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Mathematical advection-diffusion model of primary and secondary pollutants emitted from the point source with mesoscale wind and removal mechanisms

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Abstract

A numerical model is represented to study the effect of gravitational settling velocity and leakage velocity on the concentration distribution of primary and secondary pollutants emitted from the point source in an urban area with mesoscale wind. The point source characterizes pollutants emission from industrial process stacks and fuel combustion facility stacks. The article deals with the dispersion of primary and secondary pollutants emitted from point source with mesoscale wind along with large scale wind. The Crank-Nicolson's implicit finite difference method is adopted for solving partial differential equations of contaminant with wind velocity and eddy diffusivity profiles. Pollutants concentration been analysed for various removal mechanisms under stable as well as neutral condition of atmosphere. The results reveal decrease in the concentration of primary and secondary air contaminant by increasing the various removal mechanisms. In neutral condition the magnitude of concentration is less for the pollutants as compared with stable condition of atmosphere.

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Keywords: Mesoscale winds, Eddy diffusivity, Removal mechanism, Gravitational settling velocity, Leakage velocity and Finite difference technique.

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1. Introduction

Pollution is a serious problem everywhere nowa days in urban as well as around industrial areas. The rapid growth in population, transportation and industrial development has resulted in the release of all kinds of pollutants into the environment. The natural ability of the environment to tolerate and sustain development has dwindled in the face of the ever increasing discharge of pollutants. Due to the urbanization of the cities the dispersion of atmospheric contaminants has become a global problem in the recent years. The toxic gases emanating from industrial chimneys and vehicular exhausts get accumulated in large quantity over urban areas, under particular meteorological conditions. This has led to a serious health hazards in many cities around the world. An acute exposure to the elevated level of particulate air pollution has been associated with the cases of increased in the respiratory diseases, asthma, cardiopulmonary

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mortality, decline in pulmonary function and restricted life activities. Pope *et al*. [1] disclosed the chronic health diseases related with respiratory system being affected more with particulate air contamination. Brook *et al*. [2] analysed the consistent increase in the risk of cardiovascular functions due to the small period of time as well as long time exposure to the concentration of fine airborne ambient particulate substances. Riediker *et al*. [3] have also expressed the effect of particulate matter exposure associated with cardiovascular risks in younger generation. Nitu kumari and Sandeep [4] focused towards the extent as well as seriousness of the impact of particular contaminant on human beings; enumerated the impact which depends upon different factors including a kind of contaminant. Based on novel features of various anthropogenic activities they produce different kinds of contaminants, a number of models have been proposed in the literature [5–7].

Air pollution is one among various factors that attracted more attention from early 2020, which facilitated the spreading of corona virus disease, its severity and also prognosis of the disease. It is known fact that air pollution increases the cardiovascular and respiratory diseases. People suffering from such chronic diseases are prone to have high risk of mortality when infected with COVID-19. Moreover air pollution studies have shown that the increase in rate of respiratory infections from a variety of pathogens, probably by reducing host defences. In the last decade, methods have been developed to estimate outdoor concentrations of the major outdoor air pollutants particulate matter ($PM2.5$), black carbon (BC), ozone (O_3) and nitrogen dioxide (NO_2) with fine spatial resolution for the whole planet. These methods used not only data from monitoring stations but also chemical transport models, land use data and satellite observations. This has facilitated studies of very large populations, not restricted to urban areas. Recently, estimates of long-term average outdoor air concentrations on non-regulated air pollutants are becoming increasingly available, including ultrafine particulates and chemical composition of fine particles. Studies have shown that perhaps some of the previously observed health effects of $PM2.5$ might be due to these very small particles ($< 100nm$). According to Downward *et al.* [8], the health effects observed on particulate matter could potentially be attributed to these tiny particles. The mechanistic studies suggested by Ciencewicki *et al*. [9] reveal that pollutants in the particulate matter form will reduce the resistance to infections caused by bacteria or viral infections. Samet *et al.* [10] have studied the risk of pollutant NO_2 in the environment for viral infections. The results obtained from epidemiological research found that higher level of atmospheric contamination is related with lower respiratory infections, in particular among children according to Ref. [11].

While soil water can be collected in a single location, air pollution cannot be gathered in a single place. Therefore, air pollution control technologies must be implemented at the source, prior to the release of pollutants into the atmosphere. The main object of this article is to provide a mathematical model for better understanding the role of different meteorological parameters and removal mechanisms as well as transformation processes associated with the life cycle of atmospheric pollutants in urban areas. More specifically, urban air pollution plays a significant role in altering the climate of cities. Urban characteristics such as the creation of heat islands, a decrease in average speed, an increase in fog frequency, and the formation of mesoscale circulation systems significantly influence the urban climate. Basically, the primary pollutants, which are emitted directly into the atmosphere, are being converted into the secondary pollutants by means of first-order chemical reactions. The significant feature of secondary pollutants is their longer life span compared to primary pollutants, making them more hazardous to both human health and environmental protection. Many times the pollutants appear in larger particles; the effect of gravitational acceleration cannot be neglected in such cases. These pollutants come down to the ground by means of settling velocity W_s. Pollutant particles smaller than $20\mu m$ in size disperse in the environment as gases. The effects due to their falling velocity are being neglected. Molders and Olson [12] articulated the impact of precipitation on urban areas in high latitudes. Calder [13] reported that the atmospheric diffusion of particulate matter with a size greater than $20\mu m$ will have an appreciable settling velocity. The combustion of hydrocarbon fuels in residential areas, vehicular exhausts due to traffic flow, and several other major and minor sources pollute a part or whole area of an urban environment. The nature of wind flow varies accordingly with a region; large urban areas due to the formation of urban heat islands often generate their own special type of wind, known as mesoscale wind, and it plays an important role in shaping the urban pollution pattern. Dilley and Yen [14] expressed the significance of mesoscale wind in the pollutant distribution in an urban area.

Mathematical models play a crucial role in understanding the role of various meteorological parameters associated with the life cycle of atmospheric air pollutants, as well as in describing the dispersion of pollutant's concentrations. In the present article, we have discussed a numerical model for advection and diffusion of pollutants emitted from a point source on the boundary in the presence of mesoscale wind. The mesoscale wind is chosen to represent a local wind produced by the urban heat island effect. The model takes into account the realistic vertical height-dependent power law profiles for large-scale wind and eddy diffusivity, while the mesoscale wind is parameterized in the power law forms suggested by Dilley and Yen [14]. The role of different removal mechanisms of atmospheric pollutants has been discussed in the article.

One of the main removal mechanisms is dry deposition onto the surface of the earth as a result of gravitational settling and ground absorption by the soil, vegetation, buildings, or a body of water. The pollutants deposited on the surface have a significant impact on the ecosystem, as they will enter and travel through biological pathways. Secondary pollutants, due to their heavier nature, gravitationally settle to the ground. Therefore, we need to develop a mathematical model to understand secondary pollutants and how they are eliminated through settling. Rudraiah *et al*. [15] considered an atmospheric dispersal model about secondary contaminants with settling velocity. The Gaussian plume model is the basic method used to calculate the concentration of air pollution from the point source being executed by Turner [16]. Furthermore, the Gaussian plume model for point sources was also analyzed by Morgenstern *et al*. [17]. Carpenter *et al*. [18] studied the plume dispersion model for point sources too. Gifford and Hanna [19] have discussed pollutant estimates suitable for air pollution in urban areas. A mathematical model for an area source and a point resource in a city area was evaluated by Ravindranath *et al*.[20] have discussed pollutant estimates in suitable manner for the air pollution in urban area. The above-mentioned models do not talk about the effect of mesoscale wind on dispersion and diffusion of contaminants. Latha *et al*. [21] discussed an analytical model for point-source pollutants in an urban area with mesoscale wind. The mathematical model for contaminant dispersion in the atmosphere has been discussed by Kafle *et al*. [22]. Lakshminarayanachari *et al*. [23] studied how pollutants move through the air when they come from both a point source on the surface and an area source that reacts chemically. Bhaskar *et al*. [24] developed an analytical model for atmospheric contamination resulting from an elevated point source and mesoscale wind. Furthermore, Bhaskar *et al*. developed a numerical model for primary and secondary contaminants emitted from both area and point sources, incorporating chemical reaction and removal mechanisms [25].

