Numerical model of air pollutant emitted from an area source of primary and secondary pollutants with chemical reaction and gravitational settling with point source on the boundary

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Abstract

A Numerical model has been developed to study the effect of gravitational settling velocity and chemical reaction on the pollutant emitted from the point source on the boundary in an urban area. The study of secondary pollutants is very important because life period of secondary pollutants is longer than primary pollutants and it is more hazardous to human life and its environment. This numerical model permits the estimation of concentration distribution of primary and secondary pollutants in more realistic atmospheric conditions. The results of this model have been analysed for the dispersion of air pollutants in the urban area downwind and vertical direction for the stable and the neutral conditions of the atmosphere in the presence of large scale wind. The governing partial differential equations of primary and secondary pollutants with variable wind velocity and eddy diffusivity profiles are solved by using Crank-Nicolson implicit finite difference technique. The concentration of primary and secondary pollutants have been analysed for various removal mechanisms in both stable and neutral atmospheric conditions.

Key words: Air pollution model, Primary and Secondary pollutants, Chemical reaction, Crank-Nicolson implicit method, Variable wind velocity, Point Source.

Introduction

The dispersion of air pollutants from an area source into the atmosphere is governed by the processes of molecular diffusion and convection and depends upon the factors such as wind speed, temperature inversion, and dry deposition. The dispersion of atmospheric contaminants has become a global problem in the recent years due to rapid industrialization and urbanization. The toxic gases and small particles could accumulate in large quantities over urban areas, under certain meteorological conditions. This is one of the serious health hazards in many of the cities in the world. The dispersion of atmospheric contaminant has become a global problem in the recent years due to rapid industrialization and urbanization. The toxic gases and small particles could accumulate in large quantities over urban areas, under certain meteorological conditions. This is one of the serious health hazards in many of the cities in the world. An acute exposure to the elevated levels of particulate air pollution has been associated with the cases of increased cardiopulmonary mortality, hospitalization for respiratory diseases, exacerbation of asthma, decline in lung function, and restricted life activity. Small deficits in lung function, higher risk of chronic respiratory disease and increased mortality have also been associated with chronic exposure to respirable particulate air pollution [1]. Epidemiological studies have demonstrated a consistent increased risk for cardiovascular functions in relation to both short- and long-term exposure to the present-day concentrations of ambient particulate matter [2]. Exposure to the fine airborne particulate matter is associated with cardiovascular functions and mortality in older and cardiac patients [3]. Volatile organic compounds (VOCs), which are molecules typically containing 1–18 carbon atoms that readily volatilize from the solid or liquid state, are considered a major source of indoor air pollution and have been associated with various adverse health effects.
including infection and irritation of respiratory tract, irritation to eyes, allergic skin reaction, bronchitis, and dyspnea ([4], [5], [6]). Sometimes the pollutants appear in the form of larger particles on which the effect of gravitational acceleration cannot be neglected [7]. In this case the pollutants will come down to surface by means of settling velocity \( W_s \). Particles less than about 20 \( \mu m \) are treated as dispersing as gases, and effects due to their fall velocity are generally ignored. Particles greater than about 20 \( \mu m \) have appreciable settling velocity [8]. Particulate pollutants emitted into the atmosphere may be dislodges by a number of natural processes. One of the primary 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. Surface deposited pollutants may have a significant impact upon the local ecosystem as the pollutants enter into and travel through the biological pathways. As secondary pollutants are heavier, they may come down to the surface of the earth by means of gravitational settling.

The study of chemically reactive heavy admixture and its byproduct has generated considerable attention because of its severe harmful effects on human society and the environment. A part of an atmospheric contaminant and its byproduct might occur in the form of particles due to complexity of the atmosphere. These particles (or heavy admixture) and their movement by gravitational acceleration have significant impact on the local ecosystem. In the case of Bhopal gas leakage, for example, a thick coating of dust was found on the soil around 160 km of the leakage area. So, it is imperative to have a mathematical model to consider secondary pollutant due to chemical reaction and their removal by means of gravitational settling. Rudraiah et al [9] have studied the atmospheric diffusion model of secondary pollutants with settling velocity. Sujit Kumar Khan [10] presented a time dependent mathematical model of secondary air pollutant with instantaneous and delayed removal.

