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Research Article
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Mathematical Modeling of Pollutants Dispersion in the Atmosphere

Jeevan Kafle[1], Krishna Prasad Adhikari[1], Eeshwar Prasad Poudel[1,2], Ramesh Raj Pant[3,*]

[1]Central Department of Mathematics, Tribhuvan University, Kirtipur, Kathmandu, Nepal
[2]Tri-Chandra Multiple Campus, Tribhuvan University, Kathmandu, Nepal
[3]Central Department of Environmental Science, Tribhuvan University, Kirtipur, Kathmandu, Nepal

*Correspondence to: Ramesh Raj Pant, Email: ramesh.pant@cdes.tu.edu.np

Abstract: *Air pollution is one of the biggest problems in both developed and developing countries. Mathematical modeling is widely applied to assess how air pollutants impact on human and ecological health. In this paper, the fundamental behavior of the plumes along with stack height and the underlying assumptions of the Gaussian plume model were assessed. Additionally, the equation for advection and diffusion was also developed to analyze the pollutants concentration of brick kilns. Basically, the model considers the height, emission sources, eddy diffusivity, and wind profile as parameters by adopting the fundamental approaches of the model. Interestingly, the results revealed that when the stack height is reduced, pollutants are more prominent whereas when the stack height is increased, the pollutants are less prevalent along the x-axis. There is a close relationship between wind velocity and pollutants dispersion. The model illustrates that stronger winds tend to increase the dispersion of air pollutants; hence, areas with stronger winds typically have lower air pollution concentrations. The insights of this work will directly contribute to environmental sustainability by mitigating pollutants concentration, especially in the core urban areas. Additionally, the work is also applicable for the researcher and academia to select the optimal measurement techniques and ways forward for controlling the pollution level in the atmosphere.*

Keywords: Dispersion equation, Gaussian plume model, Optimal measurement, Pollution mitigation

Nomenclature

$c(x,y,z)$	Diffusing substance's average concentration at a given location (x,y,z) $[kg/m^3]$
x	Downwind distance [m]
y	Crosswind distance [m]
z	Vertical distance above ground [m]
u	Mean wind speed in a downwind direction [m/s]
H	Effective stack height above the ground [m]
Q	Contaminant emission sources [kg/s]
D	Diffusion rate [m^2/s]
D_y, D_z	Mass diffusivity in the direction of the y- and z- axes [m^2/s]
σ_y	Function of the lateral dispersion coefficient [m]
σ_z	Function of the vertical dispersion coefficients [m]
x_{max}	The downwind distance that GLMC can be found [m]
GLMC	The ground level maximum concentration of pollutants

1 Introduction

Air pollution has increased recently as a result of both anthropogenic and natural causes [1]. The major contributors of air pollution are both point and non-point sources including vehicular emissions. There are substantial evidences that air pollutants impacts human health, damages flora and fauna and non-living environment including soil and building materials [2]. Importantly, global climate change is mainly caused by atmospheric pollutants, including CO_2, CFCs, NO_x and CH_4 which is a serious concern for both developing and developed countries [3].

Environmental problems like deforestation, toxic material release, solid waste, air pollution, and many others have attracted more attention than ever due to ongoing urban expansion and population rise [4].

Urban air pollution is a major issue that it is now necessary to receive scientific and reliable information from the perspective of human and ecological health safety [4]. The advection diffusion equation is a well-known example of a major partial differential equation and is used in many environmental engineering and industrial applications, particularly in the investigation of transport processes of air pollutants [5]. The potentially toxic trace elements such as Hg, Cd, Pb and Zn are major toxic chemicals that are one of the serious issues from the human and ecological point of view [6]. The haphazard development activities and rapid urbanization including unmanaged industrialization are some of the major causes of air pollution in developing countries like Nepal. Additionally, the major air pollutants in the core urban areas of the regions are PM_{10}, $PM_{2.5}$, aerosols, dust particles, tropospheric ozone [7, 8]. Precisely, Nepal is ranked as the polluted nation in the world by the World Air Quality Report [22, 25]. However, the research revealed that the amount of air pollution that Nepal was determined to have a $PM_{2.5}$ yearly average of 48 g/m^3, down from 54.4 g/m^3 in 2019, when Nepal was still placed Ninth [22, 24]. The amount of $PM_{2.5}$ in the air in Kathmandu is very high, especially during the dry winter months (December). Urban Kathmandu air quality during this month can be described as extremely unhealthy [9]. There are some other metropolitan cities like Biratnagar and Birgunj also have similar air pollution related issues in Nepal. Thus, these issues should be solved for the sustainability of urban development and management.