In this article, the point source is considered arbitrarily on the left boundary of the city for the reason that the grid point may miss the source. In such a case, the grid points must be taken at the source point. To overcome these, the following two methods can be used:. One is to use Gaussian distribution for pollutants source at the initial line, and the other is distributing point source to its neighbouring two grid points. The second procedure is used in this numerical model for air pollutants to take into account a point source at an arbitrary point. The pollutants, after being emitted from their source, are removed from the atmosphere through various sinks like rain, fog droplets, etc. prevailing in the atmosphere. So the depletion factor responsible for these wet deposition processes is included in the model. Besides wet deposition, the removal of pollutants through dry deposition on the ground is also considered. The well-known implicit Crank-Nicolson finite difference numerical scheme, which has the advantage of being unconditionally stable and consistent, is employed to compute the concentration of pollutants in a given urban region.

In this research, our findings show that pollutant concentrations peak near the source and at ground level in additional removal systems, leading to decreased pollution levels.

2. Methodology

The dispersion of air pollutant concentrations in a turbulent atmospheric medium is specified by the equation in the K-theory approach:

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} + V\frac{\partial c}{\partial y} + W\frac{\partial c}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right) - R, \quad (1)$$

here, C represents the concentration of the pollutant in the air at any point (x, y, z) and time t. K_x, K_y, and K_z. are the coefficients of eddy diffusivity in the x, y, and z directions, respectively. U, V, and W are the wind velocity components in x, y, and z directions, respectively, and R is the reaction rate coefficient for chemical transformation.

The physical problem consists of a point source on the boundary in an urban area with finite downwind and infinite crosswind dimensions. For the present model of air pollutants, the point source is distributed around two adjacent grid points along the z-axis. We plan to calculate the concentration distribution in both the source region and the source-free region, up to a desired distance of $l = 6000$ meters downwind. The pollutants are transported horizontally by large-scale wind, which is a function of vertical height (z), as well as horizontally and vertically by local wind caused by urban heat sources, called mesoscale wind. We have taken into account the source region within the urban center, which stretches from the origin to a distance of l in the downward x direction ($0 \leq x \leq l$). In this article, we have assumed a distance of $l = 6km$. Removal mechanisms of pollutants, such as dry deposition, wet deposition, gravitational settling velocity, and leakage through the upper boundary, are assumed, as the pollutants are chemically reactive in nature. The schematic diagram of the model is shown below in Figure 1.

Primary Pollutants: In formulating the physical problem, the following assumptions are made:

1. Since bigger particles are coming down by the gravitational acceleration, the pollutants are deposited on the ground by means of gravitational settling velocity.
2. The pollutants can also be removed by dry deposition on the surface of the earth as a result of ground absorption by soil, vegetation, a building, or a body of water.
3. Pollutants leak through the boundary; we consider the leakage velocity at the top of the boundary.
4. The wind velocity and eddy diffusivity are the functions of vertical direction. And mesoscale wind velocity is a function of both horizontal and vertical direction.
5. Along the cross-wind direction, the lateral flux of pollutants is assumed to be small, i.e., $V\frac{\partial c_p}{\partial y}$ and $\frac{\partial}{\partial y}(K_y\frac{\partial c_p}{\partial y}) \to 0$ where V is the speed along y-direction and K_y is the eddy diffusivity coefficient along y-direction.
6. The horizontal advection is greater than horizontal diffusion for not too small values of wind velocity. The horizontal advection by the wind dominates over horizontal diffusion i.e., $U\frac{\partial c_p}{\partial x} \ggg \frac{\partial}{\partial x}(K_x\frac{\partial c_p}{\partial x})$ where U is wind velocity and K_x is the eddy diffusivity coefficient in x-direction.

Given the previously considered assumptions, equation (1) assumes the following form:

$$\frac{\partial c_p}{\partial t} + U(x,z)\frac{\partial c_p}{\partial x} + W(z)\frac{\partial c_p}{\partial z} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial c_p}{\partial z}\right) - \left(k + k_{wp}\right)C_p, \quad (2)$$

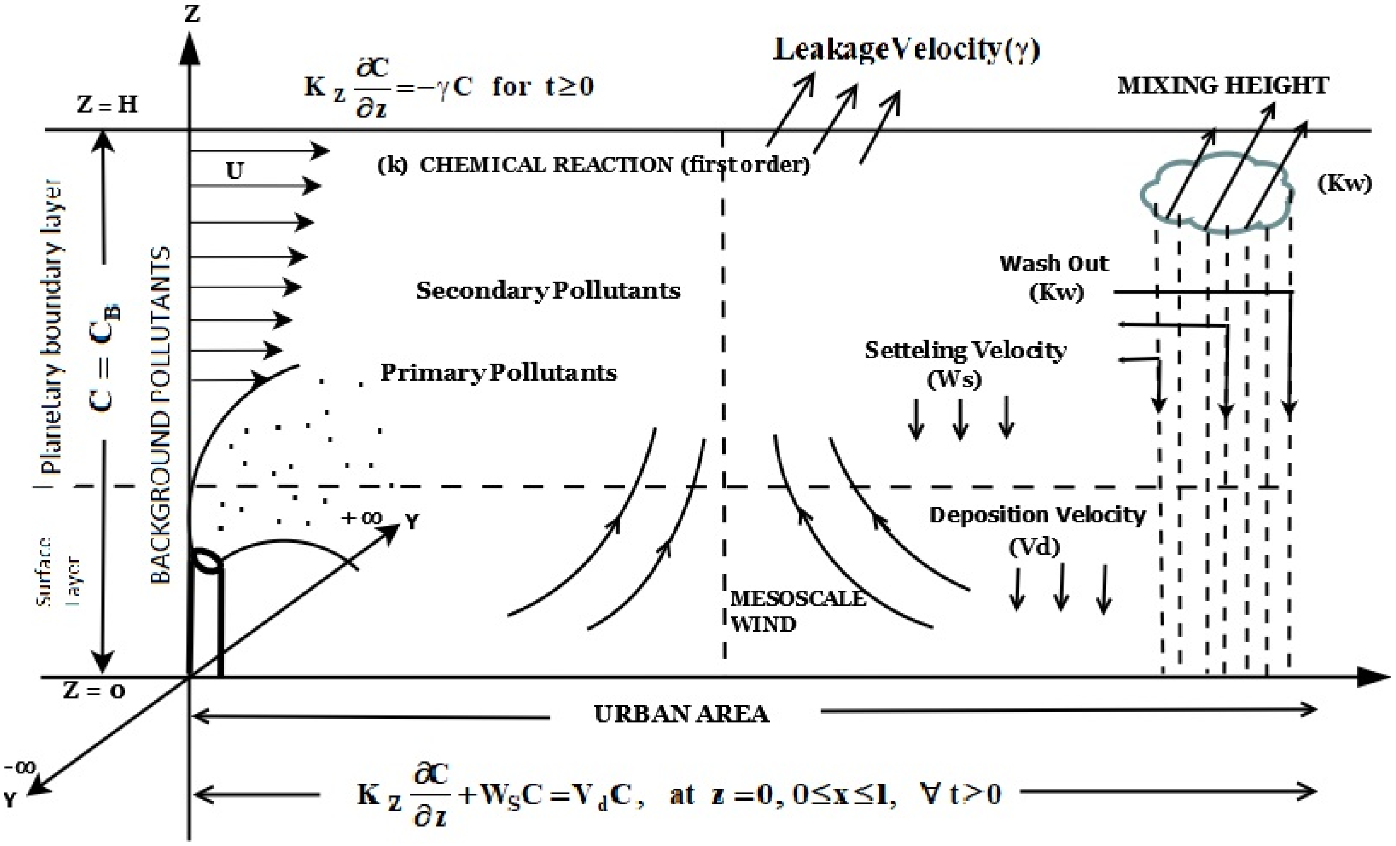

Figure 1. Physical design of the present model.