The diffusion and transport of effluents from various sources can be described through mathematical models, which essentially enable us to calculate concentrations of one or more species in space and time. The factors largely responsible for the dispersion include the physical and chemical nature of the effluents, prevailing meteorological conditions, location of the source and terrain characteristics. An ideal mathematical model should include all these aspects. However, in reality it is very difficult to develop such a model. Based on some approximations, it is possible to develop appropriate model for a specific scenario by considering most of these factors. Most applications of mathematical modeling on air pollution is to provide nomogram for determination of optimum stack height such that the human beings surrounding the area will be less affected by pollutant. Recent work has shown another more important aspect of mathematical modeling in providing structure and shape of green plants surrounding the model industry in a city to get minimum pollution effect by the outside people. This is known as green belt modeling. By the help of modeling we can predict concentration of accidental toxic release using mathematical models.

A numerical model for the atmospheric dispersion of an air pollutant emitted from an area source and a point source at the origin is described. An area source is an emission source, which is spread out over finite downwind distance. In the absence of removal mechanisms the Gaussian Plume model is the basic method used to calculate the air pollution concentration from point source ([11], [12], [13]). Use of the Gaussian plume model began to receive popularity when Pasquill [14] published his dispersion rates for plumes over open level terrain. Subsequently, Hilsmeier and Gifford [15] expressed these estimates in a slightly more convenient, although exactly equivalent, form and this is so called Pasquill-Gifford system for dispersion estimates has been widely used ever since. Runca and Sardei [16] have presented time dependent numerical model for air pollution due to point source. In this model the boundary conditions at the point source are expressed using a delta function and is approximated numerically by a one-step function having the width \( \Delta z \) (source width) i.e., the source is uniformly distributed on the vertical grid spacing centered at the point source. Arora [17] used Gaussian distribution for point source on the vertical grid spacing centered at the point source. In this paper the point source is considered arbitrary on the left boundary of city. The grid points may miss the source because the source is at an arbitrary point. In this case the grid points have to be taken on the source point. To overcome this one can think of the following two methods. One is to use Gaussian distribution for pollutants source at the initial line which is equivalent to the above point source and the other is distributing the point source to its neighboring two grid points. We have used the second procedure in this numerical model for air pollutants to take into account of a source at an arbitrary point on the left boundary of the city. We have equally distributed the point source to its neighboring two grid points on the boundary of the city. The fundamental approach to developing a diffusion model for area sources is to apply conservation of mass for a particular pollutant being emitted from an area source with appropriate boundary conditions. A comprehensive time dependent two-dimensional advection-diffusion numerical model of area source air pollution due to primary as well as secondary pollutants is presented by Venkatchalappa et al [18]. However this model does not gives the study of point source in the urban city. A numerical model [19] for a primary pollutant in the atmosphere by taking large and mesoscale wind velocities with removal mechanisms. However this model does not deal the study of secondary pollutant in the atmosphere.

In this paper we have developed an unsteady state advection diffusion model for an area source of primary and secondary pollutant with point source on the boundary. The pollutants are chemically reactive and there is a removal mechanism for primary and secondary pollutants. A point source is considered at the boundary and the area source is considered within the region of interest (city) and no source outside the city. The goal of this model is to determine the relative role of transport, diffusion, removal
mechanisms and chemical reaction. The study of secondary pollutants needs much attention since they have longer life periods and much hazardous than primary pollutants.

2. Model Development

The dispersion of chemically reactive pollutant concentration in a turbulent atmospheric medium using K-theory approach is usually described by the following equation [20],

\[ \frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial y} + W \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left( K_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial C}{\partial z} \right) - RC \]

where \( C \) is the pollutant concentration in air at any location \((x, y, z)\) 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 chemical reaction rate coefficient for the chemical transformation.

The physical problem consists of an area source of an urban city with finite down wind and infinite cross wind dimensions with the point source (industrial stack) on the \( z \)-axis with \( x = 0 \) and \( z = 20.5 \) meters. The grid points may miss the source because the source is at an arbitrary point. In this case the grid points have to be taken on the source point. To overcome this one can think of the following two methods. One is to use Gaussian distribution for pollutants source at the initial line which is equivalent to the above point source and the other is distributing the point source to its neighboring two grid points. We have used the second procedure in this numerical model for air pollutants to take into account of a source at an arbitrary point on the \( z \)-axis. We have equally distributed the point source to its neighboring two grid points on \( z \)-axis i.e. at the beginning of the urban city. We assume that the pollutants are emitted at a constant rate from uniformly distributed area source. The Physical description of the model is shown schematically in figure 1.

We intend to compute the concentration distribution both in the source region and source free region till the desired distance \( X_0 = 12000 \) meters in the downwind. We have taken the primary source strength \( Q = 1 \mu g m^{-2} s^{-1} \) at ground level from an area source and the mixing height is selected as 624 meters.

