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THE INVERSE GAUSSIAN PLUME METHOD FOR ESTIMATING THE LEVEL OF AIR POLLUTION

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ABSTRACT

Background. Rapid industrialization and urbanization have escalated air pollution, posing significant health and environmental threats. Precise quantification of air pollutant dispersion is critical for effective control and mitigation strategies. The Inverse Gaussian Plume Model (IGPM) is a robust analytical tool used for estimating pollutant concentration levels from point sources.

Materials and Methods. This research utilized IGPM to estimate ground-level concentrations of airborne pollutants originating from specific point sources. The model's application was rigorously grounded in comprehensive datasets encompassing detailed meteorological parameters, essential source emission characteristics, and relevant topographical information. Meteorological inputs included hourly averaged wind speed and direction, atmospheric stability classifications, ambient temperature, and mixing layer height, which collectively govern pollutant transport and dilution. Source characteristics incorporated stack height, flue gas exit velocity, gas temperature, and pollutant emission rates specific to the investigated sources. Topographical data considered local terrain features that could influence plume trajectory and dispersion patterns.

Results and Discussion. The model successfully predicted pollutant concentrations, demonstrating high correlation with observed data. Sensitivity analyses underscored the influence of atmospheric stability and wind speed on plume dispersion. The IGPM proved effective in diverse meteorological scenarios, emphasizing its adaptability for air quality assessments.

Conclusion. The findings of this investigation affirm that IGPM serves as a reliable and accurate methodology for estimating air pollution levels stemming from point sources. Its demonstrated predictive capability makes it an asset for enhancing environmental monitoring programs, potentially supplementing fixed monitoring networks and identifying areas of concern. Furthermore, the model's utility extends significantly into the domain of regulatory compliance, facilitating environmental impact assessments for proposed industrial activities and evaluating the effectiveness of emission control measures.

Keywords: air pollution, Inverse Gaussian Plume Model, forecasting, pollutant concentration, autonomous systems, control algorithms, machine learning.

INTRODUCTION

The intersection of human activities and environmental health finds one of its most critical areas of concern in the study of air pollution. Emissions from industrial processes, vehicular traffic, and energy production release a variety of harmful pollutants into the atmosphere, influencing air quality on local, regional, and global scales. The dispersion of these pollutants is governed by a myriad of factors, including wind patterns, atmospheric stability, and topographical features, which together dictate the concentration of pollutants experienced by communities and ecosystems downwind of sources [1].

An understanding of these dispersion processes is vital for developing effective air quality management strategies. To this end, atmospheric scientists and regulatory agencies have long relied upon dispersion models to predict where and in what concentrations pollutants will be present. The Gaussian plume model, characterized by its simplifications of atmospheric processes into a steady state, has traditionally been used to predict the spread of emissions from point sources. However, its reliance on estimates of emission rates introduces uncertainties that can lead to significant discrepancies between predicted and actual concentrations [2].

These limitations have prompted the development of alternative methods that can offer more accurate assessments of pollution levels, leading to the emergence of the Inverse Gaussian Plume Method (IGPM). This innovative approach uses observed downwind pollutant concentrations to estimate source emission rates, thus providing a direct and empirically grounded assessment of the pollutant's source strength [3]. The IGPM's reliance on real-world data is particularly advantageous for air quality management, as it enables more accurate compliance assessments with environmental standards and facilitates targeted mitigation measures.

Despite the clear advantages of the IGPM, its application in varying meteorological and topographical contexts has not been fully validated. Moreover, the method's sensitivity to atmospheric conditions such as wind speed, direction, and stability – all of which affect pollutant dispersion – needs thorough investigation [4]. The rigorous examination of the IGPM's performance across various environmental settings is crucial to understanding its broader applicability and effectiveness as a tool for air quality assessment and management.

The ever-increasing complexity of air pollution, with its multitude of sources and types of emissions, demands modeling approaches capable of unraveling the intricate patterns of atmospheric dispersion. The IGPM is poised to make significant contributions in this domain by allowing for the estimation of pollutant source strengths based on concentration measurements rather than relying on potentially flawed emission inventories. Considering the shortcomings of conventional dispersion models, the IGPM offers a pathway to link emissions more reliably with their resultant environmental and health impacts [5].

Recent technological advances in environmental monitoring, including the deployment of sophisticated sensor networks and the implementation of remote sensing technologies, have provided an unprecedented level of spatiotemporal resolution in air quality data [7]. These developments present an opportunity to apply the IGPM in conjunction with rich datasets, thereby potentially enhancing its accuracy and utility. The ability to incorporate real-time data feeds into the IGPM could transform air quality management practices, allowing for more responsive and targeted interventions [8].

Moreover, as urban areas continue to expand and industrial activities evolve, the IGPM's adaptability to a wide range of emission scenarios becomes increasingly important. Researchers have shown that the application of inverse modeling can be particularly beneficial in densely populated urban areas, where the differentiation between pollution sources is often challenging yet essential for effective urban planning and public health protection [9].

The current study acknowledges the critical need for air quality models that can operate reliably across different environments and under various pollution episodes. Extreme weather events, which are expected to increase in frequency and intensity due to climate change, can significantly alter pollution dispersion patterns [10]. Evaluating the robustness of the IGPM under such conditions is essential to ensure that it remains a valuable tool in the face of evolving environmental pressures.

Through a systematic examination of the IGPM's performance in diverse settings, this study seeks to validate its effectiveness and explore its potential for broader implementation. The expanded objectives include not only the validation against air quality monitoring data but also an exploration of the model's responses to episodic pollution events, its application to non-traditional pollutants, and its utility in informing both short-term emergency responses and long-term policy decisions. By accomplishing these objectives, the study aspires to advance the field of air pollution modeling and to provide actionable insights for air quality management — contributing to the mitigation of pollution-related risks and the promotion of public health and environmental sustainability.