To anticipate pollutant concentrations, mathematical diffusion models are now the most beneficial since they quickly produce findings and provide meaningful information [11]. The aforementioned results highlighted that the quality of atmospheric air has been seriously deteriorating in last few decades. However there are very limited studies focusing on the quality of air especially from the developing counties. Precisely, there are negligible scientific publication focusing on the quality of air by using mathematical model thus this research gap in the quality of air from the developing countries like Nepal. Taylor [4] established the modeling notion of diffusion. The main outcome of these investigations was the identification of the Gaussian nature of the average cross wind concentration. The foundation for the eventual development of atmospheric diffusion theory was established from the theoretical and experimental perspective. Additionally, Sutton [10] explained the methodology utilized to create the Gaussian diffusion theory. Hanna et al. [12] referenced two fundamental elements to explain the turbulent diffusion process that leads to the Gaussian model. Gradient transport, also referred to as eddy diffusion, is a theory that applies differential volume to a mass balance. The eddy diffusion model and statistical theory of turbulence both provide the same outcome. Hanna and Paine [13] explained about the convective nature of the dispersion of buoyant plumes from towering stacks. Schnelle [14] highlighted that any created atmospheric diffusion model shall specify that the concentration should be exactly proportional to the source strength and inversely related to the average wind speed. Park and Baik [4] explained that power functions of vertical height in an unbounded space after the advection diffusion equation for a source with a small area.

Similarly, Gayal et al. [23] studied the pollution dispersion with low wind convective circumstances. Modeling based studies were available from the developing and developed countries for getting insights on the diffusion of air pollutants. For instance, the ground level concentrations of SO_2 owing to point sources in Delhi were forecasted using the Gaussian plume model and two low wind models. In populated locations like Delhi, India, there are frequently low wind conditions. Low wind speeds (less than 2 m/s) made it difficult for Gaussian models to predict concentrations. Pramod et al. [4] have used crosswind-integrated concentrations to create a generalized analytical model for the dispersion of a pollutant produced from a continuous source in the atmospheric boundary layer. The resulting two-dimensional steady-state advection-diffusion equations explained about the eddy diffusivity as a function of vertically height and downwind path length from the source, as well as for height above the ground as a generalized function of horizontal wind speed. Romao et al. [15] investigated any errors in the solution of 3D convection diffusion equation using finite difference techniques.

The term air pollution refers to the contamination of the air as a result of the presence of compounds in the atmosphere that are hazardous to human health and the health of other living things, or that affect the environment or materials. The most polluting sources are depicted as a result of increased industrialization and urbanization. As a result, we became interested in atmospheric pollution and used the advection diffusion model to examine the pollutant dispersion in atmospheric air at various heights, from various emission sources, with various wind speeds, and at various rates of diffusion.

2 Mathematical Model

The advection diffusion model, which simulates the physical procedures involved in pollutant dispersion, is used to characterize the distribution of air pollutants. The following equation, which is time dependent, can be used to express the dispersion of pollutants [1, 4]:

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}+w\frac{\partial c}{\partial z}=\frac{\partial}{\partial x}\left(D_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial c}{\partial z}\right)+S+R, \tag{1}$$

where $c = c(x, y, z)$ represents the pollutant concentrations at any location (x, y, z) at time t; u, v, and w are the wind profiles; and D_x, D_y, and D_z are the eddy diffusivity in the downwind (x), crosswind (y), and vertical (z) directions, respectively; and S and R are the respective representations of the source and reaction term [1, 4, 17].

The Gaussian plume model takes into account the following assumptions:

1. Steady-state condition (i.e., $\frac{\partial c}{\partial t} = 0$).
2. The mean wind is blowing parallel to the x-axis, causing $v = w = 0$.
3. Neglecting downwind diffusion in favor of transport caused by the mean wind, i.e.,

$$u\frac{\partial c}{\partial x}>>\frac{\partial}{\partial x}\left(D_x\frac{\partial c}{\partial x}\right).$$

4. Source and reaction terms are both absent. i.e., $S = 0$ and $R = 0$.

After imposing the aforementioned presumptions of the Gaussian plume model, equation (1) reduce to

$$u\frac{\partial c}{\partial x}=\frac{\partial}{\partial y}\left(D_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial c}{\partial z}\right). \tag{2}$$

Assuming constant diffusivity along the y and z directions, equation (2) becomes

$$u\frac{\partial c}{\partial x}=D_y\frac{\partial^2 c}{\partial y^2}+D_z\frac{\partial^2 c}{\partial z^2}. \tag{3}$$