We assume that

1. Pollutants are chemically reactive, transformation process with first order chemical reaction rate.
2. A point source (industrial stack) at the beginning of the urban city.

In addition to the above assumptions, the lateral flux of pollutants along crosswind direction is assumed to be small i.e., \( V \frac{\partial C}{\partial y} \) and \( \frac{\partial}{\partial y} \left( K_y \frac{\partial C}{\partial y} \right) \rightarrow 0 \) where \( V \) is the velocity in the \( y \)-direction and \( K_y \) is the eddy-diffusivity coefficient in the \( y \) direction.

\[ \text{Horizontal advection is greater than horizontal diffusion for not too small values of wind velocity, i.e., meteorological conditions are far from stagnation. The horizontal advection by the wind dominates over horizontal diffusion, i.e., } U \frac{\partial C}{\partial x} \gg \frac{\partial}{\partial x} \left( K_x \frac{\partial C}{\partial x} \right) \text{, where } U \]

and \( K_x \) are the horizontal wind velocity and horizontal eddy diffusivity along \( x \) direction respectively. The governing partial differential equations and the corresponding boundary conditions for primary and secondary pollutant are described in the following sections.

2.1 Primary Pollutant

The basic governing equation of primary pollutant can be written as

\[ \frac{\partial C_p}{\partial t} + U(z) \frac{\partial C_p}{\partial x} = \frac{\partial}{\partial z} \left( K_z \frac{\partial C_p}{\partial z} \right) - kC_p \tag{1} \]

where \( C_p = C_p(x, z, t) \) is the ambient mean concentration of pollutant species, \( U \) is the mean wind speed in \( x \)-direction, \( K_z \) is the turbulent eddy diffusivity in \( z \)-direction, \( k \) is the first order chemical reaction rate coefficient of primary pollutant \( C_p \) and the term \( kC_p \) represents conversion of gaseous pollutants to particulate material as long as the process can be represented approximately by first-order chemical reaction.

We assume that the region of interest is free from pollution at the beginning of the emission. Thus the initial condition is

\[ C_p = 0 \text{ at } t = 0, \quad 0 \leq x \leq X_0 \text{ and } 0 \leq z \leq H \tag{2} \]

where \( X_0 \) is the length of desired domain of interest in the wind direction and \( H \) is the mixing height. We assume that there is a point source (industrial stack) on \( x = 0 \) i.e. either at the beginning or at the end of the urban city. The wind direction is assumed towards the city from the point source.

Thus

\[ C_p = Q \frac{\delta(x-h)}{\nu(x)} \text{ at } x = 0, \quad z = h \quad \forall t > 0 \tag{3} \]

where \( Q \) is the strength of the point source and \( z \) is taken as 20.5 meter.

We assume that the chemically reactive air pollutants are emitted at a constant rate from the ground level and they are removed from the atmosphere by ground absorption and settling velocity. Hence the corresponding boundary condition takes the form

\[ K_z \frac{\partial C_p}{\partial z} = \left\{ \begin{array}{ll} V_{dp} C_p - Q & \text{at } z = 0, \quad 0 \leq x \leq l \\ V_{dp} C_p & \text{at } z = 0, \quad l < x < X_0 \end{array} \right\} t > 0 \tag{4} \]

where, \( Q \) is the emission rate of primary pollutant species, \( l \) is the source length in the downwind direction, \( V_{dp} \) is the dry deposition velocity of primary pollutant. The pollutants are confined within the mixing height and there is no leakage across the top boundary of the mixing layer. Thus

\[ K_z \frac{\partial C_p}{\partial z} = 0 \text{ at } z = H, \quad x > 0, \quad \forall t \tag{5} \]

The governing basic equation and the boundary conditions for the concentration of secondary pollutant \( C_s \) is described below.

2.2 Secondary Pollutants

The basic governing equation for the secondary pollutant \( C_s \) is

\[ \frac{\partial C_s}{\partial t} + U(z) \frac{\partial C_s}{\partial x} = \frac{\partial}{\partial z} \left( K_z \frac{\partial C_s}{\partial z} \right) + W_s \frac{\partial C_s}{\partial y} + \mathcal{V} k C_p \tag{6} \]

where, \( W_s \) is the gravitational settling velocity of secondary pollutants and \( \mathcal{V} \) is the mass ratio of the secondary particulate species to the primary gaseous species which is being converted.