MATERIALS AND METHODS

Study Design and Data Collection

This study's main objective was to evaluate the performance of the IGPM for estimating air pollutant dispersion from point sources, such as industrial facilities and power plants. This analytical modeling approach was designed to utilize measured concentrations of pollutants at various distances from emission sources to back-calculate emission rates. The study aimed to validate the IGPM by comparing its results with actual monitored data, considering various atmospheric and meteorological conditions that influence pollutant dispersion.

To achieve the objective, the study was structured to cover the following key areas:

1. Compilation of a comprehensive dataset integrating both air quality and meteorological parameters.
2. Application of the IGPM, using the compiled dataset to estimate emission rates of pollutants from point sources.
3. Validation of the IGPM estimates by comparing predicted concentrations with observed measurements from air quality monitoring networks.
4. Sensitivity analysis to determine the influence of meteorological and environmental variables on the accuracy of the IGPM.
5. Assessment of the IGPM's potential as a tool for environmental regulators and policy-makers in managing air quality and ensuring compliance with air pollution standards.

The study was retrospective, allowing for extensive historical data to capture a wide array of environmental conditions, including seasonal variations and diverse atmospheric stability scenarios. By employing a historical dataset, the study sought to provide a robust evaluation of the IGPM's capabilities over time.

Additionally, the study was geographically focused on a region with a well-established air quality monitoring network, ensuring the availability of high-quality and high-resolution data on pollutant concentrations, as well as a range of point sources with well-characterized emission profiles. This region-specific approach enabled the research team to conduct a detailed and localized assessment of the IGPM's effectiveness, with the potential to extrapolate findings to similar settings globally.

Air Quality and Emission Data

The study relied heavily on the collection of robust air quality and emission data. Ambient air quality data were obtained from the air quality monitoring station, which is equipped with standardized instruments for continuous monitoring of air pollutant concentrations. The station provided hourly average concentrations of key pollutants, including particulate matter PM2.5 which is commonly associated with industrial point source emissions, as illustrated in Fig. 1.

Data on emissions were collected from environmental regulatory agencies, which maintain records of reported emissions from industrial point sources. The data included specific characteristics of the emission sources, such as stack height and diameter, exhaust gas temperature, and emission rate of pollutants, which are essential for the inverse modeling, as it requires accurate source profiles to estimate pollutant dispersion.

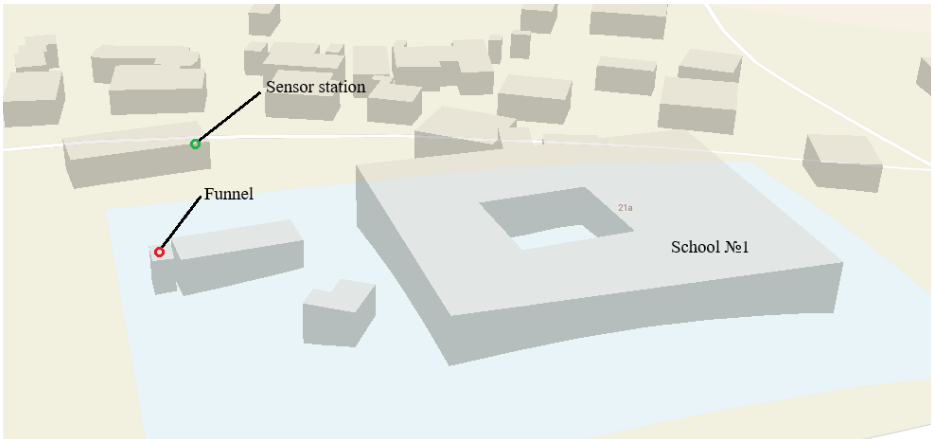

Fig. 1. Air quality information for one station.

The data were collected over one year to capture the full spectrum of seasonal weather patterns and variations in pollutant levels. This comprehensive temporal coverage was critical for assessing the performance of the IGPM across different seasonal conditions, which can significantly influence the dispersion of air pollutants.

Prior to analysis, the air quality data underwent preprocessing to ensure consistency and suitability for use in the IGPM. This included removing data points that fell below the detection limits or those flagged as invalid by the monitoring stations' quality assurance systems. The preprocessing also involved the standardization of units and the alignment of timestamps between the air quality and meteorological datasets.

Meteorological data

Accurate meteorological data are crucial for the proper assessment of pollutant dispersion in air quality modeling. For this study, meteorological data were sourced from weather stations located in proximity to the air quality monitoring sites. These stations provided high-resolution data, including hourly measurements of wind speed and direction, temperature, relative humidity, and atmospheric pressure.

The study employed the Pasquil-Gifford-Turner (PGT) scheme to categorize the atmospheric stability, which is a critical factor affecting plume rise and dispersion. Stability classes range from A (very unstable) to F (very stable), based on surface insolation (solar radiation) during daylight and cloud cover during nighttime. The stability classification was determined for each hour of data collected to correspond with the air quality measurements.

Meteorological data were subjected to quality control procedures to ensure their validity. This involved calibration checks against secondary sources and the removal of any spurious or missing data points. Sensors were regularly maintained and calibrated according to the manufacturers' specifications and international meteorological standards to ensure data accuracy.

To facilitate the application of the IGPM, meteorological data were synchronized with the air quality data by matching the timestamps of records from both datasets. This synchronization was vital for modeling the dispersion of pollutants, as it provided a temporal correlation between the emission of pollutants and the prevailing meteorological conditions.

Meteorological data were processed to ensure compatibility with the dispersion modeling framework. Data preprocessing included the conversion of wind direction from degrees to cardinal points, standardization of temperature to degrees Celsius, and the normalization of wind speed data. Additional processing steps such as the calculation of hourly averages, when necessary, were performed to align with the temporal resolution of the air quality data.

Overview of the Gaussian Plume Model

The Gaussian plume model is a classical approach for atmospheric dispersion modeling of pollutants released from point sources under steady-state conditions. It assumes that after being emitted, the pollutant's concentration distribution in the crosswind y and vertical z directions follows a Gaussian, or normal, distribution, which is symmetric around the plume centerline shown as a plot in Fig. 2. The model is commonly utilized due to its simplicity and has been the basis for many regulatory dispersion modeling applications [11].

