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MODELING OF AIR POLLUTANT DISPERSION UNDER VERY STABLE ATMOSPHERIC CONDITION

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ABSTRACT

The challenge in tracking dispersed pollutants stems from unavailability of real-time measurements to monitor pollution, primarily due to financial, temporal, and spatial limitations at all relevant locations. This study aims to model air pollutants dispersion in a highly stable atmospheric condition. In developing the model, a Gaussian distribution was utilized and refined by incorporating three additional equations to accommodate the presence of radiation inversion. The model illustrates how pollutant concentration changes in response to gravitational force. It also indicates that the vertical distribution changes depending on the depth of the mixing layer and the vertical temperature gradient (lapse rate). Nevertheless, no researchers have conducted a validation study for this model. Currently, given its simplicity, the model may be considered adequate.

KEYWORDS: pollutant dispersion; temperature inversion, stable atmospheric condition, air pollution, Gaussian model

I. INTRODUCTION

The modeling of dispersion aims to forecast the concentration of pollutants at specific point relative to their source. Air pollutants have chemical and physical characteristics that allow them to travel considerable distances from their point of emission [1]. Nevertheless, the abrupt release of these pollutants, primarily toxic gases or smog, has resulted in catastrophic incidents. For example, in 1984, a gas explosion in Bhopal, India, led to an estimated 20,000 fatalities due to gas exposure, with 120,000 individuals suffering from chronic illnesses as survivors [2]. As a result, Gaussian, Eulerian, and Lagrangian models for pollutant dispersion were developed to prevent such disasters [3-5].

It is well known that the concentration of air pollution depends on factors such as wind speed and direction, vertical mixing height and atmospheric stability [6]. The degree of stability can be determined from comparing the adiabatic lapse rate (ΓDALR) and the environmental lapse rate (Γenv.). The difference between the values of the two lapse rates results in stable, unstable or neutral condition. Stable condition occurs when the environmental lapse rate is less than adiabatic lapse rate (ΓDALR). During this atmospheric condition, cold denser air is pushed down to its original point as a result of little or no wind, vertical temperature gradient and radiation inversion [7]. Under very stable conditions, the temperature can indeed rise with altitude. This leads to a tendency for any displaced air parcel to return to its initial position. Consequently, turbulence is diminished, resulting in reduced mixing. A significant issue for the dilution of pollutants is the phenomenon known as radiation inversion. This occurs when the air temperature increases with height. Inversions are closely linked to the concentrations of pollutants present in the surrounding air. By inhibiting vertical movement and the dispersion of air pollutants, these pollutants become trapped below the inversion layer. This situation was responsible for the dense fog pollution of 1952 in London. The pollution not only resulted in loss of lives but also led to a wide array of health problems, including chronic respiratory and cardiac conditions, impaired growth, and cancer [8].

Gaussian models are extensively utilized in atmospheric dispersion modeling, primarily for regulatory purposes due to their straightforward implementation and near real-time responsiveness. AERMOD is a steady-state Gaussian plume dispersion model that currently serves as the EPA's regulatory model for near-field dispersion [9]. However, AERMOD has limitations in calm conditions. The predicted pollutant concentration by AERMOD may unrealistically escalate to high values when wind speeds below 1 m/s are entered into the model [10]. It is assumed that when the mean wind speed falls below a specific threshold (0.1 m/s), the horizontal spread of the plume encompasses 360 degrees (i.e., there is no distinct wind direction).

Numerous studies have been carried out regarding conditions characterized by low wind speeds [11-12]. Nevertheless, existing literature indicates that there is currently no model available for predicting pollutants under highly stable and windless conditions. This research modifies the Gaussian distribution to create a novel model that will successfully simulate air pollutant concentrations in stable, windless environments.

II. LITERATURE REVIEW

Currently, Gaussian-based dispersion models such as AERMOD represent the most commonly utilized approach for predicting emissions from point sources. These models demontrate the dispersion patterns surrounding a singular source in an open and uniform landscape under steady-state conditions. Numerous authors have examined the constraints of Gaussian dispersion models, especially concerning their predictive limitations [13].