The general solution to this second-order partial differential equation is

$$c=Kx^{-1}exp\left[-\left[\left(\frac{y^2}{D_y}\right)+\left(\frac{z^2}{D_z}\right)\right]\frac{u}{4x}\right]. \tag{4}$$

The rate of transfer of pollutant through any vertical plane downwind from the source is a constant for steady state, and this constant must equal the emission rate of the source, i.e.,

$$Q=\int\int uc\,dydz$$

i.e.,

$$Q=\int_{-\infty}^{\infty}Kux^{-1}exp\left[-\left[\left(\frac{y^2}{D_y}\right)+\left(\frac{z^2}{D_z}\right)\right]\frac{u}{4x}\right]dydz.$$

After integrating

$$K=\frac{Q}{4\pi x(D_yD_z)^{\frac{1}{2}}}$$

where K is an arbitrary constant whose value is determined by using the boundary conditions.

Substituting the value of K in equation (4), we get

$$c(x,y,z)=\frac{Q}{4\pi x(D_yD_z)^{\frac{1}{2}}}exp\left[-\left[\left(\frac{y^2}{D_y}\right)+\left(\frac{z^2}{D_z}\right)\right]\frac{u}{4x}\right]$$

Finally, defining the Gaussian parameters as $\sigma_y = \sqrt{2D_y \frac{x}{u}}$ and $\sigma_z = \sqrt{2D_z \frac{x}{u}}$.

The general equation to calculate the steady-state concentration of an air contaminant in ambient air resulting from a point source is given by

$$c(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} exp\left(\frac{-y^2}{\sigma_y^2}\right)\left[exp\left(\frac{-(z-H)^2}{2\sigma_z^2}\right) + exp\left(\frac{-(z+H)^2}{2\sigma_z^2}\right)\right], \tag{5}$$

where $c(x,y,z)$ is average concentration of diffusing substance at a given location (x,y,z) [kg/m^3], x is downwind distance [m], y is crosswind distance [m], and z is vertical distance above ground [m]. u mean wind speed in a downwind direction [m/s], H effective stack height above the ground [m], Q is contaminant emission rate from the source [kg/s], D is diffusion rate [m^2/s], σ_y is function of the lateral dispersion coefficient [m], and σ_z is function of the vertical dispersion coefficient [m] [12, 18, 20].

When y is equal to zero on the axis, it indicates a horizontal direction that is perpendicular to the plume axis. Height above the ground is indicated by the coordinate z, which is currently believed to be leveled and uniform. Standard deviations of the distribution c in the y and z directions, respectively, are represented by the parameters σ_y and σ_z. The final term's objective is to account for the plume's reflection at the base by assuming the source at a distance h below the surface [12, 18, 20].

3 Simulation Results and Discussion

3.1 General overview

The simulation of stack height fluctuation, concentration variation, wind flow variation, and diffusion rate variation is covered in this section. To solve the advection diffusion equation, numerous criteria were established in this study. Figure 1 explains the differences in pollutants concentration at various heights (Figure 1 a, b, c and d). Figure 2 describes the pollutants concentration by variation of emission sources (Figure 2 a, b, c and d). Similarly, Figure 3 describes the concentration of pollutants by variation of wind flow (Figure 3 a, b, c and d). Finally, Figure 4 shows the variation of diffusion for the pollutants concentration (Figure 4 a, b, c and d). Precisely, in order to assess the pollutants concentration, the nexus between the concentration of pollutants and wind speed, height, emission source, and diffusion rate is quite relevant.

3.2 Variation of height of stack

Figure 1 describes about the pollutants concentration by plume fluctuation. Here, we set the fixed values for the parameters $Q = 1$ [kg/s], $u = 1$ [m/s], and $D = 1$ [m^2/s]. Figure 1a, illustrates that the plumes are concentrated at ground level when the height choice is of 0 m. It indicates that the selection of the height at the base level resulted the dispersion of the pollutants at the same level. Figure 1b, 1 m for stack height, which shows less pollution along the x-axis, and the simulation results showed that pollution was more prevalent. Figure 1c, 2 m for stack height. According to the simulation results, pollution increased but was less visible in the x-direction as compared to Figure 1a and Figure 1b. Figure 1d, selecting stack height at 5 m. According to the simulation results, pollution is more prevalent than it is in Figure 1a, Figure 1b, and Figure 1c, which shows less pollution in the x-direction.