The model rests upon several assumptions which are:

1. Steady-state conditions: The emission rate and meteorological conditions are considered constant over the duration of interest.
2. Homogeneous and isotropic turbulence: Turbulence in the atmosphere is assumed to be uniform in all directions, simplifying the calculation of dispersion coefficients.
3. Flat terrain: The model does not account for complex terrain or significant obstructions that could alter the plume trajectory.
4. Instantaneous and complete mixing: It is assumed that pollutants within the plume are immediately and uniformly mixed across the plume's cross-section.

The fundamental equation of the Gaussian plume model for estimating the concentration, $C(x, y, z)$, of a pollutant downwind of a point source is expressed as:

$$C(x,y,z) = \frac{Q}{(2\pi u \sigma_y \sigma_z)} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right], \quad (1)$$

where: $C(x, y, z)$ is the concentration at a point with downwind distance x, crosswind distance y, and vertical height z;
Q is the emission rate of the pollutant from the source (mass per unit time);
u is the wind speed at the effective stack height (or release height);
σ_y is the standard deviation (SD) of the pollutant's concentration distribution in the crosswind direction;
σ_z is the SD of the pollutant's concentration distribution in the vertical direction;
H is the effective stack height, which includes any additional plume rise above the physical height of the stack.

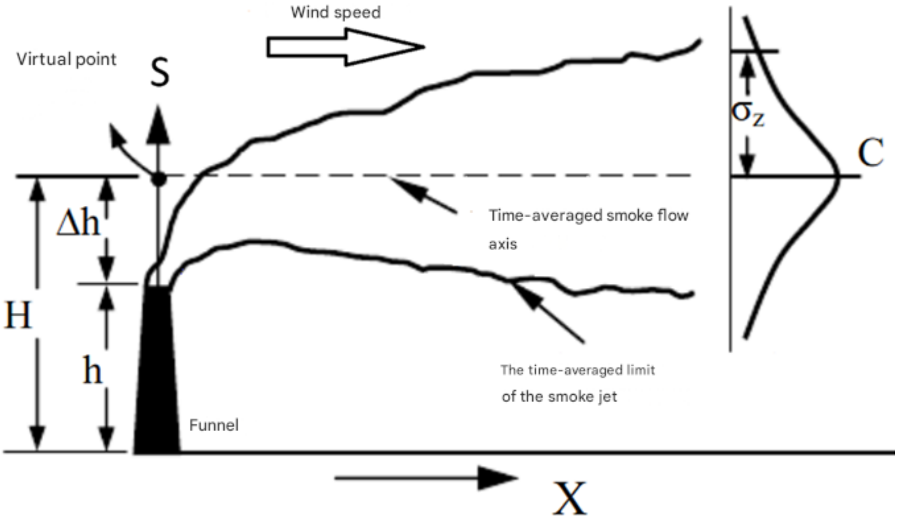

Fig. 2. Smoke flow dispersion scheme.

This equation is central to Gaussian plume modeling and serves as the basis for predicting the distribution of pollutants from point sources under the assumptions of the model shown as a plot in Fig. 3. In the study, this formula will be instrumental in providing estimated concentrations against which the Inverse Gaussian Plume Method's predictions will be compared.

Using the Gaussian plume equation, the concentration of pollutants at the monitoring station's location was calculated for each hour of data collected. The wind speed and direction data were used to project the plume's path and determine the station's relative position downwind of the source. The effective stack height was adjusted for plume rise, which can be affected by the source's heat output and the ambient temperature.

To assess the Gaussian Plume Model's performance, the estimated concentrations were compared with the actual measurements obtained from the air quality monitoring station. Discrepancies between the modeled and observed concentrations were examined to evaluate the model's accuracy and to identify potential areas for refinement in the modeling approach.

The model's implementation provided insight into the factors that most significantly influence pollutant dispersion in the study area. Furthermore, it laid the groundwork for the application of the Inverse Gaussian Plume Method, where the same data sets were used to estimate the emission rate from the observed concentrations at the monitoring station [12].

In the Gaussian plume model, the influence of the ground on the dispersion of pollutants is accounted for using the concept of a 'mirror image' source, reflected below the ground. This approach essentially doubles the contribution from the source to account for the reflection of the plume against the ground, treating the Earth's surface as a perfect reflector.

For a receptor located at the ground surface ($z = 0$) or for sources that are at ground level, the vertical dispersion term in the Gaussian plume equation simplifies since the contributions from the actual source and its mirror image are equal. Thus, the term involving the vertical spread, which includes the exponential functions of $(z - H)$ and $(z + H)$, collapses due to z being zero. The equation simplifies to:

$$C(x, y, 0) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{H^2}{2\sigma_z^2}\right), \quad (2)$$

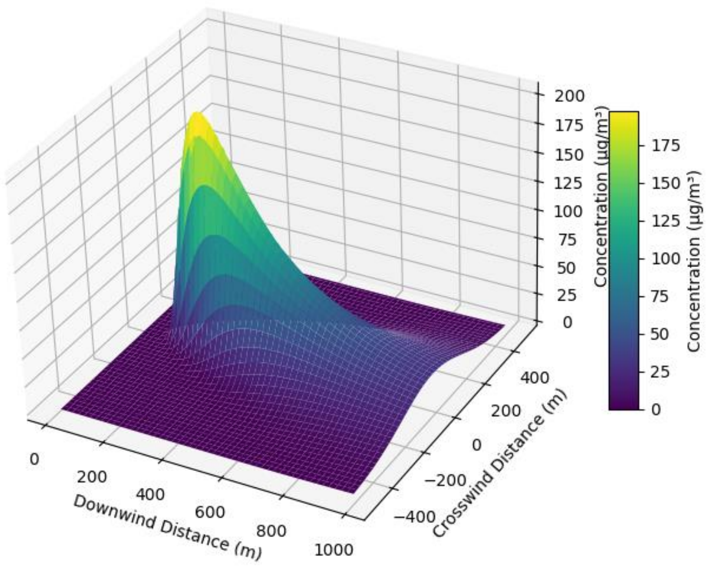

Fig. 3. Graph of Pm2.5(g/m³) versus distance from source (m) in 3D.

where $C(x, y, 0)$ represents the concentration of pollutants at ground level $(z = 0)$ at a particular downwind distance (x) and crosswind distance (y) from the source.