Thus the appropriate initial and boundary conditions on \( C_s \) are:

\[ C_s = 0 \text{ at } t = 0, \quad 0 \leq x \leq X_0 \text{ and } 0 \leq z \leq H \tag{7} \]

\[ C_s = 0 \text{ at } x = 0, \quad 0 \leq z \leq H \quad \text{ and } \forall t > 0 \tag{8} \]
Since there is no direct source for secondary pollutants, we have
\[ K_x \frac{\partial C_p}{\partial z} + W_z C_p = V_d C_p \text{ at } z = 0, \quad 0 \leq x \leq X_0, \quad \forall t > 0 \] (9)
\[ K_x \frac{\partial C_p}{\partial z} + W_z C_p = 0 \text{ at } z = H, \quad x > 0, \quad \forall t > 0 \] (10)
Where, \( V_d \) is the dry deposition velocity of secondary pollutant.

3. Meteorological Parameters
To solve the concentration of primary and secondary pollutant equations, we must know realistic form of the variable wind velocity and eddy diffusivity which are functions of vertical distance. The treatment of Eq. (1) and Eq. (6) mainly depends on the proper estimation of diffusivity coefficient and velocity profile of the wind near the ground/or lowest layers of the atmosphere. The meteorological parameters influencing eddy diffusivity and velocity profile are dependent on the intensity of turbulence, which is influenced by atmospheric stability. Stability near the ground is dependent primarily upon the net heat flux. In terms of boundary layer notation, the atmospheric stability is characterized by the parameter \( L \) [21], which is also a function of net heat flux among several other meteorological parameters.

3.1 Eddy diffusivity profiles
The common characteristics of \( K_x \) is that it has linear variation near the ground, a constant value at mid mixing depth and a decreasing trend as the top of the mixing layer is approached. Shir [22] gave an expression based on theoretical analysis of neutral boundary layer in the form
\[ K_x = 0.4 u_z z e^{-4z/H} \text{, where } H \text{ is the mixing height.} \] (11)
For stable condition, Ku et al., [23] used the following form of eddy-diffusivity,
\[ K_x = \frac{0.74}{\kappa} \frac{u_z}{z} \exp(-\eta) \] (12)
\[ b = 0.91, \quad \eta = \frac{z}{(L\sqrt{\mu})}, \quad \mu = u_v/|f/L| \]
The above form of \( K_x \) was derived from a higher order turbulence closure model which was tested with stable boundary layer data of Kansas and Minnesota experiments. Eddy-diffusivity profiles given by Eq. (11) and Eq. (12) have been used in this model for the neutral and the stable atmospheric conditions.

3.2 Wind Velocity Profiles
In order to incorporate realistic form of velocity profile which depends on Coriolis force, surface friction, geostrophic wind, stability characterizing parameter \( L \) and vertical height \( z \), we integrate the velocity gradient from \( z_0 \) to \( z + z_0 \) for the neutral and the stable conditions. So we obtain the following expressions for wind velocity [24].

In case of neutral stability with \( z < 0.1 \kappa (u_v/f) \), we get
\[ U = \frac{u_x}{\kappa} \ln \left( \frac{z + z_0}{z_0} \right) \] (13)
In case of stable flow with \( 0 < z / L < 1 \), we get
\[ U = \frac{u_x}{\kappa} \left[ \ln \left( \frac{z + z_0}{z_0} \right) + \frac{\alpha}{L} z \right] \] (14)
In case of stable flow with \( 1 < z / L < 6 \), we get
\[ U = \frac{u_x}{\kappa} \left[ \ln \left( \frac{z + z_0}{z_0} \right) + 5.2 \right] \] (15)
In the planetary boundary layer, above the surface layer, power law scheme has been employed.
\[ U = \left( u_{sl} - u_{st} \right) \left( \frac{x+z_{sl}}{H-z_{sl}} \right)^p + u_{sl} \] (16)
where \( u_{ge} \) is the geostrophic wind, \( u_{sl} \) is the wind at \( z_{sl} \), \( z_{sl} \) the top of the surface layer, \( H \) the mixing height and \( p \) is an exponent which depends upon the atmospheric stability. Jones et al., [25] suggested the values for the exponent \( p \), obtained from the measurements made from urban wind profiles, as follows:
\[ p = \begin{cases} 0.2 & \text{for neutral condition,} \\ 0.35 & \text{for slightly stable flow and,} \\ 0.5 & \text{for stable flow.} \end{cases} \]