Interestingly, at the medium level of stack height the dispersion of pollutants is maximum and the further increasing trend of height resulted the decreasing trends of pollutants dispersion (Figure 1). The modeling output of our result is consistent with previous work [18]. The results are consistent in all the cases illustrates of Figure 1a to d. Interestingly with increasing height of stack in y-axis the dispersion of pollutants are dramatically reduced in the x-axis. To the simulation results, pollution is more prevalent along the x-axis but less prevalent along the y-axis.

In two of the cases, the source is either on the ground (H = 0) or somewhat raised over floor level (H = 1), (H = 2), and (H = 5) in order to understand the usual altitude of the plume solution. Contour plots are used to represent the concentrations for the two source heights in Figure 1a, Figure 1b, Figure 1c, and

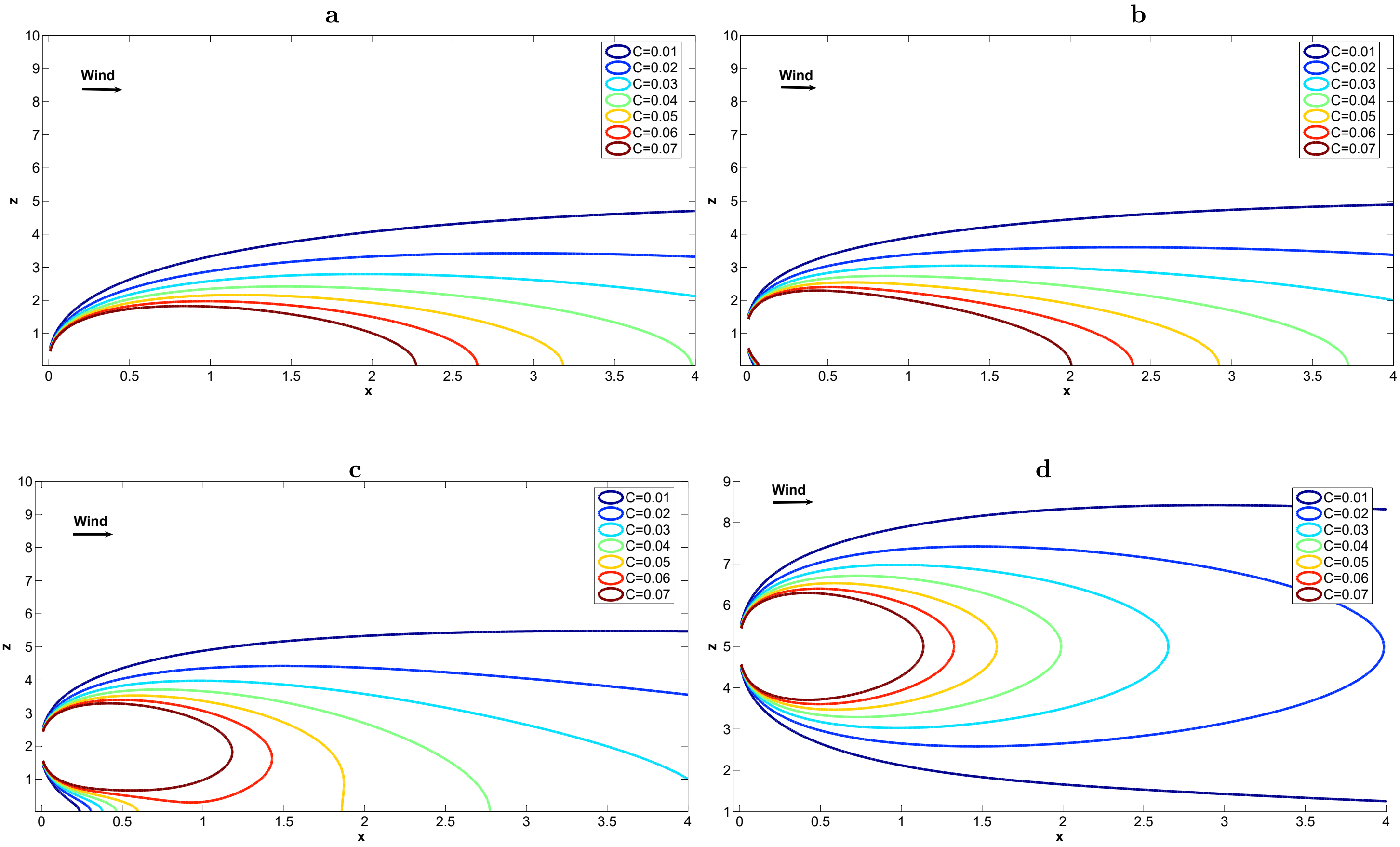

Figure 1: Contour plots of concentration $c(x, y, z)$ for a ground-level source (a) H = 0, (b) H = 1 m, (b) H = 2 m, and (d) H = 5 m in the vertical plane y = 0. A red square indicates the location of the contamination source.