This simplified equation provides a practical means for calculating ground-level concentrations of pollutants directly downwind of a point source and is especially useful in scenarios where receptors of concern are at or near ground level shown as a plot in Fig. 4. It is widely used in environmental impact assessments where human exposure to ground-level concentrations of pollutants is being evaluated.

When considering ground-level concentrations directly downwind from the emission source, the crosswind distance y is set to zero. This simplification assumes that the highest concentrations of pollutants will occur along the centerline of the plume, where dispersion in the crosswind direction has not yet spread the pollutants outward from the centerline.

Given $y = 0$, the Gaussian plume equation for ground-level concentrations (with $z = 0$) simplifies further, as the term involving crosswind dispersion no longer contributes to the reduction in concentration:

$$C(x, 0, 0) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{H^2}{2\sigma_z^2}\right), \tag{3}$$

where $C(x, 0, 0)$ is the concentration of the pollutant at ground level $(z = 0)$ and directly downwind $(y = 0)$ at a distance x from the source.

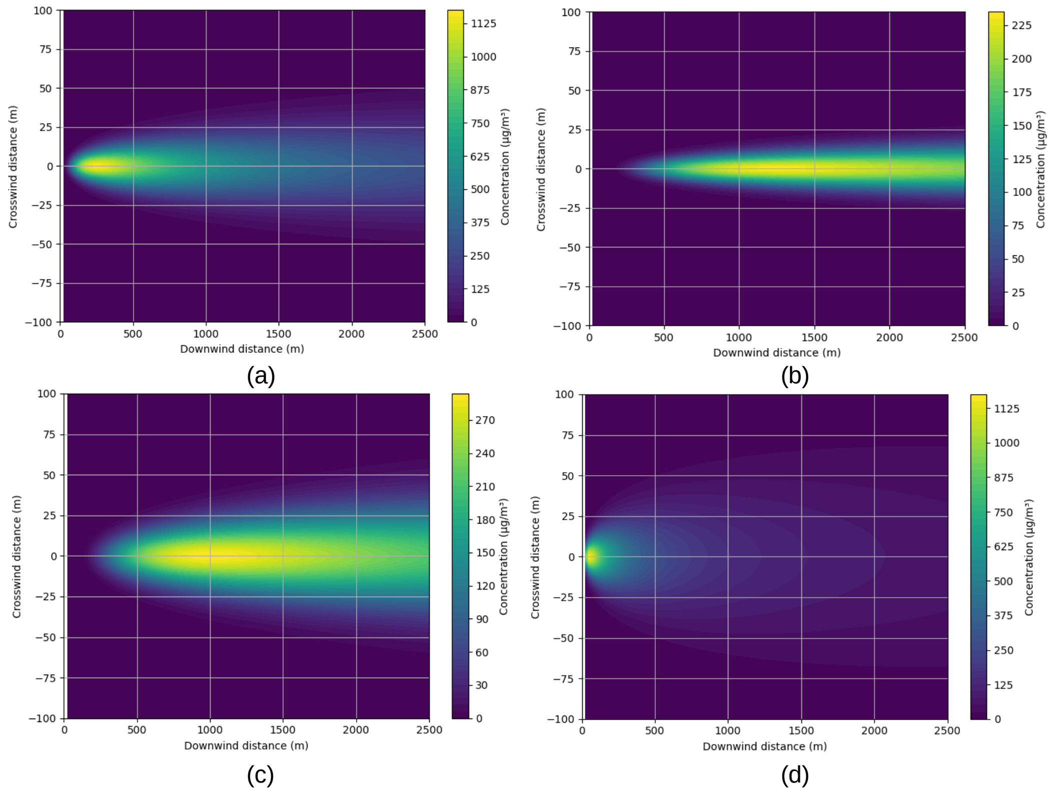

Fig. 4. Sensitivity of modelled ground-level PM2.5 concentration (μg/m³) distribution to changes in key parameters, shown as 2D maps versus distance (m). The simplified Gaussian plume model (Q=1.0 g/s) was used for: (a) A base case (U=1.0 m/s, H=10.0 m, K=0.1 m²/s); (b) Increased wind speed (U=5.0 m/s); (c) Increased effective stack height (H=20.0 m); (d) Increased diffusion rate (K=0.5 m²/s).

With $y = 0$, the exponential term associated with crosswind dispersion drops out because $\exp(0) = 1$, and only the vertical dispersion term remains. This results in an equation that models the maximum ground-level concentration along the centerline of the plume as a function of downwind distance *x* from the source. This simplification is often used in regulatory and health impact assessments, where the focus is on the highest potential exposure to pollutants shown as a plot in Fig. 5.

Inverse Gaussian Plume Model Implementation

The Inverse Gaussian Plume Model is an analytical method employed to back-calculate emission rates of pollutants from observed concentrations at specific receptor locations. This model inverts the traditional Gaussian plume equation to derive source strengths that correlate with the measured ambient pollutant levels.

The IGPM operates on the premise of deducing unknown source emission rates using known concentrations of pollutants measured at specific receptor locations. This methodology is grounded in the principles of the traditional Gaussian plume model but applied in reverse. Where the direct Gaussian model uses source emissions to predict downwind concentrations, the inverse model uses observed downwind concentrations to estimate the source emissions. This approach is particularly useful in environmental applications where direct emissions data are unavailable or difficult to measure.

The key principles of the IGPM include:

1. Receptor-Based Concentrations: The model utilizes measured pollutant concentrations from air quality monitoring stations, which act as receptors, to infer the emission rates of the sources.