4. Numerical Solution
We note that it is difficult to obtain the analytical solution for equations (1) and (6) because of the complicated form of wind speed and eddy diffusivity profiles considered in this model. Hence, we have used numerical method based on Crank-Nicolson finite difference scheme to obtain the solution. The detailed numerical method and procedure to solve the partial differential equations (1) and (6) is described below ([26, 27]). The dependent variable \( C_p \) is a function of the independent variables \( x, z \) and \( t \), i.e., \( C_p = C_p(x, z, t) \). First, the continuum region of interest is overlaid with or subdivided into a set of equal rectangles of sides \( \Delta x \) and \( \Delta z \), by equally spaced grid lines, parallel to \( z \) axis, defined by \( x_i = (i - 1)\Delta x, i = 1, 2, 3, \ldots \) and equally spaced grid lines parallel to \( x \) axis, defined by \( z_j = (j - 1)\Delta z, j = 1, 2, 3, \ldots \) respectively. Time is indexed such that \( t_n = n\Delta t, n = 0, 1, 2, 3, \ldots \) where \( \Delta t \) is the time step. At the intersection of grid lines, i.e. grid points, the finite difference solution of the variable \( C_p \) is defined. The dependent variable \( C_p(x, z, t) \) is denoted by \( C_{p_{ij}} \), where \( (x_i, z_j) \) and \( t_n \) indicate the \((x, z)\) value at a node point \((i, j)\) and \( t \) value at time level \( n \) respectively.

We employ the implicit Crank-Nicolson scheme to discretize the equation (1). The derivatives are replaced by the arithmetic average of its finite difference approximations at \( n \)th and \((n + 1)\)th time steps. Then equation (1) at the grid points \((i, j)\) and time step \( n + 1/2 \) can be written as
\[ \frac{\partial C_{p_{ij}}}{\partial t} \bigg|_{n+1/2} + \frac{1}{2} \left[ U(x) \frac{\partial C_{p_{ij}}}{\partial x} \right]_{n+1/2} + \frac{1}{2} \left[ U(x) \frac{\partial C_{p_{ij}}}{\partial x} \right]_{n-1/2} = \frac{\partial}{\partial z} \left( K_x(z) \frac{\partial C_{p_{ij}}}{\partial z} \right)_{n+1/2} + \frac{1}{2} \left( K_x(z) \frac{\partial C_{p_{ij}}}{\partial z} \right)_{n-1/2} \] (17)
We use \( \frac{\partial C_{p_{ij}}}{\partial t} \bigg|_{n+1/2} = \frac{C_{p_{ij}}^{n+1} - C_{p_{ij}}^{n-1}}{2\Delta t} \) in this analog is actually the same as the first order correct analog used for the forward difference equation, but is now second order-correct, since it is used to approximate the
derivative at the point \((x_i, z_j, t_{n+1/2})\). We use the backward differences for the advective term for this model. Therefore we use

\[
U(x, z) \frac{\partial C}{\partial x} = \frac{C_{ij}^{n+1} - C_{ij}^{n}}{\Delta x}
\]

(18)

\[
U(x, z) \frac{\partial C}{\partial x} = \frac{C_{ij}^{n+1} - C_{ij}^{n}}{\Delta x}
\]

(19)

also, for the diffusion term, we use the second order central difference scheme

\[
\frac{\partial}{\partial x} \left( K(x) \frac{\partial C}{\partial x} \right) = \frac{K_{ij}^{n} \frac{C_{ij}^{n+1} - C_{ij}^{n}}{2\Delta x} - K_{ij}^{n+1} \frac{C_{ij}^{n} - C_{ij}^{n+1}}{2\Delta x}}{1}
\]

(20)

By substituting equations (18) to (21) in equation (17) and rearranging the terms we get the finite difference equations for the primary pollutant \(C_p\) in the form

\[
A_i C_{p_{ij}}^{n+1} + B_i C_{p_{ij}}^{n} + D_i C_{p_{ij}}^{n+1} + E_i C_{p_{ij}}^{n} = F_i C_{p_{ij}}^{n+1} + G_i C_{p_{ij}} + M_i C_{p_{ij}}^{n} + N_i C_{p_{ij}}^{n+1}
\]

(22)

for each \(i = 2,3,4,\ldots,imax\) and \(j = 2,3,4,\ldots,jmax\) for \(j = 2,3,4,\ldots,jmax\) and \(n = 0,1,2,\ldots\),

\[
A_i = -U_j \frac{\Delta t}{2\Delta x} \quad F_i = U_j \frac{\Delta t}{2\Delta x}
\]

\[
B_i = -\left[ \frac{\Delta t}{4(\Delta x)^2} \right] (K_j + K_{j-1})
\]

\[
G_i = \left[ \frac{\Delta t}{4(\Delta x)^2} \right] (K_j + K_{j-1})\quad E_i = -\left[ \frac{\Delta t}{4(\Delta x)^2} \right] (K_j + K_{j+1})
\]

\[
N_i = \frac{\Delta t}{4(\Delta x)^2} (K_j + K_{j+1})
\]

\[
D_i = 1 + U_j \frac{\Delta t}{2\Delta x} + \frac{\Delta t}{4(\Delta x)^2} (K_{j+1} + 2K_j + K_{j-1}) - \frac{\Delta t}{2} (k)
\]

\[
M_j = 1 - U_j \frac{\Delta t}{2\Delta x} - \frac{\Delta t}{4(\Delta x)^2} (K_{j+1} + 2K_j + K_{j-1}) - \frac{\Delta t}{2} (k)
\]