Figure 1d, respectively. The maximum concentration occurs simultaneously at (0, 0, H) as the source, and the pollutant is carried moving away from (0, 0, H) in the shape of an extended plume. It demonstrates that when H = 0, the highest ground-level concentration occurs near the origin (Figure 1a or is transferred to a point if the source is high, further downwind (Figure 1b, Figure 1c, and Figure 1d). We concluded that when the stack height was reduced, pollution was more prominent along the x-axis, and when the stack height was increased, pollution was less prevalent along the x-axis. When the source is stronger, the concentration increases when $(H > 0)$ reaches a maximum of $c_{max} = \frac{2Q}{\pi u H^2 e}$ at the downstream location $x_{max} = \frac{uH^2}{4D}$ along the plume centerline $y = 0$ [18].

3.3 Variation of emission sources

For the scenario of various pollutant concentrations along the x-direction. Figure 2 describes pollutant concentration by variation of emission sources. Figure 2a, we decide to set the pollutant emission source at $Q = 0.5$ kg/s. We observed that the dispersion was more apparent and less likely to increase in height in the x-direction, and pollution proceeded more quickly in that direction. Figure 2b, we choose the pollutant emission source $Q = 1$ kg/s with the assumption that the height was slightly higher than expected and that the rate of x-axis dispersion was increasing. Figure 2c and 2d show the pollutant dispersion along the x-axis and an increase in height due to our choice of $Q = 2$ kg/s and $Q = 5$ kg/s as the pollution emission