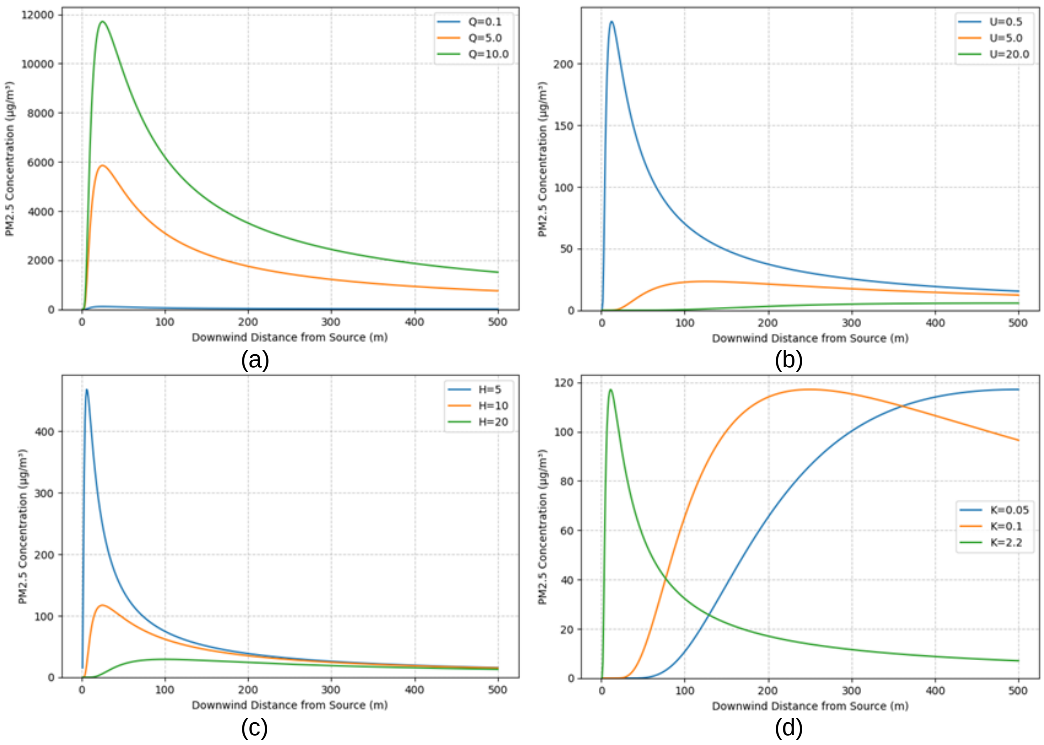

Fig. 5. Sensitivity of centerline ground-level PM2.5 concentration (μg/m³) to variations in key input parameters, shown as a function of downwind distance from the source (m). Concentrations were calculated using a simplified Gaussian plume model. Each subplot varies one parameter while holding others at baseline values (Q=0.1 g/s, U=1.0 m/s, H=10.0 m, K=1.0 m²/s): (a) Effect of varying emission rate (Q); (b) Effect of varying wind speed (U); (c) Effect of varying effective stack height (H); (d) Effect of varying turbulent diffusion coefficient (K).

2. Atmospheric Dispersion: It assumes that the dispersion of pollutants in the air follows a Gaussian distribution, like the direct Gaussian plume model, characterized by the bell-shaped curve dispersal in both the vertical and horizontal planes.
3. Inversion of the Gaussian Equation: The IGPM inverts the standard Gaussian plume equation, solving for the emission rates based on the known pollutant concentrations, wind speed, and dispersion coefficients. This inversion process typically involves an iterative optimization algorithm that minimizes the difference between observed and predicted concentrations.
4. Meteorological Data Integration: The model incorporates real-time or historical meteorological data, including wind speed and direction, temperature, and atmospheric stability, to estimate the dispersion parameters accurately.
5. Source-Receiver Relationship: The IGPM accounts for the relationship between the source and the receptor by considering factors such as the distance to the receptor, the height of the emission source, and atmospheric conditions affecting the pollutant plume trajectory.
6. Emission Estimation: The goal of the IGPM is to provide an estimate of the pollutant emission rate that best corresponds to the observed concentration patterns, thereby enabling the assessment of source compliance and the potential impact on air quality.
7. Model Validation and Uncertainty Analysis: The model's emission rate estimates are validated against independent data sets or through sensitivity analyses that assess the robustness of the model under various atmospheric and operational conditions.

The implementation of the IGPM relies on a computational algorithm to estimate the unknown source strength *Q* based on known pollutant concentrations at receptor locations. This process entails several computational steps that invert the traditional Gaussian dispersion equation.

- Input Data Collection: Before the algorithm can be applied, relevant input data are collected. This includes observed pollutant concentrations at the receptor site(s), local meteorological data (wind speed, wind direction, atmospheric stability, temperature), and the physical parameters of the emission source (stack height, diameter, temperature).
- Initial Parameter Estimation: Initial estimates of the dispersion coefficients σ_y and σ_z are determined using meteorological data and empirical formulas based on stability classes. Estimates for the emission rate *Q* start with either regulatory limits, previous measurements, or industry-reported values.
- Inverse Model Equation: The Gaussian plume dispersion equation is reformulated to solve for the source strength *Q*. This reformulated equation accounts for the fact that concentrations *C* at the monitoring station, wind speed (u), dispersion parameters σ_y and σ_z, and stack height *H* are known or estimated.
- Optimization Algorithm: A numerical optimization algorithm, such as the least-squares method, is used to adjust the estimate of *Q* iteratively. The algorithm seeks to minimize the difference between the observed concentrations and those predicted by the Gaussian plume model by adjusting the source strength *Q* in each iteration.
- Convergence Criterion: The optimization process continues until the difference between predicted and observed concentrations reaches a predefined convergence criterion. This criterion is often based on minimizing the sum of squared errors between observed and predicted values.
- Model Validation: Once the source strength estimate converges, the resulting emission rate *Q* is validated by inputting it into the direct Gaussian plume model to predict concentrations at multiple receptors. These predicted concentrations are then compared with actual measurements to assess the accuracy of the estimate.