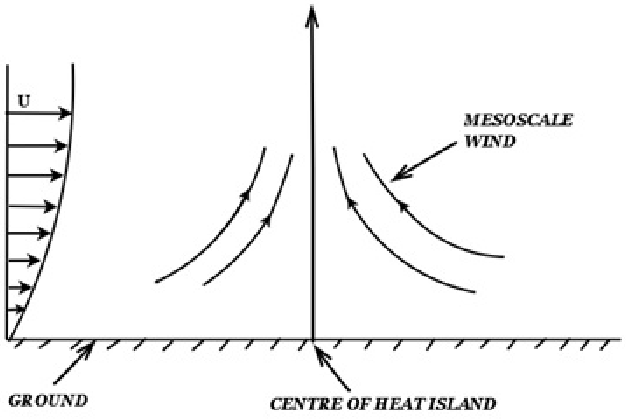

Figure 2. A virtual urban heat island and mesoscale winds.

where $C_p = C_p(x, z, t)$ denotes the mean concentration of pollutant species, k_{wp} the washout coefficient of primary pollutants, and k is the first-order chemical reaction rate coefficient for the transformation. At the beginning of the emission, the region of interest is free from pollution. Therefore, the initial stage condition is provided by,

$$C_p = 0 \text{ when } t = 0,\ \ 0 \leq x \leq l \text{ and } 0 \leq z \leq H. \tag{3}$$

The wind direction determines the length of the desired domain of interest (l), while the mixing height (H) equals $624m$. We assume the presence of a point source (industrial stack) at $x = 0$, which corresponds to the start of the urban area. The wind direction is assumed to be toward the city from the point source. Thus,

$$C_p = Q_1 \frac{\delta(z - z_1)}{U(z)} \text{ at } x = 0,\ z = z_1 \text{ and } \forall\ t > 0, \tag{4}$$

where Q_1 represents the strength of the point source, and we take z to be 20.5 meters. The pollutants are confined within the mixing height, and there is a leakage across the top boundary of the mixing layer. Thus,

$$K_z \frac{\partial C_p}{\partial z} = -\gamma_p C_p \quad x > 0,\ z = H,\ \forall\ t. \tag{5}$$

Secondary Pollutants: The basic governing equation for the secondary pollutant C_s is,

$$\frac{\partial c_s}{\partial t} + U(x, z)\frac{\partial c_s}{\partial x} + W(z)\frac{\partial c_s}{\partial z} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial c_s}{\partial z}\right) + W_S \frac{\partial c_s}{\partial z} + V_g k C_p. \tag{6}$$

Vg is the mass ratio of secondary particulate species to the primary gases that are being converted. k is the first-order coefficient with respect to wet deposition. The following assumptions were made in the derivation of equation (6):

1. The removal of secondary pollutants C_s occur by the process of dry deposition on the surface of the earth.

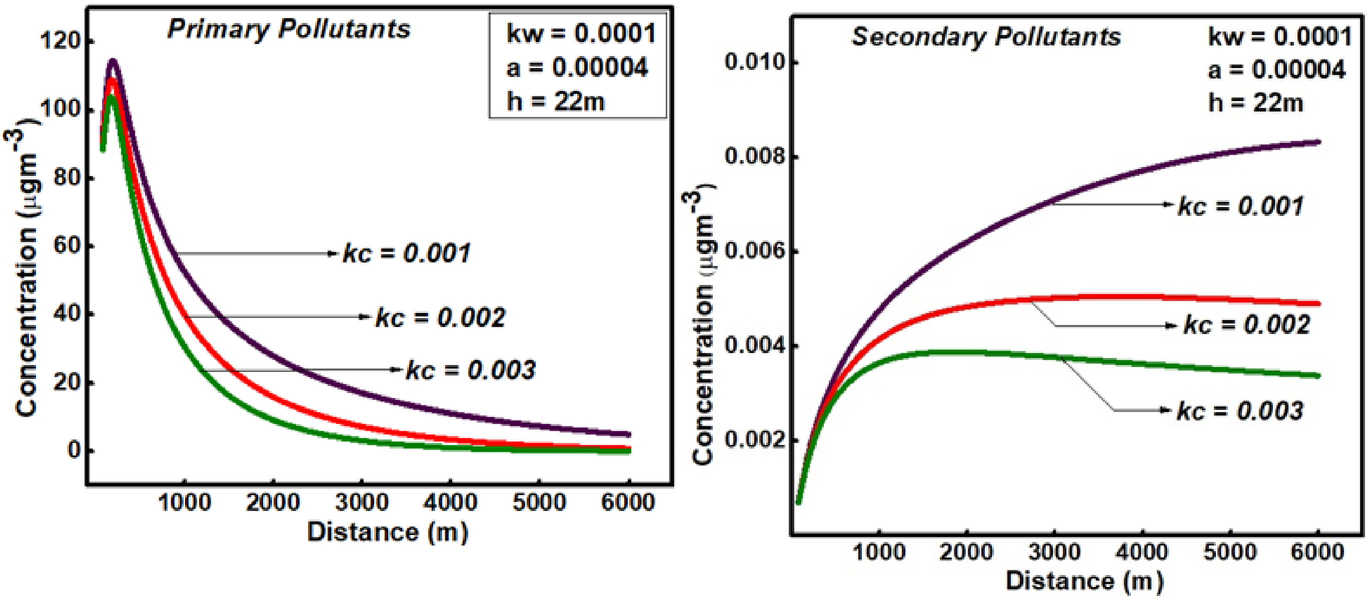

Figure 3. Ground level concentration verses distance of pollutants for different k_c under neutral condition.

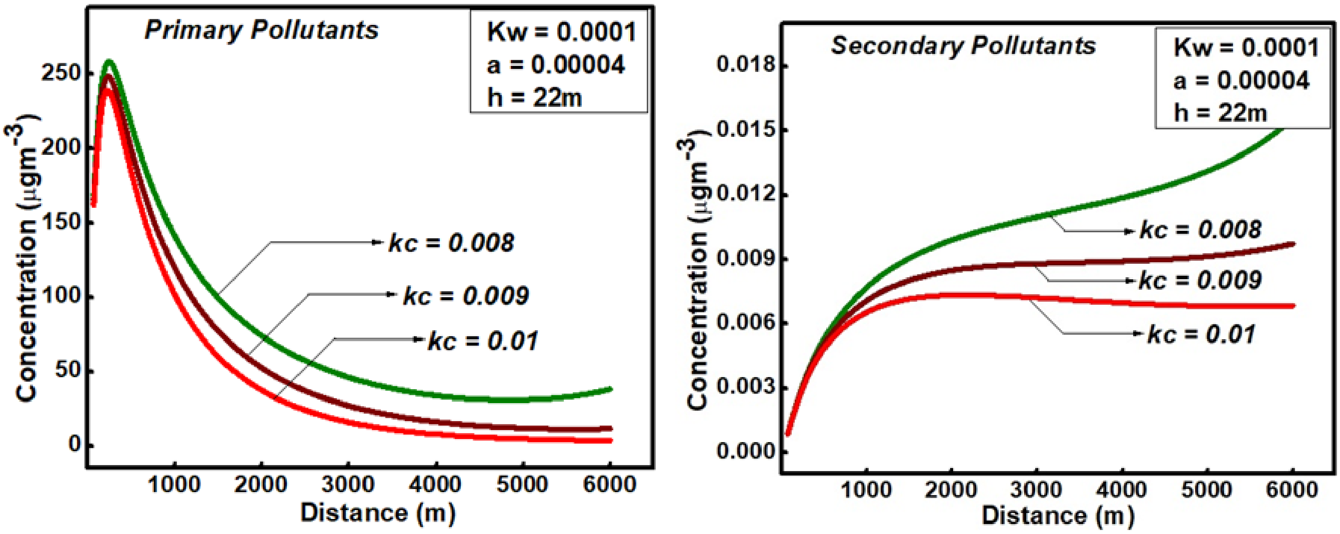

Figure 4. Ground level concentration verses distance of pollutants for different k_c under stable condition.

2. Dry deposition on the earth surface is due to the ground absorption by soil, vegetation, buildings etc.
3. By means of rainout/washout the wet deposition of secondary pollutants occurs and larger size particle pollutants are removed by gravitational settling.