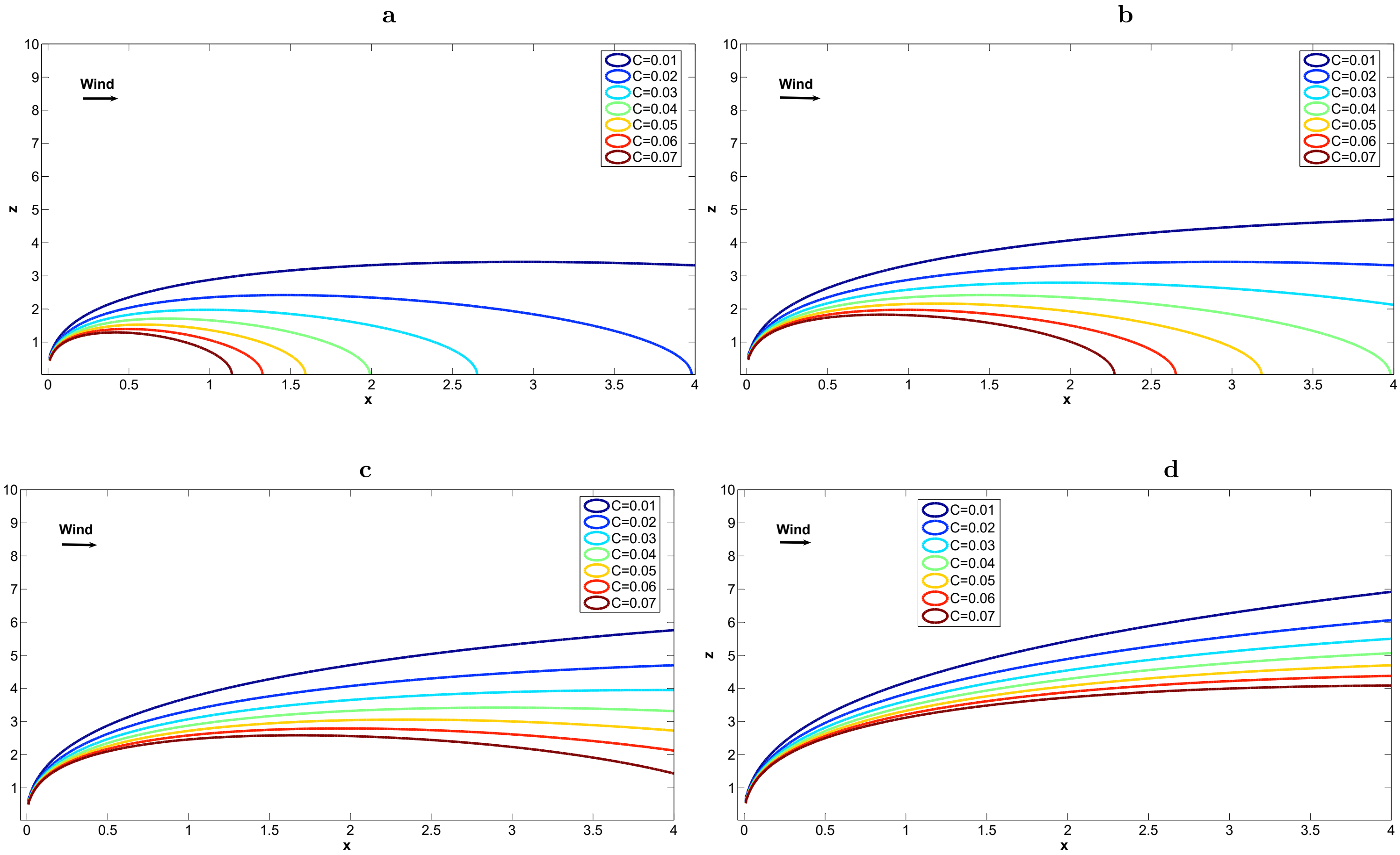

Figure 2: Contour plots of concentration $c(x, y, z)$ for a ground-level source (a) Q = 0.5 kg/s, (b) Q = 1 kg/s, (c) Q = 2 kg/s, and (d) Q = 5 kg/s in the vertical plane y = 0.

source.

Finally, we draw the conclusion that a large number of emission sources contributed to high directional dispersion and a slightly increased height, and that if the emission source slightly decreases, the height will also slightly decrease and the dispersion length will also decrease in the x-direction.

3.4 Variation of mean wind velocity

Wind direction and speed can be used to understand how air pollution moves. Managers of the quality of the air can locate probable sources of pollution by observing the direction and speed of the wind. On the other hand, it can be used to illustrate why there might be lower levels of air pollution close to a pollutant source if the dominant wind has carried the pollutant from somewhere else, like a burning factory. The best course of action to protect the health of both people and the environment can be determined by understanding the movement of air pollution. Figure 3 describes the concentration of pollutants by variation of wind flow for the case of different concentrations of pollutants along the x-direction. First of all we choose the condition with $u = 1$ m/s. In this condition more advection along the x-direction resulted in fast dispersion of the atmosphere (Figure 3a). Similarly, we assumed $u = 3$ m/s. Given this situation relatively more advection was observed in x-direction which indicates that the atmospheric pollutants will disperse here to