Qian and Venkatram,[14] worked on two steady-state models: an advection-diffusion equation and AERMOD to predict dispersion for surface releases under low wind-speed conditions (less than 2 ms^{-1} at the tower level of 1 m). A comparison of model predictions with data from two tracer (SO2) studies, namely the Prairie Grass experiment and the Idaho Falls experiment, reveals that approximately 50% of the concentration estimates fall within a factor of two of the actual observations; however, the variability is significant: the 95% confidence interval for the ratio of observed to estimated concentrations is around 4.

Misra et al.[15] identified a negative correlation between simulated hourly nitrogen oxides (NOx) and observed concentrations, revealing unrealistically high concentration in proximity to the emission source when utilizing the Gaussian model AERMOD.

Kesarkar [16] assessed the efficacy of AERMOD in relation to gaseous pollutants through a study aimed at analyzing the dispersion of PM10 in Pune, India. In this investigation, AERMOD was integrated with a regional weather prediction model (WRF). The parameters for the planetary boundary layer and surface layer necessary for AERMOD were derived from the WRF model. The findings indicated that the model tended to underpredict concentrations throughout the city.

Numerous studies have highlighted considerable variability in the predicted AERMOD concentrations for inert pollutants, which varies according to the type of source utilized.[17,18] Certain studies have indicated comparable results (i.e., elevated concentrations predicted with an area source characterization), while others have shown contrasting results (i.e., increased concentrations predicted with a volume source characterization). Pasch et al.[18] performed an analysis on a theoretical freeway expansion project, demonstrating that an AERMOD area-source characterization resulted in PM concentrations that were 2.6 times greater than those predicted by employing a limited number (i.e., 22) of large volume sources for the freeway characterization; however, this concentration disparity diminished to merely 10 percent higher when a substantial number (i.e., 968) of small volume sources were utilized for the freeway characterization. Given certain limitations inherent in AERMOD (and most other plume models), there are circumstances where the application of an alternative model may be warranted.

III. MODEL ASSUMPTION

To study the dispersion of air pollutant in free atmosphere under stable condition, the development of the model depends on the following assumption:

1. Transportation of mass is by concentration gradient(Diffusion).
2. No pollutant dilution, wind velocity is zero.
3. Atmosphere is very stable as it is characterized by temperature gradient and temperature inversion.
4. Movement in uplift motion in z-direction is not completely zero, but is small to ignore.
5. Variable depth of mixing layer.

IV. MODEL SET UP

Consider the instantaneous release of a fixed mass flux($\dot{m}$) of pollutant into the air. The concentration(c) of the pollutant resulting from the release is shown by

$$\dot{m} = D\frac{\partial c}{\partial x} \quad (1)$$

where

$\dot{m}$ = mass flux (kg/m^{2}s)

D = molecular/eddy diffusivity (m^2/s)

As the mass of gas is diffusing through a unit cross section **∂**x, the change of mass becomes

Mass flux moving in = Mass flux moving out (the gradient is -ve, therefore, mass flux is negative)

$$- D\frac{\partial c}{\partial x} = -\left(D\frac{\partial c}{\partial x} + D\frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) \partial x\right) \quad (2)$$

Rate of change of mass = change of concentration

$$-\frac{\partial c}{\partial t}\partial x = - D\frac{\partial^2 c}{\partial x^2}\partial x \quad (3)$$

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \quad (4)$$

Solving [4] by dimensional variable; making the equation as a single variable. So expressing D and t as a single variable

$Dt = m^2/s \times s = m^2$ (5)

$x^2 = m^2$

By dimensional consideration,

$$\frac{m^2}{m^2} = \frac{x^2}{Dt} = s \qquad (6)$$

therefore, $s = \frac{x}{\sqrt{Dt}}$ (7)

where s is a new variable

Solving (4) with initial conditions :

$x = 0, \quad t = 0, \quad c = c_o$

$x \to \infty, \; c = 0$

$$\frac{\partial c}{\partial t} = \frac{\partial c}{\partial s}\frac{\partial s}{\partial t} = -\frac{x}{2t\sqrt{Dt}}\frac{\partial c}{\partial s} \qquad (8)$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial c}{\partial s}\frac{\partial s}{\partial x} = \frac{x}{\sqrt{Dt}}\frac{\partial c}{\partial s} \qquad (9)$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial c}{\partial x} \qquad (10)$$

Substituting (9) into (10)