The initial and boundary conditions on secondary pollutants C_s are as follows-

$$C_s = 0 \text{ when } t = 0, \ 0 \le x \le l \text{ and } 0 \le z \le H. \tag{7}$$

$$C_s = 0 \text{ when } x = 0, \ 0 \le z \le H \text{ and } \forall \ t > 0. \tag{8}$$

There is no direct source of secondary pollutants, and they are being removed by ground deposition and settling velocity from the atmosphere. The corresponding boundary conditions are expressed as follows:

$$K_z \frac{\partial c_s}{\partial z} + W_{gs} C_s = V_{ds} C_s \text{ with } z = 0, \ 0 \le x \le l \ \forall \, t > 0. \tag{9}$$

The secondary pollutants have a V_{ds} dry deposition velocity and a W_{gs} gravitational settling velocity. The pollutants are confined within the mixing height; hence, there will be a leakage across the top boundary of the mixing layer. Thus,

$$K_z \frac{\partial C_s}{\partial z} = -\gamma_s C_s \text{ at } x = 0, \ z = H \text{ and } \forall \ t > 0. \tag{10}$$

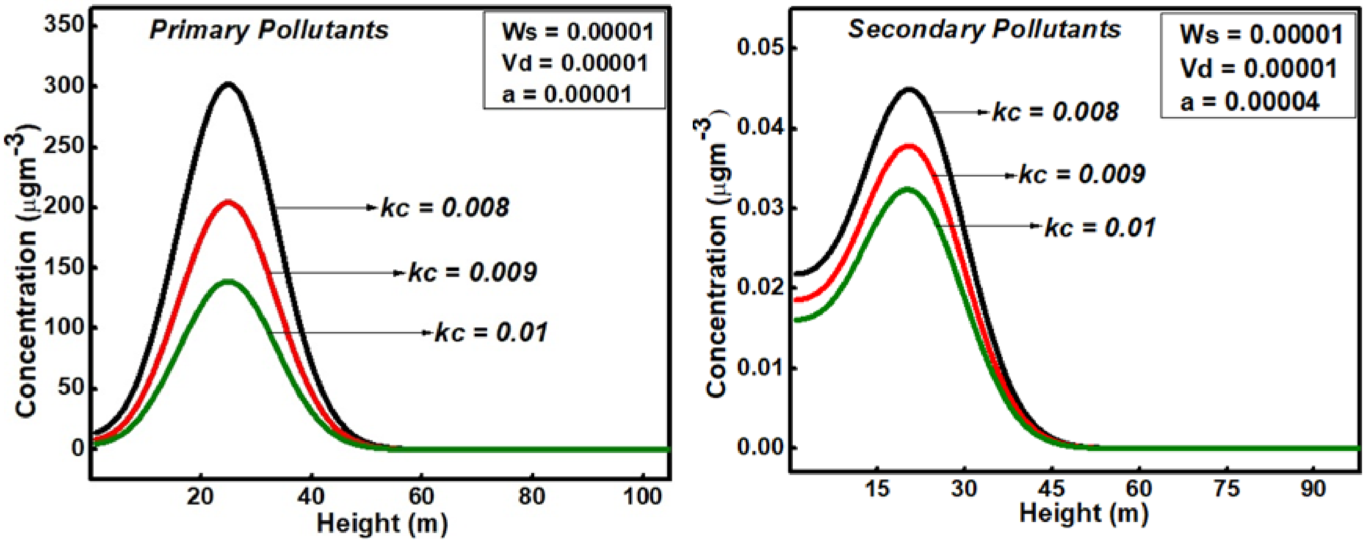

Figure 5. Concentration versus Height of Pollutants with removal mechanism Ws and Vd under Stable Condition for different values of k_c and $Kw = 0.0001$.

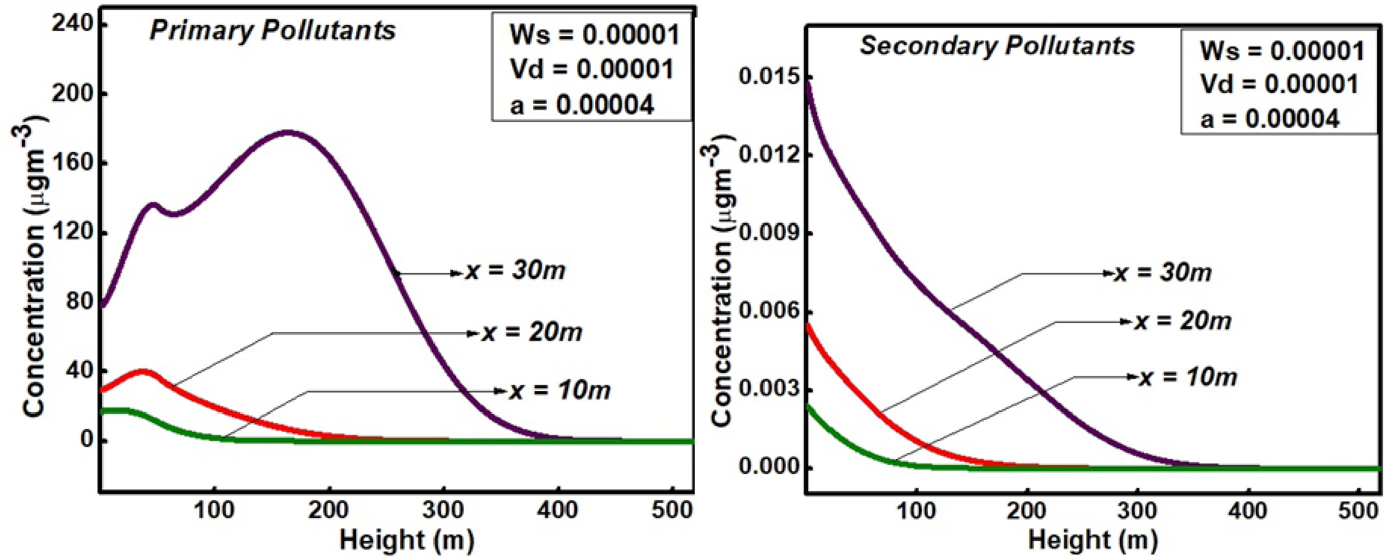

Figure 6. Concentration versus height of pollutants for different distances with removal mechanism W_s and V_d under neutral condition with $\gamma = 0.006$.

2.1. Meteorological parameters

In order to solve equations (2) and (6), one should know the realistic form of the variable wind velocity and eddy diffusivity, both of which are functions of vertical distance. The meteorological parameters that influence the eddy diffusivity and velocity profile are dependent on the intensity of turbulence, which is influenced by the stability of the atmosphere. It is essential to know the wind speed and eddy diffusivity at each grid point. The stability near the ground depends primarily upon the net heat flux.

2.2. Eddy diffusivity profiles

The characteristics of K_z are that it has a linear variation near the ground, a constant value at mid mixing depth, and a decreasing trend at the top of the mixing layer. Shir [26] provided an expression for the neutral condition based on the hypothetical analysis.

$$K_z = 0.4 u_* z e^{-4z/H}, \tag{11}$$

where u_* is friction velocity, L is the stability length parameter according to Ref. [27]. For stable atmospheric conditions, the eddy diffusivity is given by Ku *et al*. [28].