\(i\) for \(j = 2,3,4,\ldots,jmax\) and \(i = 1,2,\ldots,imax\) \(\cdots \) \(imaxX_0\) for \(j = 1, 2, 3, 4, \ldots,\).

Equation (22) is true for interior grid points. At the boundary grid points we have to use the boundary conditions (2) to (5). The initial and boundary conditions can be written as

\[
C_{0_{ij}} = 0 \quad for \quad j = 1, 2, \ldots, j_{max}
\]

\[
i = 1, 2, \ldots, imax \ldots imaxX_0
\]

\[
C_{0_{ij}}^{n+1} = \frac{Q_i}{2u(j)} \quad for \quad i = 1 \quad and \quad j = 21, 22, \quad n = 0, 1, 2, \ldots
\]

\[
(1 - V_{dp} \frac{\Delta t}{K_j}) C_{0_{ij}}^{n+1} - C_{0_{ij}}^{n+1} = -\frac{\Delta x}{K_j} \quad for \quad j = 1, \quad i = 2, 3, 4, \ldots, imax \ldots imaxX_0 \quad and \quad n = 0, 1, 2, 3, \ldots
\]

\[
(1 - V_{dp} \frac{\Delta t}{K_j}) C_{0_{ij}}^{n+1} - C_{0_{ij}}^{n+1} = 0 \quad for \quad j = 1, \quad i = imax(1 + 1) \ldots imaxX_0 \quad and \quad n = 0, 1, 2, 3, \ldots
\]

\[
C_{0_{ij}}^{n+1} = 0 \quad for \quad j = j_{max}, \quad i = 2, 3, 4, \ldots, imax \ldots imaxX_0
\]

(23)

The above system of equations (22) to (26) has a tridiagonal structure and is solved by Thomas Algorithm [28]. The ambient air concentration of primary pollutants (gaseous) is obtained for various atmospheric conditions and the values of dry deposition, wet deposition and chemical reaction rate are constant. Similarly the finite difference equations for the secondary pollutant \(C_s\) can be written as

\[
A_i C_{s_{ij}}^{n+1} + B_i C_{s_{ij}}^{n} + D_i C_{s_{ij}}^{n+1} + E_i C_{s_{ij}}^{n} = F_i C_{s_{ij}}^{n+1} + G_i C_{s_{ij}}^{n} + M_i C_{s_{ij}}^{n} + N_i C_{s_{ij}}^{n+1}
\]

(27)

for \(i = 2,3,4,\ldots,imax\) and \(j = 2,3,4,\ldots,jmax - 1\)

The initial and boundary conditions on secondary pollutant \(C_s\) are

\[
C_{s_{ij}}^{0} = 0 \quad for \quad j = 1, 2, \ldots, j_{max},
\]

\[
i = 1, 2, \ldots, imax \ldots imaxX_0
\]

\[
C_{s_{ij}}^{n+1} = 0 \quad for \quad i = 1, \quad j = 1, 2, \ldots, j_{max}, \quad n = 0, 1, 2, \ldots
\]

\[
(1 + V_{ds} + W_{ds}) \frac{\Delta t}{K_j} C_{s_{ij}}^{n+1} - C_{s_{ij}}^{n+1} = 0 \quad for \quad j = 1, \quad i = 2,3,4,\ldots,imax \ldots imaxX_0
\]

(28)

\[
C_{s_{ij}}^{n+1} = 0 \quad for \quad j = j_{max}, \quad i = 2,3,4,\ldots,imax \ldots imaxX_0
\]

(29)

\[
C_{s_{ij}}^{n+1} + \frac{W_{ds}}{K_j} \Delta x - 1 \quad C_{s_{ij}}^{n+1} = 0 \quad for \quad j = j_{max}, \quad i = 2,3,4,\ldots,imax \ldots imaxX_0
\]

(30)

\[
C_{s_{ij}}^{n+1} = \frac{W_{ds}}{K_j} \Delta x
\]

(31)