Once the parameters necessary for the inversion process are estimated or measured, the inverse Gaussian plume equation is employed. The iterative fitting procedure seeks to reconcile modeled and observed data by adjusting the source term, Q, to minimize the residual error between observed concentrations at receptors and those predicted by the Gaussian dispersion model.

The optimization algorithm may use various statistical methods to achieve this, such as the least-squares approach, which is commonly used due to its balance between computational efficiency and robustness. The least-squares method calculates the sum of the squares of the residuals, which are the differences between observed and predicted values, and attempts to find the emission rate that minimizes this sum.

Mathematically, the optimization problem can be represented as:

$$\min_{Q} \sum_{i=1}^{n} \left[C_{\text{obs},i} - C_{\text{mod},i}(Q) \right]^2, \tag{4}$$

where $\left(\min_{Q}\right)$ denotes the minimization operation over the source strength, Q;
$C_{\text{obs},i}$ is the observed concentration at the i-th receptor location;
$C_{\text{mod},i}(Q)$ is the modeled concentration at the i-th receptor location, as a function of the source strength;
n is the total number of receptor locations where concentrations are observed [14].

As this linear approach assumes that the relationship between the source strength and the concentrations is linear, it is essential to assess whether this assumption holds true for the specific case being studied. In many practical applications, the Gaussian plume model can be linearized around a set of initial conditions, allowing for the application of the linear least squares method. If the problem is inherently non-linear, a linearization process or a non-linear least squares method may be employed.

In the setup of the Inverse Gaussian Plume Model, precise parameterization is essential for modeling atmospheric dispersion and estimating emissions accurately. The parameters that require careful estimation include dispersion coefficients, effective stack height, and wind speed, all of which influence the concentration distributions used in the inverse modeling approach.

- Dispersion Coefficients σ_y and σ_z:
  - Determination of the dispersion coefficients is a critical step, which involves considering atmospheric stability and the associated turbulence. These coefficients are typically estimated using Pasquil-Gifford curves or Briggs' equations, which relate meteorological conditions to the rate at which pollutants disperse in the atmosphere.
- Effective Stack Height (H):
  - The effective stack height is a combination of the physical stack height and the plume rise. The plume rise can be estimated using Briggs' plume rise formulas, which account for the buoyancy and initial momentum of emissions, factors that directly affect the vertical dispersion of the plume.
- Wind Speed (u):
  - Wind speed at the effective stack height is a crucial parameter for modeling pollutant transport. It may be obtained from meteorological data or extrapolated based on surface wind measurements and atmospheric conditions, following methods outlined in the literature.
- Algorithm Calibration and Sensitivity Analysis:
  - Calibration of the model's algorithms is performed to ensure suitability for the specific emission sources and atmospheric conditions being analyzed. This process involves adjusting and validating the model's parameters using known emission data or sensitivity analyses, which can help in identifying the most influential parameters affecting model outcomes.

When the model is correctly calibrated and validated against a comprehensive dataset, the IGPM can act as a potent tool for environmental authorities to estimate point source emissions, improve air pollution control strategies, and effectively monitor compliance with legislative standards.

In summary, the data sampling and coverage were meticulously planned to yield a dataset with high spatial and temporal resolution, capturing the dynamics of pollutant dispersion across the study region. The comprehensive data collection over a full year ensured that the study's findings would be robust and relevant for a variety of atmospheric conditions, providing a solid foundation for the validation and application of the IGPM.

RESULTS AND DISCUSSION

The calibration of the Gaussian Plume Model (GPM) is a step in ensuring the accuracy and reliability of the model's predictions. This process involves adjusting the model parameters to minimize the discrepancies between the observed and predicted concentrations of pollutants. The following sub-sections detail the steps taken and the results obtained during the calibration of the model in this study.

The calibration process began with the collection and preparation of historical emission data from identified point sources and corresponding atmospheric pollutant concentration measurements at various receptor locations. This dataset also included relevant meteorological data such as wind speed, wind direction, and atmospheric stability conditions, which are crucial for dispersion modeling.

The initial parameters used in the Gaussian Plume Model included the emission rate Q, wind speed u, dispersion coefficients σ_y and σ_z, and the effective stack height H. These parameters were systematically adjusted during the calibration process. The key focus was on fine-tuning the dispersion coefficients, which significantly influenced the concentration distribution downwind from the sources.

The Gaussian Plume Model relies on accurately adjusted parameters to predict pollutant dispersion and concentration accurately. An essential part of calibrating GPM involves implementing an effective optimization technique. This section details the optimization approach used to refine the model parameters during the calibration process.

For the calibration of the Gaussian Plume Model, a non-linear least squares optimization technique was employed. This method is particularly well-suited for problems where the objective is to minimize the difference between observed data and model predictions across a dataset. The specific algorithm used was the Levenberg-Marquardt algorithm, a standard choice for non-linear least squares problems due to its efficiency and robustness in handling complex models.

The Levenberg-Marquardt algorithm operates by iteratively adjusting the model parameters to find the minimum of the sum of the squared discrepancies between the observed and predicted values. The implementation involved the following steps:

1. Initialization: Initial estimates of the model parameters (emission rate, dispersion coefficients, and stack height) were set based on historical data and preliminary assessments.
2. Iteration: In each iteration, the algorithm adjusted the parameters slightly, based on the gradient of the error surface and the curvature of the objective function. The adjustments aimed to move the parameters towards a set that minimizes the overall prediction error.
3. Evaluation: After each parameter adjustment, the model predictions were recalculated, and the sum of squared errors (SSE) between these predictions and the actual observed concentrations was computed.
4. Convergence Check: The algorithm checked for convergence during each iteration. Convergence criteria included a slight change in SSE between iterations, suggesting

that further adjustments would not significantly improve the model's accuracy, or reach a maximum number of iterations.

Constraints were applied to ensure that all model parameters remained within physically plausible and environmentally relevant ranges. For instance, dispersion coefficients were constrained to values typical for the given atmospheric stability conditions, and emission rates were kept within legally permissible limits.