$$K_z = \frac{\kappa u_* z}{0.74 + 4.7z/L} e^{-b\eta}, \tag{12}$$

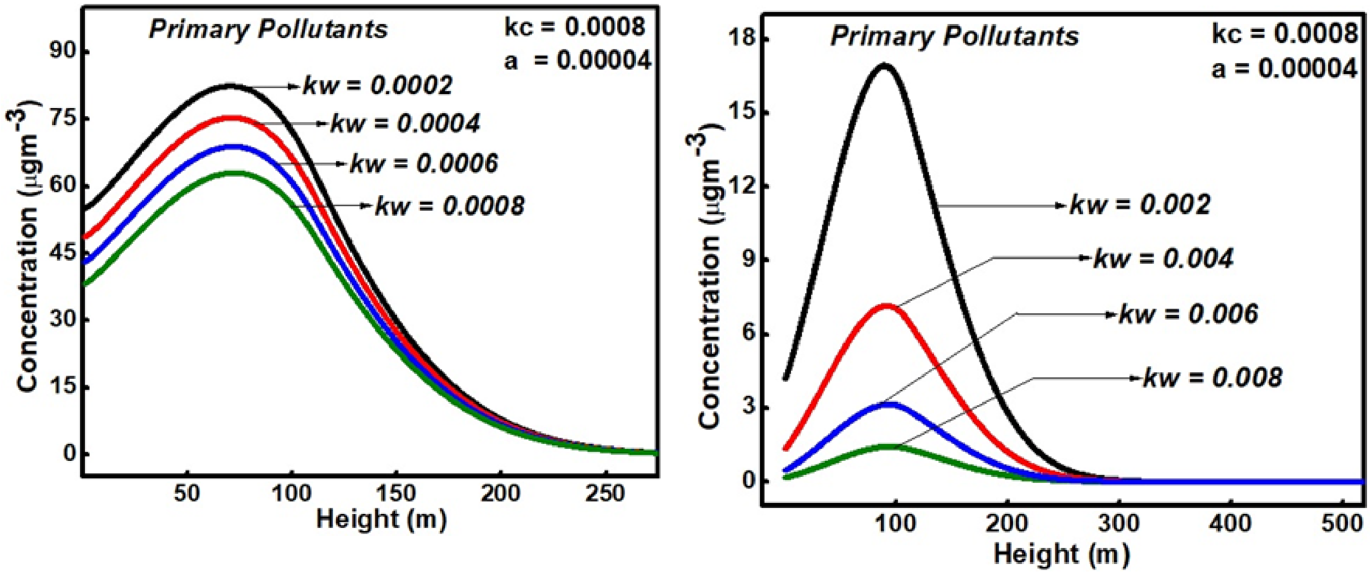

Figure 7. Concentration versus height of primary pollutants for different K_w with removal mechanism Kc =0.0008 at X=6 km and X= 3km under stable condition.

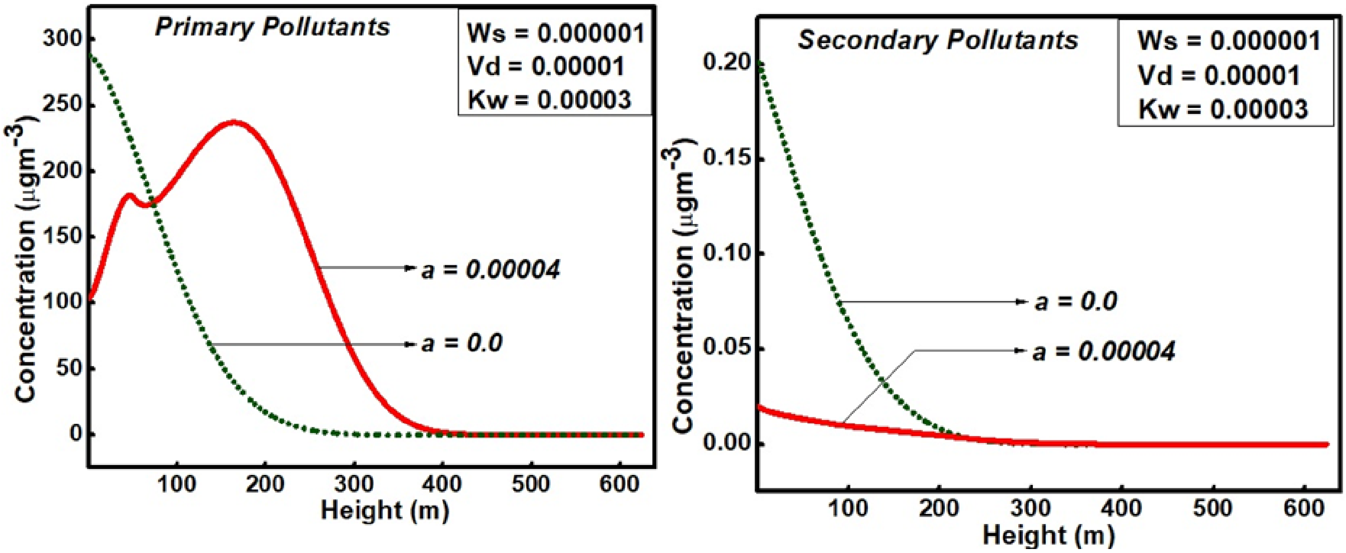

Figure 8. Concentration versus height of pollutants with and without mesoscale winds along with removal mechanism under Neutral condition.

where $b = 0.91; \eta = z/L\sqrt{\mu}$ with $\mu = u_*/|fL|$. k is the Karman's constant. Eddy diffusivity profiles given by equation (11) and equation (12) have been used in this model, developed for neutral and stable atmospheric condition.

2.3. *Wind velocity profiles*

Wind velocity inside the atmospheric boundary layer has a very important role in transporting pollutant material, which usually increases with elevation. Very frequently used expressions for velocity profiles are the logarithmic, log-linear, and power law profiles. The velocity profile is given by $U = u_l(z/z_l)^p$ u_l and, z_l, are reference velocity and elevation, respectively.

2.4. *Mesoscale wind velocity profiles*

It is a known fact that in a large city, the generation of heat causes the rising of air at the centre of the city, and hence the city can be called a 'heat island'. This raising of air forms an air circulation, and this circulation is competitive at larger heights. This circulation is called 'mesoscale circulation' and in urban areas it is schematically depicted as in Figure 2.

In order to incorporate a realistic form of velocity profile in our model, which depends upon Coriolis force, surface friction geostrophic wind, stability characterising parameter L, and vertical height z, we integrate the velocity gradient $\frac{\partial U}{\partial z} = \frac{u_* \phi_M}{kL}$ with a lower limit z_0 to an upper limit $z + z_0$ for stable and neutral conditions to obtain the expression for wind velocity accord-

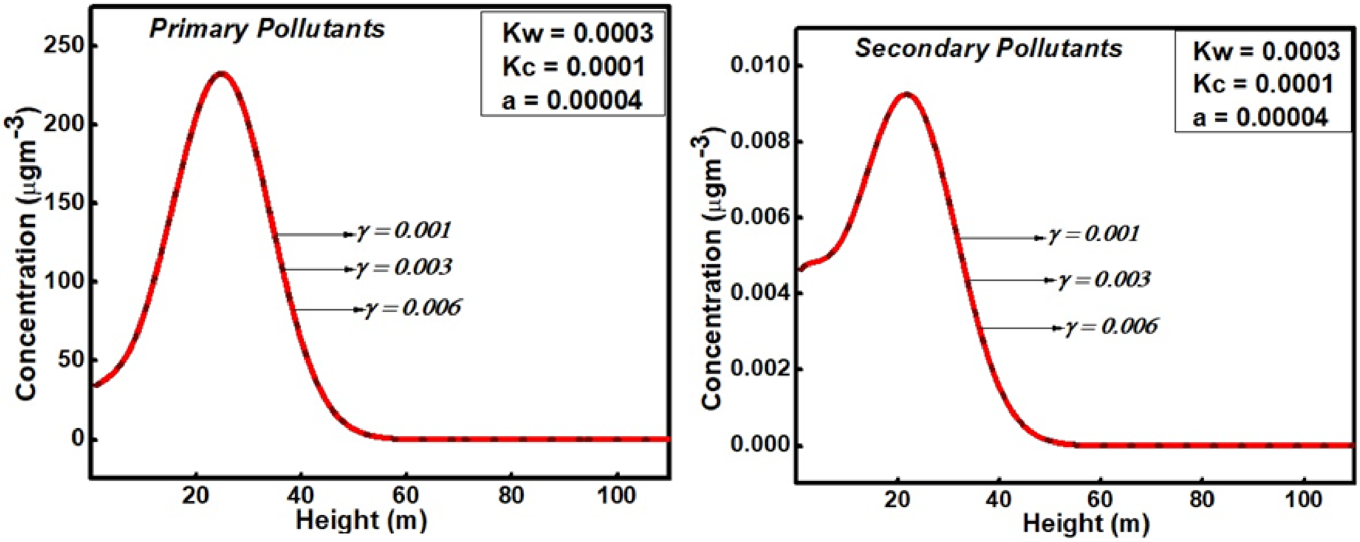

Figure 9. Concentration versus height of pollutants with leakage velocity along with removal mechanism under stable condition.