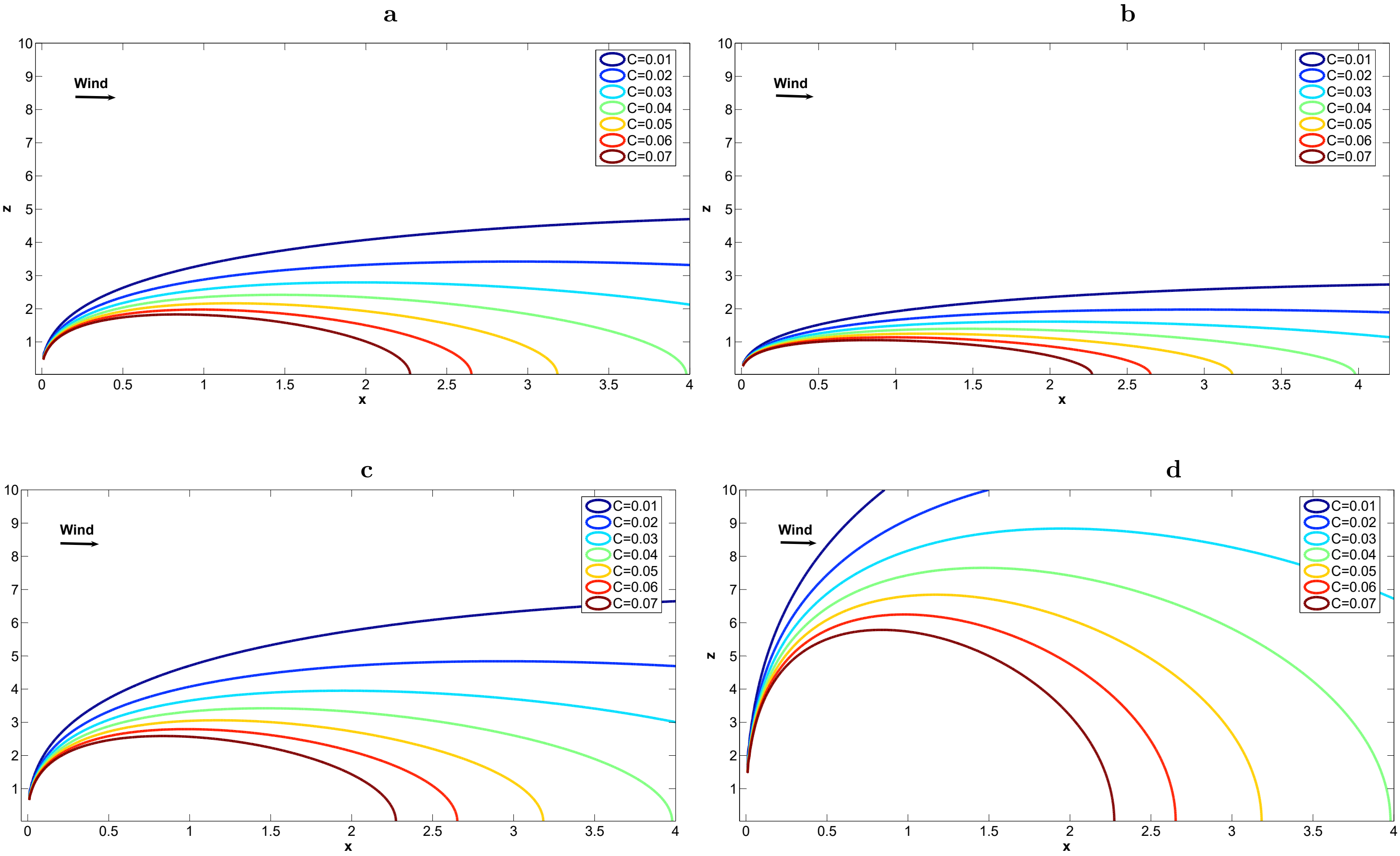

Figure 3: Contour plots of concentration $c(x, y, z)$ for a ground-level source (a) u = 1 m/s, (b) u = 3 m/s, (b) u = 0.1 m/s, and (d) u = 0.5 m/s in the vertical plane $y = 0$.

ground surface (Figure 3b). Adding, we assume $u = 0.1$ m/s . Pollutants in the atmosphere moved up and away from the earth relatively less. When the wind speed is set to $u = 0.5$ m/s, the pollutant has a high average speed and obtains some height. We choose the different wind speed (u) in the equation which gives the change the pollutants concentration along the x-direction. We conclude from Figure 3 that increased approximation wind flow results in a change in the x-direction, or an increase in ground level concentration. Similarly, decreased approximation wind flow results in averaged dispersion of pollutants and an increase in height.

Pollution in one region can have an impact on the quality of the air in a large area because wind takes air pollutants away from their original source and can spread them elsewhere. As a rule, places with stronger winds will have lower air pollution concentrations due to the increased dispersion of air pollutants that higher wind speeds often cause. The air becomes more turbulent during the day as the ground warms up, which causes air contaminants to scatter in the air and pollutants tend to diffuse less when the air is cooler at night because of the result of more stable conditions. Measurements of wind direction and speed can be helpful for a wide range of air quality-related tasks.