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial}{\partial x}\left[\frac{x}{\sqrt{Dt}}\frac{\partial c}{\partial s}\right] \qquad (11)$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{1}{Dt}\frac{\partial^2 c}{\partial s^2} \qquad (12)$$

$$D\frac{\partial^2 c}{\partial x^2} = \frac{D}{Dt}\frac{\partial^2 c}{\partial s^2} \qquad (13)$$

Equating (8) and (13), we have:

$$-\frac{x}{2t\sqrt{Dt}}\frac{\partial c}{\partial s} = \frac{D}{Dt}\frac{\partial^2 c}{\partial s^2} \qquad (14)$$

Making $\frac{\partial^2 c}{\partial s^2}$ the subject of formula to get:

$$\frac{\partial^2 c}{\partial s^2} = -\frac{x}{2t\sqrt{Dt}}\frac{\partial c}{\partial s} \times \frac{Dt}{D} \qquad (15)$$

$$\frac{\partial^2 c}{\partial s^2} = \frac{x}{2\sqrt{Dt}} \qquad (16)$$

Recall that s = $\frac{x}{\sqrt{Dt}}$, therefore $\frac{x}{2\sqrt{Dt}} = -\frac{s}{2}$ (17)

Equating (15) and (16) we have:

$$\frac{\partial^2 c}{\partial s^2} = -\frac{s}{2}\frac{\partial c}{\partial s} \quad (18)$$

Solve (17) with boundary conditions:

S = 0 , c = c_0

S = ∞, c = 0

$$\int \frac{\partial\left(\frac{\partial c}{\partial s}\right)}{\left(\frac{\partial c}{\partial s}\right)} = -\int \frac{s}{2}\partial s \quad (19)$$

$$\ln \frac{\partial c}{\partial s} = -\frac{s^2}{4} + c \quad (20)$$

$$\ln e^{\frac{\partial c}{\partial s}} = e^{-s^2/4} + c \quad (21)$$

$$\frac{\partial c}{\partial s} = c_1 e^{-s^2/4} \quad (22)$$

$$\int \partial c = c_1 \int_0^s e^{-s^2/4}\partial s \quad (23)$$

$$c = c_1 \int_0^s e^{-s^2/4}\partial s + c_2 \quad (24)$$

Recall $\int e^{-cx^2}\partial x = \sqrt{\frac{x}{4c}}\mathrm{erf}\left(\sqrt{cx}\right)$ erf is the error function

Applying the boundary condition: s = 0, c = c_0

$$c_0 = c_1\sqrt{\frac{s}{4}}\left(\sqrt{s}\right) \quad (25)$$

$$c_0 = c_1\frac{0}{2} + c_2 \quad (26)$$

$$c_0 = c_2 \quad (27)$$

For s → ∞, c = 0 (28)

$$c = c_1 \int_0^\infty e^{-s^2/4}\partial s + c_2 \quad (29)$$

Recall $\int_0^\infty e^{-s^2}\partial s = \frac{\sqrt{\pi}}{2}$, where $\frac{\sqrt{\pi}}{2}$ is error function

$$0 = c_1\frac{\sqrt{\pi}}{2} + c_2 \quad (30)$$

$$c_2 = -\frac{c_1\sqrt{\pi}}{2} \quad (31)$$

$$c_1 = -\frac{2c_2}{\sqrt{\pi}} = -\frac{2c_0}{\sqrt{\pi}} \quad (32)$$

Substitute equations (27) and (32) into (24)

$$C = -\frac{2c_0}{4\sqrt{\pi}}\int_0^s e^{-s^2}\,\partial s + c_0 \quad (33)$$

$$C = c_0 - \frac{1}{2\sqrt{\pi}}c_0\int_0^s e^{-s^2}\,\partial s \quad (34)$$

Bell shaped Gaussian distribution

$$C = c_0\exp\left[-\left(\frac{x}{2\sqrt{Dt}}\right)^2\right] \quad (35)$$

Applying Lateral distribution function, we have

$$C = \frac{Q}{\sqrt{2\pi}} \quad \sigma_y\exp\left(\frac{-y^2}{2\sigma_y}\right) \quad (36)$$

where: $\int_{-\infty}^{\infty} c(x)\partial x = Q$

$\sqrt{Dt} = \sigma_y$, $Dt = \sigma_y^2$

In a very stable atmosphere, with no wind, the gas is being moved by inertia force. Therefore,