ing to Refs. [14, 23] as seen in equation (15, 19, 23, 27). The stability condition for neutral case:

$$\text{For} \quad z < 0.1\kappa\frac{u_*}{f} \quad \text{we get} \quad u = \frac{u_*}{\kappa}\ln\left[\frac{z+z_0}{z_0}\right]. \qquad (13)$$

$$u_e = -a(x-x_0)\ln\left[\frac{z+z_0}{z_0}\right], \ a \ \text{proportionality constant}.(14)$$

$$U(x,z) = u + u_e = \left(\frac{u_*}{\kappa} - a(x-x_0)\right)\ln\left[\frac{z+z_0}{z_0}\right]. \qquad (15)$$

The mesoscale wind w_e is obtained on integrating the continuity equation as,

$$w_e = a\left[z\ln\left[\frac{z+z_0}{z_0}\right] - (z+z_0)\ln(z+z_0)\right]. \qquad (16)$$

The stability condition for stable case:

$$\text{For} \quad 0 < \frac{z}{L} < 1 \quad \text{we get} \quad u = \frac{u_*}{\kappa}\left[\ln(\frac{z+z_0}{z_0}) + \frac{\alpha}{L}z\right].(17)$$

$$u_e = -a(x-x_0)\left[\ln(\frac{z+z_0}{z_0}) + \frac{\alpha}{L}z\right]. \qquad (18)$$

$$U(x,z) = u+u_e = \left(\frac{u_*}{\kappa} - a(x-x_0)\right)\left[\ln(\frac{z+z_0}{z_0}) + \frac{\alpha}{L}z\right].(19)$$

$$w_e = a\left[z\ln\left(\frac{z+z_0}{z_0}\right) - (z+z_0)\ln(z+z_0) + \frac{\alpha}{2L}z^2\right]. \qquad (20)$$

$$\text{For} \quad 1 < \frac{z}{L} < 6 \quad u = \frac{u_*}{\kappa}\left[ln\left(\frac{z+z_0}{z_0}\right) + 5.2\right]. \qquad (21)$$

$$u_e = -a(x-x_0)\left[\ln\left(\frac{z+z_0}{z_0}\right) + 5.2\right]. \qquad (22)$$

$$U(x,z) = u+u_e = \left(\frac{u_*}{\kappa} - a(x-x_0)\right)\left[\ln\left(\frac{z+z_0}{z_0}\right) + 5.2\right].(23)$$

$$w_e = a\left[z\ln\left(\frac{z+z_0}{z_0}\right) + z_0\ln(z+z_0) + 4.2z\right]. \qquad (24)$$

In the planetary boundary layer above the surface layer power law scheme is being employed for both stable ($z/L \geq 6$) and neutral atmospheric stability condition ($z \geq 0.1\,\kappa\frac{u_*}{f}$).

$$u = (u_g - u_{sl})\left(\frac{z-z_{sl}}{H-z_{sl}}\right)^p + u_{sl}. \qquad (25)$$

$$u_e = -a(x-x_0)\left[\left(\frac{z-z_{sl}}{H-z_{sl}}\right)^p + u_{sl}\right]. \qquad (26)$$

$$U(x,z) = u + u_e = \left[(u_g - u_{sl}) - a(x-x_0)\right]\left(\frac{z-z_{sl}}{H-z_{sl}}\right)^p$$
$$+ (1 - a(x-x_0))u_{sl}. \qquad (27)$$

$$w_e = a\left[(u_g - u_{sl})\left(\frac{z-z_{sl}}{p+1}\right)\left(\frac{z-z_{sl}}{H-z_{sl}}\right)^p + zu_{sl}\right], \qquad (28)$$

where u_g is the geostrophic wind, z_{sl} is the top of the surface layer. x_0 is the x-coordinate of the center of the heat island, and H is the mixing height. The exponent, p, is dependent on the atmospheric stability. We have used the value of p as,

$$\boldsymbol{p} = \begin{cases} 0.2 & \text{for} \quad \text{neutral case} \\ 0.35 & \text{for} \quad \text{slightly stable flow} \\ 0.5 & \text{for} \quad \text{stable flow} \end{cases}$$

The wind velocity profiles are valid for $x \leq (\frac{u_*}{a\kappa} + x_0)$. So the range of validity increases indefinitely as mesoscale wind decreases. The mesoscale wind velocity depends on the value of '$\boldsymbol{a}$', and $\boldsymbol{a} = 0.00004$ is considered for the model.

2.5. Numerical technique

In the present model, we have used the numerical method, which is based on the Crank-Nicolson finite difference scheme, to discretise the equations (2) and (6) to get the solution. The derivatives are replaced by the arithmetic average of its finite difference approximations at the n^{th} and $(n+1)^{th}$ time steps. The equation (2) at the grid points (i, j) and time step $(n+\frac{1}{2})$ is given as,

$$\frac{\partial C_p}{\partial t}\Big|_{ij}^{n+\frac{1}{2}} + \frac{1}{2}\left[U(x,z)\frac{\partial C_p}{\partial x}\Big|_{ij}^{n} + U(x,z)\frac{\partial C_p}{\partial x}\Big|_{ij}^{n+1}\right] + \frac{1}{2}[W(z) \frac{\partial C_p}{\partial z}\Big|_{ij}^{n} + W(z)\frac{\partial C_p}{\partial z}\Big|_{ij}^{n+1}] = \frac{1}{2}[\frac{\partial}{\partial x}\left(K_z(z)\frac{\partial C_p}{\partial z}\Big|_{ij}^{n}\right) + (K_z(z)\frac{\partial C_p}{\partial z}\Big|_{ij}^{n+1})] - \frac{1}{2}\left(k + k_{wp}\right)\left(C_{pij}^{n} + C_{pij}^{n+1}\right), \quad (29)$$

where $i = 1, 2, 3, \cdots$ and $j = 1, 2, 3, \cdots$ with $n = 0, 1, 2, \cdots$

$$\text{Using} \quad \frac{\partial C_p}{\partial t}\Big|_{ij}^{n+\frac{1}{2}} = \frac{C_{pij}^{n+1} - C_{pij}^{n}}{\Delta t}. \quad (30)$$

$$U(x,z)\frac{\partial C_p}{\partial x}\Big|_{ij}^{n} = U_{ij}\left[\frac{C_{pij}^{n} - C_{pi-1j}^{n}}{\Delta x}\right]. \quad (31)$$

$$U(x,z)\frac{\partial C_p}{\partial x}\Big|_{ij}^{n+1} = U_{ij}\left[\frac{C_{pij}^{n+1} - C_{pi-1j}^{n+1}}{\Delta x}\right]. \quad (32)$$

$$W(z)\frac{\partial C_p}{\partial z}\Big|_{ij}^{n} = W_j\left[\frac{C_{pij}^{n} - C_{pij-1}^{n}}{\Delta z}\right]. \quad (33)$$

$$W(z)\frac{\partial C_p}{\partial z}\Big|_{ij}^{n+1} = W_j\left[\frac{C_{pij}^{n+1} - C_{pij-1}^{n+1}}{\Delta z}\right]. \quad (34)$$

$$\text{Also} \quad kC\Big|_{ij}^{n+\frac{1}{2}} = k\left[\frac{C_{pij}^{n} + C_{pij}^{n+1}}{2}\right]. \quad (35)$$

$$k_{wp}C\Big|_{pij}^{n+\frac{1}{2}} = k_{wp}\left[\frac{C_{pij}^{n} + C_{pij}^{n+1}}{2}\right]. \quad (36)$$

And second order central difference for,

$$\frac{\partial}{\partial z}(K_z(z))\frac{\partial C_p}{\partial z}\Big|_{ij}^{n} = \frac{1}{2(\Delta z)^2} \left[(K_{j+1} + K_j)(C_{pij+1}^{n} - C_{pij}^{n}) - (K_j + K_{j-1})(C_{pij}^{n} - C_{pij-1}^{n})\right]. \quad (37)$$

$$\frac{\partial}{\partial z}(K_z(z))\frac{\partial C_p}{\partial z}\Big|_{ij}^{n+1} = \frac{1}{2(\Delta z)^2} \left[(K_{j+1} + K_j)(C_{pij+1}^{n+1} - C_{pij}^{n+1}) - (K_j + K_{j-1})(C_{pij}^{n+1} - C_{pij-1}^{n+1})\right]. \quad (38)$$

