

TIME DEPENDENT TWO DIMENSIONAL MATHEMATICAL MODEL OF AIR POLLUTION DUE TO AREA SOURCE OF PRIMARY AND SECONDARY POLLUTANTS WITH TRANSFORMATION PROCESSES, GRAVITATIONAL SETTLING AND LEAKAGE VELOCITY

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1. Introduction

Atmospheric diffusion models are being widely used to study the complicated relationships between air quality and emission sources as a function of meteorological and source conditions. The dispersion of air pollutant from an area source into the atmosphere is governed by the process of molecular diffusion and convection and depends upon the factors such as wind speed, temperature inversion, dry deposition etc. 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 [4-6]. Principal sources of air-pollution are industries, automobiles and household indoor pollutants. The life cycle of pollutants includes emission, dispersion and removal by dry deposition on the surface of the earth. One of the most effective ways to assess the impact of various pollutants on the environment of a particular area is through mathematical modeling. Mathematical models are important tools and can play a crucial role in the methodology developed to predict air quality.

Mathematical models used in the air pollution field range from simple empirical models to very complex numerical models. In general, these models are based on the equation governing the pollutant concentration with the physical principles of mass conservation. The governing equation is solved with the initial and boundary conditions for a given source emission rate. However, due to the complexity of the atmospheric circulation patterns in the urban areas and inadequate data availability, various empirical approaches have been sought for practical purposes, based on either statistical theory, or observed features, or some time even arbitrary assumptions.

There are numerous models to deal with the dispersion of pollutants emitted from point source and area sources [7-9]. In these models eddy-diffusivity and velocity profile are all considered as constant. A realistic variation form of eddy – diffusivity profile has been considered in the case of time dependent one dimensional model in the absence of removal mechanism [10]. Gradient transfer hypothesis reveals that the eddy – diffusivity K_z is a function of vertical height z and several meteorological parameters including stability length L . An analytical time dependent one dimensional model for the region above the surface layer considering two sources, one continuous in surface layer and the other one instantaneous at a particular height above the surface layer was presented [11]. This model considers atmospheric parameters which are variable wind speed, atmospheric stability, surface roughness, mixing height and diffusivity. A

time dependent mathematical model of an air pollutant with instantaneous and delayed removal was developed [12]. In these models eddy-diffusivity and velocity profiles are all considered constant. The mathematical model with chemically reactive pollutants without considering mesoscale wind was discussed [13; 14]. A two dimensional numerical model with mesoscale wind was developed [15]. But they have not considered the effect of the gravitational settling velocity and a point source on the boundary.

In this paper we formulate a mathematical model to study the effect of removal mechanisms namely leakage of pollutants through the top of the boundary layer, wet deposition due to rainout or washout, dry deposition and gravitational settling on the concentration distribution of primary and secondary pollutants. In the model, we consider transformation of primary pollutant to secondary pollutants through chemical reaction. From the practical point of view there may be leakage of some amount of pollutants through the top of the boundary (mixing height). In practice, the height of surface layer is a function of drag coefficient, geotropic wind and total turning of its direction in the friction layer. This effect has been taken into account in this model.

2. Model Development

The mathematical formulation of the area source air pollution model is based on the conservation of mass equation which describes advection, turbulent diffusion, chemical reaction, removal mechanisms and emission of pollutants. It is assumed that the terrain is flat, the wind velocity is a function of height ie $u = u(z)$. The equation for the concentration of pollutants can be expressed as follows

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

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.

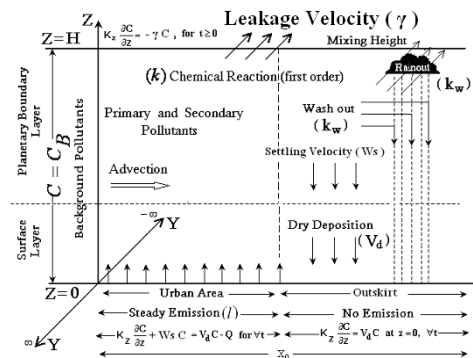


FIGURE 1. Physical layout of the model.

The physical problem consists of an area source which is spread out over the surface of the city with finite down wind and infinite cross wind dimensions. We assume that the pollutants are emitted at a constant rate from uniformly distributed area source. We have considered the source region within the urban centre $(0 \leq x \leq l)$ which extends up to $l = 6$ km from the origin and source free region beyond l $(l \leq x \leq X_0)$. We compute the concentration distribution till the desired down wind distance $X_0 = 12$ km i.e. $0 \leq x \leq X_0$. The pollutants are considered to be chemically reactive and form secondary pollutants by means of first order chemical conversion. We assume that the pollutants undergo the removal mechanisms, such as dry deposition, wet deposition, gravitational settling velocity and leakage through the upper boundary. The Physical description of the model is shown schematically in figure 1.