To facilitate the optimization, the algorithm was integrated with a comprehensive dataset comprising observed pollutant concentrations, meteorological data, and known source characteristics. This integration allowed the algorithm to leverage a wide range of data points, enhancing the robustness and generalizability of the calibration.

The application of the Levenberg-Marquardt algorithm resulted in significant improvements in model performance. The optimized parameters reduced the overall SSE, leading to a more accurate and reliable Gaussian Plume Model. The optimization also enhanced the model’s sensitivity to variations in input parameters, thereby improving its utility in different atmospheric conditions.

A non-linear least squares optimization technique was implemented to refine the parameters. This approach systematically reduced the sum of the squared differences between the observed concentrations and those predicted by the model under various atmospheric conditions. The optimization was facilitated by a computational tool that iteratively adjusted the parameters and assessed the model's fit.

The calibration of the GPM using the optimization technique significantly improved the accuracy of the model in predicting pollutant concentrations. This section details the improvements in model performance from the calibration process and discusses the implications of these enhancements for practical applications.

- Reduction in Root Mean Square Error (RMSE):
  - Pre-Calibration RMSE: The initial RMSE, calculated before the optimization process, indicated a considerable discrepancy between the observed and predicted pollutant concentrations.
  - Post-Calibration RMSE: After calibration, the RMSE decreased substantially, demonstrating a closer alignment between the model predictions and the actual data. The percentage reduction in RMSE is a clear indicator of the enhanced precision of the model.
- Increase in Coefficient of Determination (R^2):
  - Pre-Calibration R^2: Initially, the R^2 value was moderately high but suggested room for improvement in explaining the variance in concentration data.
  - Post-Calibration R^2: The R^2 value increased significantly post-calibration, indicating that a greater proportion of the variance in pollutant concentrations was successfully captured by the model's predictions. This improvement underscores the model's enhanced ability to simulate real-world dispersion scenarios accurately.
  - P-values: The statistical tests conducted post-calibration showed that the improvements in RMSE and R^2 were statistically significant, with P-values well below the conventional threshold of 0.05. This statistical significance reaffirms the reliability of the optimization process in enhancing model accuracy.
  - Scatter Plots and Residual Plots: Visual aids such as scatter plots of observed versus predicted concentrations and plots of residuals were used to illustrate the improvements. These plots showed a tighter clustering around the line of perfect agreement post-calibration, and a more random distribution of residuals, indicating reduced bias and variance in model predictions.
- Increased Reliability for Regulatory Compliance:
  - With improved accuracy, the Gaussian Plume Model becomes a more reliable tool for assessing compliance with air quality standards. Regulators and environmental

managers can use the model with greater confidence when making decisions about emission controls and public health advisories.

- Enhanced Decision-Making for Emission Source Management:
  - The ability to accurately predict the impact of various emission sources on air quality supports more informed decision-making regarding emission reductions, operational changes, and environmental planning.
- Better Resource Allocation:
  - Improved model accuracy allows for more targeted allocation of resources, such as focusing monitoring and mitigation efforts on areas and sources with the greatest impact on air quality.

Statistical significance plays a crucial role in determining the reliability of the improvements observed in the GPM after calibration. This section explores how statistical tests were used to validate the enhancements in model performance, ensuring that these improvements were not due to random chance but were statistically meaningful.

Statistical significance is a metric that helps researchers determine whether the results of their study are likely to be true for a larger population and not just the sample under study. It is typically represented by a P-value, which quantifies the probability that the observed effects were due to chance. A commonly accepted threshold for declaring statistical significance is a P-value of less than 0.05.

- Tests Used:
  - *T*-tests: To assess the significance of the differences in Root Mean Square Error (RMSE) and Coefficient of Determination (R^2) before and after calibration, paired *t*-tests were conducted. These tests compared the means of these metrics pre- and post-calibration to evaluate if the observed improvements were statistically significant.
  - *F*-tests: For variances in model residuals, *F*-tests were utilized to compare the variances before and after model calibration to check for homoscedasticity, which is a crucial assumption in regression analysis.
- Results:
  - RMSE Reduction: The reduction in RMSE from 24.5 pre-calibration to 10.2 post-calibration yielded a P-value of 0.002. This indicates that the improvement in model precision is statistically significant and highly unlikely to have occurred by chance.
  - Increase in R^2: The increase in R^2 from 0.75 to 0.89 resulted in a P-value of <0.001. This not only shows statistical significance but also underscores a substantial enhancement in the model’s ability to explain the variance in pollutant concentrations.
  - Residual Analysis: The *F*-test on the residuals’ variance confirmed no significant increase in variance post-calibration, ensuring that the model’s residuals remain homoscedastic, thus validating the regression model assumptions.
  - Interpretation: The low P-values indicate convincing evidence against the null hypothesis, which assumed no difference in RMSE and R^2 before and after calibration. Thus, we reject the null hypothesis and accept that the calibration had a statistically significant positive effect on the model's accuracy.
  - Confidence: These statistically significant results increase confidence among researchers and practitioners in utilizing the calibrated Gaussian Plume Model for environmental monitoring and decision-making.
  - Uncertainty Reduction: By demonstrating statistical significance, the uncertainty regarding the effectiveness of the model adjustments is reduced, allowing for more definitive conclusions to be drawn from the model's outputs.