Equation (29) can be rewritten as,

$$A_{ij}C_{i-1j}^{n+1} + B_jC_{ij-1}^{n+1} + D_{ij}C_{ij}^{n+1} + E_jC_{ij+1}^{n+1} = F_{ij}C_{i-1j}^{n} + G_jC_{ij-1}^{n} + M_{ij}C_{ij}^{n} + V_jC_{ij+1}^{n}. \quad (39)$$

For each $i = 1, 2, \cdots imax$, with $j = 1, 2, \cdots jmax - 1$ also $n = 0, 1, 2, \cdots$ Here
$A_{ij} = -\left[U_{ij}\frac{\Delta t}{2\Delta x} + W_j\frac{\Delta t}{2\Delta z}\right]$: $B_j = -(k_j + k_{j-1})\frac{\Delta t}{4(\Delta z)^2}$.
$E_j = -(k_{j+1} + k_j)\frac{\Delta t}{4(\Delta z)^2}$: $F_{ij} = U_{ij}\frac{\Delta t}{2\Delta x} + W_j\frac{\Delta t}{2\Delta z}$.
$G_j = (k_j + k_{j-1})\frac{\Delta t}{4(\Delta z)^2}$: $V_j = (k_{j+1} + k_j)\frac{\Delta t}{4(\Delta z)^2}$.
$D_{ij} = 1 + U_{ij}\frac{\Delta t}{2\Delta x} + W_j\frac{\Delta t}{2\Delta z} + (k_{j+1} + 2k_j + K_{j-1})\frac{\Delta t}{4(\Delta z)^2} + (k + k_{wp})\frac{\Delta t}{2}$.
$M_{ij} = 1 - U_{ij}\frac{\Delta t}{2\Delta x} + W_j\frac{\Delta t}{2\Delta z} - (k_{j+1} + 2k_j + K_{j-1})\frac{\Delta t}{4(\Delta z)^2} - (k + k_{wp})\frac{\Delta t}{2}$.
$imax$ is i value about $x = l$. Also $jmax$ is j value about $z = H$.
The conditions at the boundary from equation (3) to equation (5) are being discretized: The initial boundary condition given in equation (3) implies,

$$C_{pij}^{0} = 0 \text{ at } j = 1, 2, \cdots jmax, \text{ and } i = 1, 2, \cdots imax.$$

Boundary condition given in equation (4) becomes,

$$C_{pij}^{n+1} = \frac{Q_1}{2U_{ij}} \text{ for } i = 1,\ j = j_s j_{s+1} \text{ and } n = 0, 1, 2, \cdots$$
$$= 0 \text{ for } i = 1\ j = 1, 2 \cdots j_{s-1} j_{s+2} j_{s+3} \cdots j_{max}$$
$$n = 0, 1, 2 \cdots$$

And boundary condition given in equation (5) imply,

$$C_{pijmax}^{n+1} - (1 - \gamma_p\frac{\Delta z}{k_{jmax}})C_{pimaxj}^{n+1} = 0 \text{ for } j = jmax,$$
$$i = 2, 3, \cdots imaxl$$

A similar method is adopted to obtain the finite difference equations for the secondary pollutant C_s; thus, equation (6) can be discretized as:

$$\frac{\partial C_s}{\partial z}\Big|_{ij}^{n+\frac{1}{2}} + \frac{1}{2}\left[U(x,z)\frac{\partial C_s}{\partial x}\Big|_{ij}^{n} + U(x,z)\frac{\partial C_s}{\partial x}\Big|_{ij}^{n+1}\right] + \frac{1}{2}\left[W(z)\frac{\partial C_s}{\partial z}\Big|_{ij}^{n} + W(z)\frac{\partial C_s}{\partial z}\Big|_{ij}^{n+1}\right] = \frac{1}{2}\left[\frac{\partial}{\partial x}(K_z(z))\frac{\partial C_s}{\partial z}\Big|_{ij}^{n} + (K_z(z))\frac{\partial C_s}{\partial z}\Big|_{ij}^{n+1})\right] + \frac{1}{2}\left[W_S\frac{\partial C_s}{\partial z}\Big|_{ij}^{n} + W_S\frac{\partial C_z}{\partial z}\Big|_{ij}^{n+1}\right] + \frac{1}{2}\left[V_gk(C_{pij}^{n} + C_{pij}^{n+1})\right]. \quad (40)$$

Equation (40) can be rewritten as:

$$\bar{A}_{ij}C_{i-1j}^{n+1} + \bar{B}_jC_{sij-1}^{n+1} + \bar{D}_{ij}C_{sij}^{n+1} + \bar{E}_jC_{sij+1}^{n+1} = \bar{F}_{ij}C_{i-1j}^{n} + \bar{G}_jC_{sij-1}^{n} + \bar{M}_{ij}C_{sij}^{n} + \bar{V}_jC_{sij+1}^{n} \quad (41)$$

For each $i = 1, 2, 3, \cdots imax$, $j = 1, 2, 3, \cdots jmax - 1$, and $n = 0, 1, 2, \cdots$.
And $imax$ is the i value at $x = l$ and $jmax$ is value of j at $z = H$.
The initial and boundary conditions of secondary pollutant C_s are discretized as,
Boundary condition given by equation (7) becomes,

$$C_{sij}^{0} = 0 \text{ for } j = 1, 2, 3, \cdots jmax, \ i = 1, 2, 3, \cdots imax.$$

The boundary conditions given by equation (8) and equation (9) successively can be written as,

$$C_{sij}^{n+1} = 0 \text{ for } i = 1 \text{ and } j = 1, 2 \cdots jmax \,\&\, n = 0, 1, 2 \cdots .$$

$$(1+(V_d+W_{gs})\frac{\Delta z}{k_j})C_{sij}^{n+1} - C_{sij+1}^{n+1} = 0 \text{ for } j = 1, \; i = 2, 3, 4, \cdots imaxl.$$

Also the boundary condition given by equation (10) becomes,

$$C_{sijmax-1}^{n+1} - (1-\gamma_s\frac{\Delta z}{k_{jmax}})C_{sijmax}^{n+1} = 0 \text{ for } j = jmax, i = 2, 3 \cdots imaxl.$$

Here, $\bar{A}_{ij} = -\left[U_{ij}\frac{\Delta t}{2\Delta x} + (W_j - W_S)\frac{\Delta t}{2\Delta z}\right]$: $\bar{B}_j = B_j$: $\bar{E}_j = E_j$.
$\bar{F}_{ij} = U_{ij}\frac{\Delta t}{2\Delta x} + (W_j - W_S)\frac{\Delta t}{2\Delta z}$: $\bar{G}_j = G_j$: $\bar{V}_j = V_j$.
$\bar{D}_{ij} = 1 + U_{ij}\frac{\Delta t}{2\Delta x} + (W_j - W_S)\frac{\Delta t}{2\Delta z} + (k_{j+1} + 2k_j + K_{j-1})\frac{\Delta t}{4(\Delta z)^2} - (V_g k)\frac{\Delta t}{2}$.
$\bar{M}_{ij} = 1 - U_{ij}\frac{\Delta t}{2\Delta x} - (W_j - W_S)\frac{\Delta t}{2\Delta z} - (k_{j+1} + 2k_j + K_{j-1})\frac{\Delta t}{4(\Delta z)^2} + (V_g k)\frac{\Delta t}{2}$.
Also V_d and W_{gs} denote the deposition velocity and gravitational settling velocity of secondary pollutant C_s respectively.