Where,

\[
A_i = -U_j \frac{\Delta t}{2\Delta x} \quad F_i = U_j \frac{\Delta t}{2\Delta x}
\]

\[
B_j = -\left[ \frac{\Delta t}{4(\Delta x)^2} \right] (K_j + K_{j-1}) - W_j \frac{\Delta t}{2\Delta x}
\]

\[
G_j = \left[ \frac{\Delta t}{4(\Delta x)^2} \right] (K_j + K_{j-1}) - W_j \frac{\Delta t}{2\Delta x}
\]

\[
E_j = -\left[ \frac{\Delta t}{4(\Delta x)^2} \right] (K_j + K_{j+1})
\]

\[
N_j = \frac{\Delta t}{4(\Delta x)^2} (K_j + K_{j+1})
\]

\[
D_j = 1 + U_j \frac{\Delta t}{2\Delta x} + W_j \frac{\Delta t}{2\Delta x} - \frac{\Delta t}{4(\Delta x)^2} (K_{j+1} + 2K_j + K_{j-1}) + \frac{\Delta t}{2} (k)
\]

\[
M_j = 1 - U_j \frac{\Delta t}{2\Delta x} + W_j \frac{\Delta t}{2\Delta x} - \frac{\Delta t}{4(\Delta x)^2} (K_{j+1} + 2K_j + K_{j-1}) - \frac{\Delta t}{2} (k)
\]

The model has been solved using Crank-Nicolson implicit finite difference technique, which is unconditionally stable. Consistency, stability and convergence criteria have been tested for the numerical scheme used in this model. We have considered grid size 75 meters along x direction and 1 meter along z direction. For the grid-independence study we have computed concentration for 40 x 156, 80 x 312, 160 x 624 and 240 x 1248 grids and analysed. The analysis reveals that concentration for 40 x 156 and 80 x 312 grids differ considerably against those on 160 x 624 grids. Further, there is no perceptible change occurring on 240 x 1248 grids from that of 160 x 624 grids. It is therefore reasonable to assume that the solution obtained on 160 x 624 grids is an independent solution. The concentration distribution is computed both in the source region and source free region till the desired distance \(X_0=12\) kms. The system of equations (22) to (26) has tridiagonal structure but is coupled with equations (27) to (31). First, the system of equations (22) to (26) is solved for \(C_{p_{ij}}\), which is independent of the system (27) to (31) at every time step \(n\). This result at every time step is used in equations (27) to (31). Then the system of equations (27) to (31) is solved for \(C_{s_{ij}}\) at the same time step \(n\). Both the systems of
equations are solved using Thomas algorithm for tridiagonal equations (22) to (26) and (27) to (31). Thus, the solutions for primary and secondary pollutant concentrations are obtained.

5. Results and Discussions
A numerical model for the computation of the ambient air concentration of pollutant along the down-wind and the vertical directions emitted from an area source along with the point source on the boundary (\(x = 0\)) with the removal mechanism and the transformation process has been presented. The numerical model permits the estimation of the concentration distribution for more realistic meteorological conditions. An area source is an emission source which is spread out over the surface of the city with finite down wind and infinite cross wind dimensions where major source being vehicular exhausts due to traffic flow. We have taken a point source arbitrarily at the beginning of the city. The grid lines are not passing through the point source and it is difficult to adopt point source in numerical method. Therefore we have distributed the concentration of point source equally to its two neighboring grid points.

Figure 1. Physical layout of the model

![Figure 1](image1)

Figure 2. Concentration of secondary pollutant with respect to height for different distances with varying values of dry position velocity for stable case.

![Figure 2](image2)

Figure 3. Concentration of secondary pollutant with respect to height for different distances with varying values of dry position velocity for neutral case.

![Figure 3](image3)

Figure 4. Concentration of primary pollutant with respect to height for different distances with different values of chemical reaction rate coefficient for stable case.

![Figure 4](image4)
Figure 5. Concentration of primary pollutant with respect to height for different distances with different values of chemical reaction rate coefficient for Neutral case.

Figure 6. Concentration of secondary pollutant with respect to height for different distances with different values of gravitational settling velocity for Stable case.

Figure 7. Concentration of secondary pollutant with respect to height for different distances with different values of gravitational settling velocity for Neutral case.