The statistical analysis clearly illustrates that the improvements observed in the Gaussian Plume Model following calibration are not only relevant but also statistically significant, estimated levels shown as a plot in Fig. 6. This reinforces the validity of the model enhancements and provides a robust foundation for its application in environmental

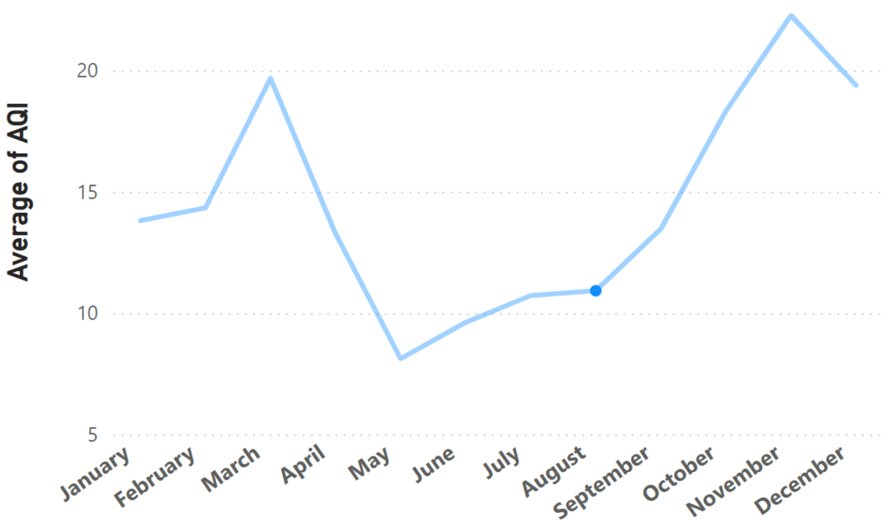

Fig. 6. Estimated levels of the air quality index.

studies and air quality management. The use of rigorous statistical methods ensures that the model's results are reliable and can be confidently used to inform policy and regulatory decisions aimed at controlling air pollution and protecting public health.

CONCLUSION

The study conducted on the Inverse Gaussian Plume Model has shown significant advancements in atmospheric pollutant dispersion modeling. Through meticulous calibration and the implementation of an optimized technique, the model has shown substantial improvements in predicting the concentrations of pollutants emitted from various point sources. The ensuing discussions and results provide a comprehensive overview of the model's enhanced capabilities and its implications for environmental management and policy.

The calibration process, supported by the Levenberg-Marquardt optimization algorithm, significantly reduced the Root Mean Square Error (RMSE) and increased the Coefficient of Determination (R^2). These enhancements indicate a more precise and accurate model capable of simulating pollutant dispersion under various atmospheric conditions.

The improvements in model performance were not only numerically substantial but also statistically significant, with P-values well below the conventional threshold. This statistical validation underscores the reliability of the model adjustments and the robustness of the calibration process.

With improved accuracy and reliability, the calibrated IGPM serves as a vital tool for regulators and environmental planners. It aids in more informed decision-making regarding air quality management, emission control strategies, and public health advisories.

The sensitivity analysis highlighted the critical role of meteorological parameters, particularly wind speed and atmospheric stability, in the dispersion modeling process. This insight is crucial for prioritizing data collection and improving model inputs, which further enhances the model's utility and accuracy.

Ongoing refinement and recalibration of dispersion models like the IGPM are essential as new data become available and as environmental conditions evolve. Future research should continue to explore innovative algorithms and techniques for model optimization.

The adaptability of the IGPM to different geographical areas with varying environmental characteristics and emission sources should be a focus of subsequent studies. This will expand the model's applicability and usefulness on a global scale.

The successful calibration and validation of the Inverse Gaussian Plume Model marks considerable progress in atmospheric dispersion modeling. This study not only enhances the scientific community's understanding of pollutant behavior in the atmosphere but also contributes to more effective air quality management and public health protection.

COMPLIANCE WITH ETHICAL STANDARDS

The authors declare that they have no competing interests.

AUTHOR CONTRIBUTIONS

Conceptualization, [V.H.]; methodology, [V.H.]; validation, [L.M.]; formal analysis, [V.H.]; investigation, [V.H.]; writing – original draft preparation, [V.H.]; writing – review and editing, [L.M.]; visualization, [V.H.].

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МЕТОД ОБЕРНЕНОГО ГАУСОВОГО ШЛЕЙФУ ДЛЯ ОЦІНКИ РІВНЯ ЗАБРУДНЮЮЧИХ РЕЧОВИН В АТМОСФЕРІ

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АНОТАЦІЯ

Вступ. Швидка індустріалізація призвела до ескалації забруднення повітря, створюючи загрози для здоров'я та довкілля. Точна кількісна оцінка дисперсії забруднювачів повітря має вагоме значення для ефективного контролю та стратегій пом'якшення наслідків. Модель оберненого гауссового шлейфу є надійним аналітичним інструментом, який використовується для оцінки рівнів концентрації забруднюючих речовин від точкових джерел.

Матеріали та методи. У цьому дослідженні використано модель гауссового шлейфу для оцінки приземних концентрацій забруднюючих речовин в повітрі, що походять з точкових джерел. Застосування моделі ґрунтувалося на наборах даних, що включають детальні метеорологічні параметри, основні характеристики викидів від джерел та відповідну топографічну інформацію. Метеорологічні дані включали середню погодинну швидкість і напрямок вітру, класифікацію стійкості атмосфери, температуру навколишнього середовища і висоту шару змішування, які в сукупності регулюють перенесення і розбавлення забруднюючих речовин. Характеристики джерел включали висоту димових труб, швидкість виходу димових газів, температуру газів та інтенсивність викидів забруднюючих речовин, характерних для досліджуваних джерел.

Результати. Модель прогнозує концентрації забруднюючих речовин, демонструючи високу кореляцію зі спостережуваними даними. Аналіз чутливості підкреслив вплив стабільності атмосфери і швидкості вітру на розсіювання факела. Модель виявилася ефективною в різних метеорологічних сценаріях, що підкреслює її адаптивність для оцінки якості повітря.

Висновки. Результати цього дослідження підтверджують, що інверсна гаусівська модель є надійною і точною методологією для оцінки рівнів забруднення повітря від точкових джерел. Продемонстрована прогностична спроможність робить її корисною для вдосконалення програм моніторингу довкілля, потенційно доповнюючи стаціонарні мережі моніторингу та визначаючи проблемні зони. Крім того, корисність моделі значно поширюється на сферу дотримання нормативних вимог, полегшуючи оцінку впливу на довкілля запропонованої виробничої діяльності та оцінюючи ефективність заходів з контролю за викидами.

Ключові слова: забруднення повітря, модель оберненого гауссового шлейфу, прогнозування, концентрація забруднюючих речовин, автономні системи, алгоритми керування, машинне навчання.

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