3. Results and discussion

In the present numerical model, the effects of gravitational settling velocity and leakage velocity on the pollutants emitted from the point source in the presence of mesoscale winds are being analysed. The point source characterizes the emission of pollutants from manufacturing processes and fuel ignition facility stacks. The present model speculates on the distribution of primary and secondary pollutants released from a point source in the presence of mesoscale wind and large-scale wind. We select the mesoscale wind to stimulate the local wind that the urban city's heat island generates. We have analysed the concentration of pollutants for various removal mechanisms under neutral and stable atmospheric conditions. Primary pollutants undergo chemical reactions to form secondary pollutants, such as the oxidation of sulphur dioxide to form sulphate. Since secondary pollutants have a longer life period and are more harmful than primary pollutants, it is crucial to analyse them. To determine ambient air concentration, one must know the distribution of primary and secondary pollutants in the city. The results show that increasing the gravitational settling velocity decreases the magnitude of secondary air pollutants' concentration. The concentration magnitude is lower for air pollutants in a neutral state compared to those in a stable state of the atmosphere.

The calculation of pollutant concentration in the atmosphere, both along wind direction and in vertical direction, considers the point source (industrial stack) as an arbitrary point on the boundary, in accordance with the numerical scheme. The point source, which is the industrial stack at $x = 0$, is situated at a height of $z = z_1 = 20.5m$ to the left of the urban area. Source strength is being evenly distributed between adjacent points of the point source along the z-axis. The source region is extending up to $l = 6km$ downwind from the origin, and the mixing height is taken as $624m$ above which the pollutants do not rise due to the temperature profile of the atmosphere. The model has been solved using the Crank-Nicolson finite difference technique, which is unconditionally stable. The primary and secondary pollutants are removed from the atmosphere by rainout/washout, dry deposition, wet deposition, and gravitational settling velocity in terrain. We consider a grid size of $75m$ along the x-direction and $1m$ along the z-direction to analyze the dispersion of primary and secondary pollutants under stable and neutral conditions of the atmosphere. The results of the present model have been exhibited graphically from Figure 3 to Figure 9.

Figures 3 and 4 illustrate how the ground level concentration varies with the distance of primary and secondary pollutants for different values of k_c, the removal mechanism W_s, and the leakage velocity γ, which corresponds to the dry deposition velocity V_d. From the graph, it is clear that the concentration of pollutants decreases with the increase in the value of k_c. The magnitude of the concentration is greater in the case of a stable atmospheric condition and less in the neutral condition. Similarly, the concentration of the primary pollutant is higher than that of the secondary pollutants. Thus, the presence of mesoscale winds causes a decrease in the concentration of the pollutants in the neutral condition.

Under the removal mechanisms of $W_s = 0$ and $V_d = 0$, the concentration of the secondary pollutant reaches its maximum under stable atmospheric conditions. And when it is taken $W_s = 0.0001$ and $V_d = 0.0001$, there is a decrease in the magnitude of concentration of the secondary pollutant as compared to $W_s = 0$ with $V_d = 0$, from Figure 4.

A similar effect is noticed in the neutral condition of the atmosphere. We observe that the presence of mesoscale wind tends to lower the concentration of pollutants in neutral conditions compared to stable conditions. A similar effect is observed for ground-level concentration versus height of the pollutants.

From Figure 5, it is clear that the maximum concentration is near the source, which is at $h = 23m$. There is a peak found in the graph for the different values of k_c in the presence of mesoscale wind. With the removal mechanisms W_s and V_d, we find a decrease in the concentration of pollutants with an increase in the height from the source. The graph (Figure 5) clearly illustrates this under stable atmospheric conditions. Also, it is observed that the pollutant concentration is higher in the stable condition of the atmosphere.

Figure 6 illustrates the ground level concentration of primary and secondary pollutants as a function of distance, for various removal mechanisms $W_s = 0.00001$ and $V_d = 0.00001$, with a leakage velocity of $\gamma = 0.006$. The graphs show values of $W_s = 0$ and $V_d = 0$. In the neutral condition of the atmosphere, the concentration of pollutants reaches its maximum. And when the removal mechanism has $W_s = 0.00001$ and $V_d = 0.00001$, the concentration of the pollutant is found to have decreased. Thus, an increase in the values of the removal mechanism decreases the magnitude of the concentration of pollutants-secondary pollutants in particular.

A similar kind of effect is found in stable atmospheric conditions. But in stable conditions, the concentration of pollutants is higher than in neutral conditions. The presence of mesoscale wind also contributes to the decrease in the magnitude of pollutant concentration. The effect is observed around height $h = 200m$ in the case of primary pollutants and $h = 300m$ in the case of secondary pollutants.

Figure 7 illustrates how the concentration of primary pollutants varies with height at different values of k_w, given a fixed value of $k_c = 0.0008$, at distances of $X = 6000m$ and $X = 3000m$. From the graph, it is clear that as the distance increases, the concentration of the pollutant decreases, and an increase in the values of k_w will also decrease the magnitude of the concentration of the primary pollutant. We observed that when k_w takes the values from 0.0002 to 0.0008, the concentration of the pollutants rises from $35\mu gm^{-3}$ to $77\mu gm^{-3}$. Similarly, when k_w takes the values 0.002 to 0.008, the concentration value decreases from $17\mu gm^{-3}$ to $1\mu gm^{-3}$. The removal mechanism's impact on the pollutant concentration is thus demonstrated.

In figure 8, the effect of removal mechanisms W_s, V_d, and k_w on the concentration of primary and secondary pollutants with and without mesoscale winds is being depicted. From the graph, we notice that the presence of mesoscale winds reduces the concentration of both primary and secondary pollutants under a neutral atmosphere. A similar effect has been noticed in the case of stable conditions, with the magnitude of concentration higher for primary as well as secondary pollutants.

Figure 9 illustrates the ground-level concentration versus height in a stable atmospheric condition for pollutants with varying leakage velocities; γ= 0.001, γ= 0.003, and γ= 0.006, expressed in k_w, when mesoscale winds are present. As shown in the graph, leakage velocity does not affect pollutant concentration. This is because the mixing height is taken as $624m$, and the point source is considered at $z = 20.5m$; hence, there is no effect of leakage velocity on the pollutant concentration in a stable atmospheric condition.

4. Conclusion

In this article, a two-dimensional numerical model for determining the concentration of pollutants emitted from the point source in the presence of a mesoscale with gravitational settling velocity is presented. To study how gravitational settling speed and removal mechanisms like dry deposition, wet deposition, and leakage velocity affect the concentration distribution of primary and secondary pollutants over an urban area is the most important part of the model. The results are examined pollutants in a neutral and stable atmosphere in an urban area. This model takes into account a more realistic form of variable wind and eddy diffusivity profiles. The effects of settling velocity and removal mechanisms near the point source are negligible. Such removal mechanisms significantly reduce the concentration of pollutants throughout the entire city region, with the exception of the area near the source. Also, the effect of gravitational settling velocity on primary and secondary pollutants is being noticed individually; the concentration of pollutants will decrease in the urban region as wet deposition increases with respect to height and distance for stable and neutral atmospheric conditions. Under stable atmospheric conditions, the concentration of primary pollutants is high in the surface region, while the concentration of secondary pollutants is high near the lower atmosphere. But under neutral atmospheric conditions, the concentration of pollutants reaches higher heights, thus reducing the concentration of pollutants at the ground surface. This phenomenon indicates the enhanced vertical diffusion of pollutants under neutral atmospheric conditions in the presence of mesoscale winds. We find that the leakage velocity of pollutants does not significantly affect the concentration distribution. This is because the source is located at ground level, and the top of the mixing layer, where the pollutants leak, is located far away from the source. Therefore, leakage has no effect on the concentration of pollutants. Thus, it can be concluded from air contamination's point of view that a stable atmospheric condition is unfavourable, but a neutral atmospheric situation is convenient for the lives of animal beings as well as plants in urban areas.

This study emphasizes how crucial it is to put into practice efficient air quality management techniques, including eco-environmentally friendly transit, environmentally friendly building techniques, and more stringent emission standards. Additionally, public awareness campaigns and community engagement campaigns are essential for promoting environmental accountability. By forming alliances between cities, businesses, and government organizations, we can create more all-encompassing strategies to fight air pollution. In the end, this cooperative strategy is crucial for producing sustainable urban ecosystems that are advantageous to present and future generations.

Data Availability

We do not have any research data outside the submitted manuscript file.

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