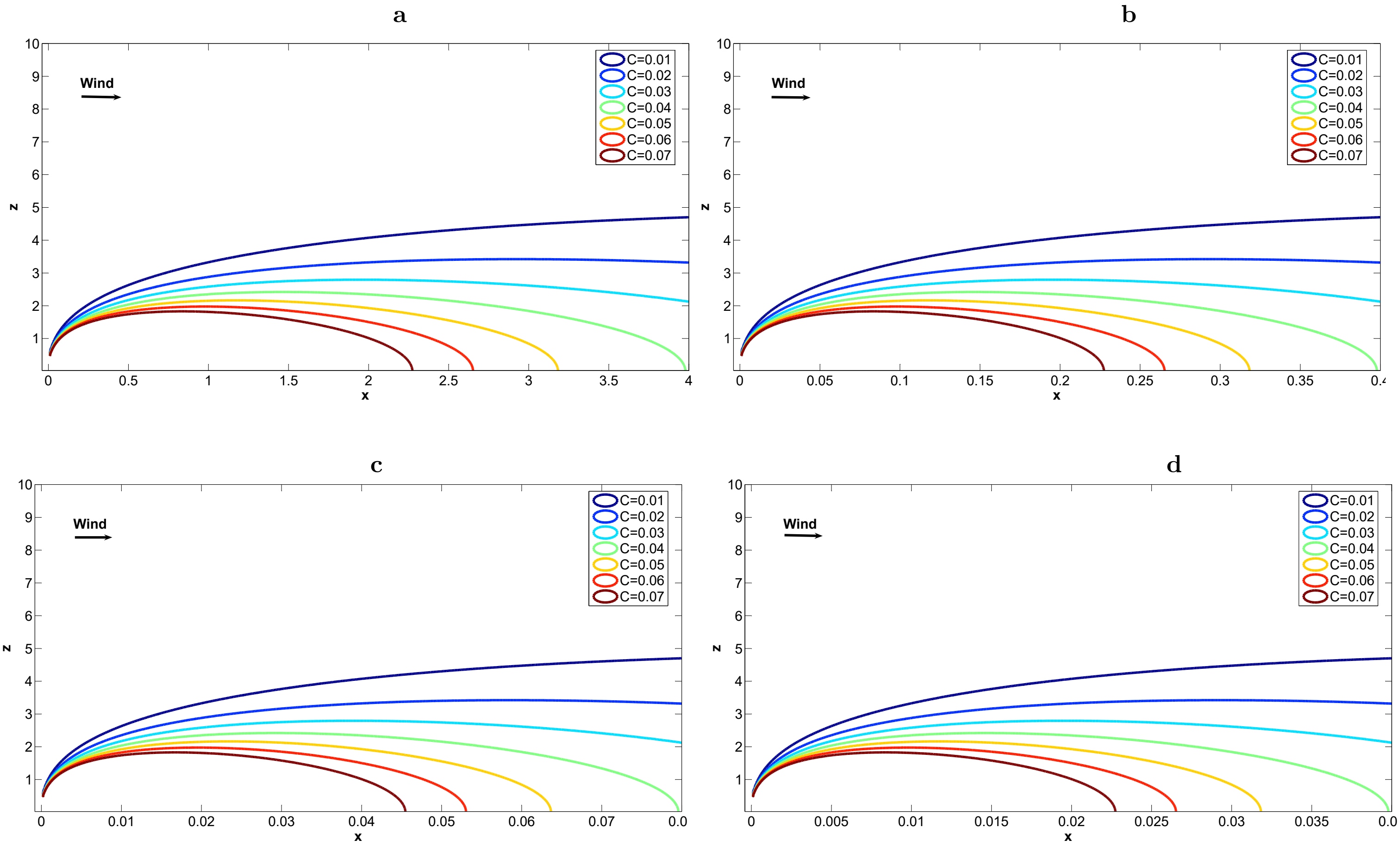

Figure 4: Contour plots of concentration $c(x, y, z)$ for a ground-level source (a) D = 1 m^2/s, (b) D = 10 m^2/s, (b) D = 50 m^2/s, and (d) D = 100 m^2/s in the vertical plane $y = 0$.

3.5 Variation of diffusion rate

Figure 4 depicts the pollutants concentration by variation of diffusion rate along the x-axis. Figure 4a, we choose the diffusion of pollution to be $D = 1$ m^2/s. We observed that the pollutants were normal advect along the x-direction. Figure 4b, we set the pollutants diffusion rate to $D = 10$ m^2/s. Compared to Figure 4a, this affects the diffusion rate in the x-direction more quickly. Figure 4c and 4d, We set the pollutants diffusion rate to $D = 50$ m^2/s and $D = 100$ m^2/s. When compared to slower diffusion rates, this changes the diffusion rate in the x-direction relatively quick.

Hence, we concluded that the change in the diffusion rate, substantially disperse the pollutants in x-direction. Finally, it is emphasized that weak diffusion rates change the x-axis into slow dispersed and strong diffusion rates resulting in speedy dispersion at ground level.

4 Conclusion

This research work looks closely at the mathematical foundations of atmospheric dispersion modeling, which involves a Gaussian plume model to find the solution to the advection-diffusion problem. By the application of the two-dimensional dispersion equations, it is analyzed for eddy diffusivity, upwind distance from the source, horizontal wind speed, emission sources and downwind height above the ground of the pollutants which demonstrate the effectiveness of the existing model that could be applicable for forecasting a continuous range of dispersion. The pollution was more pronounced when the stack height was lower whereas it was less pronounced along the x-axis when the stack height was higher. Meanwhile, the pollutant will spread slowly in the atmosphere when there is a strong weight of the emission source but the pollutant will disperse quickly when there is a light weight of the source. Regarding wind speed, increasing the speed causes the pollutant to be dispersed widely at ground level while decreasing the speed resulted in the pollutant being dispersed slowly. By altering the diffusion rate, the dispersion of pollutants also alters, and the pollutants substantially disperse in the x-direction. This research contributes to the practical application of air quality management, especially in urban areas, and provides insight to policymakers and other concerned stakeholders on how to minimize the concentration of pollutants in the atmosphere.

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