Inertia force = gravitational force

ma = mg

a = g (37)

Recall that velocity (u) = acceleration × time

u = at = gt (38)

Vertical distribution of a gas (H_z) is a function of temperature lapse rate, depth of mixing height($\bar{z}$) and time of travel of gas particle(t).

$$H_z = f(\Gamma, \bar{z}, t) \quad (39)$$

$$H_z \;\alpha\; \sqrt{\frac{\Gamma_{env}}{\Gamma_d}} \quad (40)$$

$$H_z \;\alpha\; \sqrt{\frac{1}{\bar{z},}} \text{ and } \sqrt{t^2} \quad (41)$$

Therefore, $H_z = k_z \sqrt{\frac{\Gamma_{env}}{\Gamma_d}} \times \sqrt{\frac{t^2}{\bar{z},}}$ (42)

where: $\frac{\Gamma_{env}}{\Gamma_d}$ = ratio of environmental lapse rate to dry adiabatic lapse rate ($^oC/m$)

k_z = Dispersion coefficient value for free atmosphere ($50m^2/sec$)

$\bar{z}$ = Depth of mixing layer (m)

Depth of mixing height was estimated based on Venkatram, [19] as:

$$\bar{z} = 2400 u_*^{3/2} \quad (43)$$

Therefore, a modified 2D model for predicting concentration dispersion is given as:

$$C = \frac{Q}{\sqrt{2\pi}} \frac{1}{\sigma_{ygt H_z}} \exp\left(\frac{-y^2}{2\sigma_y}\right) \quad (44)$$

where: C is concentration, Q is emission rate(g/m^3), H_z is vertical distribution of a gas (m), σ_y is lateral dispersion coefficient(m), t is time of travel of gas particle in x-direction, g is gravity constant ($9.8m/s^2$)

Comparison of the modified 2D model with AERMOD

AERMOD uses the following formulation [11] to estimate the ground-level concentration from a surface release during stable conditions:

$$C = \frac{Q}{\sqrt{2\pi\, \sigma_z U_e}} H(x, y) \left[\exp\left(-\frac{(H_{s-z})^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(-H_{s-z})^2}{2\sigma_z^2}\right)\right] \quad (45)$$

where Q = source pollutant emission rate, in g/s, H_z is the effective stack height, U_e is effective wind speed, σ_z is vertical plume spreads, z is the receptor height, H is height of emission plume centerline above ground level (m) , exp is the exponential function

A significant distinction exists between the utilization of a 2D model and the intricate 3D AERMOD model that reflects real-world scenarios, where diverse flow patterns, wind directions, and velocities influence the behavior of particles. Consequently, AERMOD is unable to directly replicate stagnation conditions (i.e., the absence of wind). Furthermore, the value of σ_z varies throughout the day and across different seasons, while background concentrations are affected by fluctuating wind conditions. AERMOD is specifically tailored for near-field and steady-state scenarios; however, it possesses certain inherent limitations when applied to source-receptor relationships. For instance, AERMOD does not account for causal effects (i.e., the time required for pollutants to move from point A to point B), treats the airflow trajectory as a straight line, and depends on spatially uniform meteorological conditions.

V. CONCLUSION

In the course of developing this model, a Gaussian distribution was utilized and refined by incorporating three additional equations to account for the occurrence of radiation inversion. Every model, grounded in accurate assumptions, has inherent limitations, as the outcomes are contingent upon the quality of the data collected. Consequently, the acceptability of the results from dispersion models is influenced by the perspective of the modeler and the evaluation of other researchers.

Moreover, each model is tailored for a specific purpose and is not suitable for alternative applications. It is crucial to note that the Gaussian plume model is only applicable when the wind velocity is greater than zero. Therefore, risk assessments for hazardous installations typically necessitate the modeling of the dispersion of toxic or flammable gases across various potential accident scenarios under a range of representative wind conditions.

VI. RECOMMENDATION

It is advisable to model the dispersion of air pollutants while considering subsidence inversion. This particular type of inversion occurs when descending air leads to an increase in temperature and pressure as an inversion layer develops above. Additionally, modeling for radiation inversion should be conducted in valleys, as the denser, cooled air tends to descend to the valley floor.

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