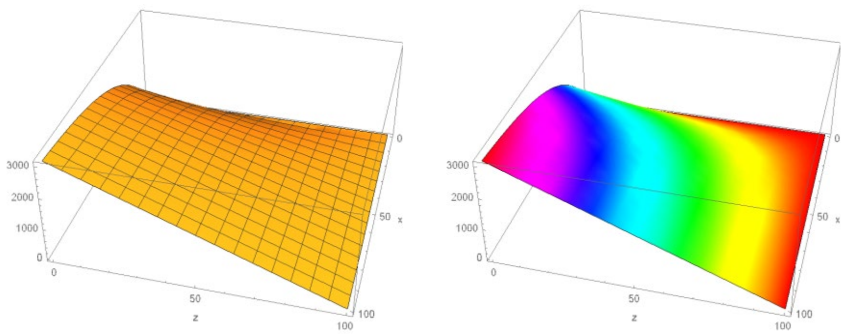


Figure 4
Representation of the numerical solution with parameters of the stability class m = 0.1; n = 0.9

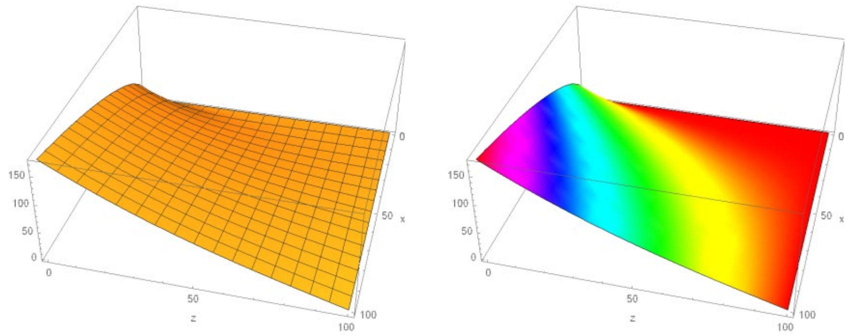


Figure 5
Special case of a numerical solution - Gaussian model (m=n=0)

Conclusions and Directions for Further Research

Monitoring and analyzing pollutant emissions into the atmosphere remains a significant challenge today. With the growing relevance of air pollution, modern research builds upon a long history of technical and technological advancements. Mobile sources of pollutants, contributing nearly a quarter of greenhouse gas emissions and significantly impacting urban air quality, present a particular challenge. Research is increasingly focused on understanding the dispersion processes, generating models and enhancing monitoring systems to track pollutant emissions.

As data availability improves, so does the need to develop models that generate reliable estimates, support decision making and inform both short-term and long-term action plans. This trend aligns with innovative research programs and technological advancements, which are producing tools and systems capable of data collection, analysis and forecasting. These advancements enable the formulation of recommendations and measures to mitigate air pollution risks.

Each applied model requires thorough evaluation to assess its capabilities, performance, strengths, and weaknesses, with verification using available field observations wherever possible [14-15, 18, 32-36]. This paper explores the development, limitations, and application of analytical and numerical models for a selected theoretical case (a line source), using initial limitations and parameter values from the literature and the author's selection. The results demonstrate significant agreement between analytical and numerical solutions, as illustrated for selected cases and shown graphically.

Assumptions for comparing analytical and numerical solutions include the strength of the source, stability conditions according to Pasquill's classification (1974), initial obstacles, assuming low vegetation (up to half of meter) and K and u parameters determined using Robert's function. Additionally, values of m, n and the Gamma function were based on Abramowitz and Stegun (1964). The same assumptions were applied during the development of the numerical solution.

A particular issue in developing the numerical solution is determining boundary conditions and their limitations (Neumann, Dirichlet Condition) for solving PDE. The presented solutions can be used to develop further models for continuous line sources or discrete points that might be interpolated as line. Representations for the chosen case are given for stability classes $m = 0.9$; $n = 0.1$, $m = 0.1$; $n = 0.9$, and $m = n = 0.0$ which represent the Gaussian model.

Besides that, the presented study highlights the interdisciplinary nature of the field and suggests future research directions, such as analyzing functional connectivity, threshold values of parameters and training models based on real data. Comparing model parameters and boundary conditions with measured data can refine and validate solutions, ensuring they meet field standards. Further development and evaluation are necessary to effectively integrate these models into real-world simulations. Furthermore, further research could be directed toward testing for specific air pollutants in particular cases, referencing air quality monitoring stations wherever possible to validate the model's results.

Acknowledgement

This work was supported by the University of Criminal and Police Studies, which recognizes the significance of theoretical research and its practical applications in forensic studies.

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