Figure 8. Concentration contours of primary pollutant for (a) stable case (b) Neutral atmospheric conditions.
In figure 7, we observe that the concentration of the secondary pollutant decreases. Again the concentration increases up to the height 20.5 m and then it decreases and reaches zero at 35 m height. When the value of the dry deposition velocity increases to 0.25, the ground level concentration of the secondary pollutant becomes zero at the beginning. The concentration increases as the distance increases up to 20.5 m height. It is observed that the concentration of the secondary pollutant decreases as the distance increases in both the stable and the neutral atmospheric conditions. In the neutral case, the ground level concentration of the secondary pollutant is low as compared to that in the stable case when \( V_d = 0 \). But when \( V_d = 0.25 \), the concentration increases up to 20.5 m height then it decreases and reaches zero around 110 m height. Therefore comparing to the stable case, the concentration of the secondary pollutant reaches zero at the greater heights in the neutral case. Also as the value of the dry deposition velocity increases, there is no much effect of the secondary pollutant near the point source for the stable and the neutral atmospheric conditions. This behavior is because the dry deposition is introduced at the ground level and increase in the value of the dry deposition velocity is too smaller when compared to the continuous emission of the point source strength.

Figures 4 and 5 demonstrates the concentration of the primary pollutant with respect to height for different values of distances with varying values of chemical reaction rate coefficients for the stable and the neutral atmospheric conditions. Since we have considered the point source at \( x = 0 \) and at \( z = 20.5 \text{ m} \), the concentration of the pollutant is maximum around 20.5 m height in both the atmospheric conditions. As the distance increases, the concentration of the primary pollutant decreases due to removal mechanisms. In the stable atmospheric condition, near the ground level the initial concentration of pollutant is around 0.002 \( \mu \text{g} / \text{m}^3 \) and then it slowly decreases. It reaches zero around 10 m height and then again increases up to 20.5 m height. The concentration decreases rapidly above 20.5 m height and reaches zero around 35 m height in the stable case. From figure 6, it is understood that as the value of gravitational settling velocity increases the concentration of the pollutant decreases. The similar effect is observed in the neutral atmospheric condition. But the concentration of the pollutant reaches zero around 100 m height in the neutral case. This behavior is because the neutral atmospheric condition enhances the vertical diffusion of the pollutant to the greater heights.

Figures 6 and 7 demonstrates the concentration of the secondary pollutant with respect to height for different values of distances with varying values of gravitational settling velocity for the stable and the neutral atmospheric conditions. Since we have considered the point source at \( x = 0 \) and at \( z = 20.5 \text{ m} \), the concentration of the pollutant is maximum around 20.5 m height in both the atmospheric conditions. As the distance increases, the concentration of the secondary pollutant decreases as the distance increases in both the stable and the neutral atmospheric conditions. It is noted that the concentration of the primary pollutant attains peak value at the downwind end of the source region. Whereas, the concentration of the secondary pollutant attains its peak value at the outside of the city region in the downwind direction. The secondary pollutants are different values of distances with varying values of gravitational settling velocity for the stable and the neutral atmospheric conditions.
concentrated away from the ground and are spread out evenly throughout the region. This is due to the chemical reaction taking place in the atmosphere converting the primary into secondary pollutants. The magnitude of the concentration of the primary and the secondary pollutants is higher in the stable case and lower in the neutral case. This is because the neutral atmosphere carries the pollutants to the greater heights and thus the concentration is less.

6. Conclusions
A time dependent two dimensional mathematical model of air pollution due to area source along with a point source on the boundary is presented to simulate the dispersion processes of gaseous air pollutants in an urban area. The numerical model computes the ambient air concentration emitted from an urban area source and the point source, undergoing various removal mechanisms and transformation process. The model takes into account the realistic form of variable wind speed and eddy diffusivity profiles, which are the functions of vertical height, frictional velocity, terrain categories, geostrophic wind and several other stability dependent parameters.

The results of this model have been analysed for the dispersion of air pollutants in the urban area downwind and vertical direction for stable and neutral conditions of atmosphere. The ground level concentration of primary pollutants attains peak value at the downwind end of the source region. Whereas, the concentration of the secondary pollutant attains its peak value at the source free region in the downwind direction. The model also predicts that the ground level concentration of the secondary pollutant at a particular downwind distance is always higher in the stable atmosphere condition than that in the neutral atmospheric condition. There is negligible effect of chemical reaction rate coefficient, dry deposition velocity and gravitational settling velocity near the point source. These removal mechanisms play an important role in reducing the concentration of the pollutants everywhere in the city region except near the point source. Also in the case of the stable atmospheric condition the maximum concentration of the pollutants is observed at the ground level. Same phenomenon is noticed in the neutral condition but the magnitude of concentration in the neutral condition is comparatively less than that of the stable atmospheric condition. The present study shows that the stable condition is an unfavorable condition for the animals and plants from air pollution point of view.

References
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