Further we assume that

- ❖ Pollutants leak through the top of the boundary i.e we consider leakage velocity at the top boundary.
- ❖ Pollutants are chemically reactive, transformation process with first order chemical reaction rate.

The governing partial differential equation for primary pollutant is described below.

a. Primary Pollutant

The basic governing equation of primary pollutant can be written as

$$\frac{\partial C_p}{\partial t} + U(z) \frac{\partial C_p}{\partial x} = \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) - (k + k_{wp}) C_p, \quad (1)$$

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_{wp} is the first order rainout/washout coefficient of primary pollutant C_p and k is the first order chemical reaction rate coefficient of primary pollutant C_p .

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

$$C_p = 0 \quad \text{at } t = 0, \quad 0 \leq x \leq X_0 \quad \text{and} \quad 0 \leq z \leq H, \quad (2)$$

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 no background pollution of concentration entering at $x = 0$ into the domain of interest. Thus

$$C_p = 0 \quad \text{at } x = 0, \quad 0 \leq z \leq H \quad \text{and} \quad \forall t > 0. \quad (3)$$

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

$$K_z \frac{\partial C_p}{\partial z} + W_s C_p = \begin{cases} V_{dp} C_p - Q & \text{at } z = 0 \quad 0 < x \leq l \\ V_{dp} C_p & \text{at } z = 0 \quad l < x \leq X_0 \end{cases} \quad \forall t > 0, \quad (4)$$

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 and W_s is the gravitational settling velocity of primary pollutants. Here we have considered emission of pollutants within a distance of l which is a city distance in the x -direction i.e the pollutants are assumed to be emitted within the city. The pollutants are confined within the mixing height with some amount of leakage across the top boundary of the mixing layer. Thus

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

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

b. Secondary Pollutants

The basic governing equation for the secondary pollutant C_s is

$$\frac{\partial C_s}{\partial t} + U(z) \frac{\partial C_s}{\partial x} = \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_s}{\partial z} \right) - k_{ws} C_s + V_g k C_p, \quad (6)$$

where, k_{ws} is the first order wet deposition coefficient of secondary pollutants and V_g 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:

$$C_s = 0 \quad \text{at } t = 0, \quad \text{for } 0 \leq x \leq X_0 \quad \text{and} \quad 0 \leq z \leq H, \quad (7)$$

$$C_s = 0 \quad \text{at } x = 0, \quad \text{for } 0 \leq z \leq H \quad \text{and} \quad \forall t > 0. \quad (8)$$

Since there is no direct source for secondary pollutants, we have

$$K_z \frac{\partial C_s}{\partial z} + W_{gs} C_s = V_{ds} C_s \quad \text{at } z = 0, \quad 0 \leq x \leq X_0, \quad \forall t > 0, \quad (9)$$

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

where V_{ds} is the dry deposition velocity, γ_s is the leakage velocity at the top of the boundary and W_{gs} is the gravitational settling velocity of the secondary pollutant C_s .

3. Meteorological Parameters

To solve equations (1) and (6) we must know realistic form of the variable wind velocity and eddy diffusivity which are functions of vertical distance. The treatment of equations (1) and (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 , which is also a function of net heat flux among several other meteorological parameters [16]. It is defined by

$$L = -\frac{u_*^3 \rho c_p T}{\kappa g H_f}, \tag{11}$$

where u_* is the friction velocity, H_f the net heat flux, ρ the ambient air density, c_p the specific heat at constant pressure, T the ambient temperature near the surface, g the gravitational acceleration and κ the Karman's constant ≈ 0.4 . $H_f < 0$ and consequently $L > 0$ represents stable atmosphere, $H_f > 0$ and $L < 0$ represent unstable atmosphere and $H_f = 0$ and $L \rightarrow \infty$ represent neutral condition of the atmosphere.

The friction velocity u_* is defined in terms of geostrophic drag coefficient c_g and geostrophic wind u_g such that

$$u_* = c_g u_g, \tag{12}$$

where c_g is a function of the surface Rossby number $R_0 = u_* / fz_0$, where f is the Coriolis parameter due to earth's rotation and z_0 is the surface roughness length. The value of c_{gn} , the drag coefficient for a neutral atmosphere is in the following form [24].

$$c_{gn} = \frac{0.16}{[\log_{10}(R_0) - 1.8]}. \tag{13}$$

The effect of thermal stratification on the drag coefficient can be accounted through the relations: $c_{gus} = 1.2 c_{gn}$ for unstable flow,

$c_{gs} = 0.8 c_{gn}$ for slightly stable flow and

$c_{gs} = 0.6 c_{gn}$ for stable flow.

In order to evaluate the drag coefficient, the surface roughness length z_0 may be computed according to the relationship developed [17]. i.e., $z_0 = \frac{\overline{Ha}}{2\overline{A}}$, where \overline{H} is the effective height of roughness elements, a is the frontal area seen by

the wind and \overline{A} is the lot area (i.e., the total area of the region divided by the number of elements).

Finally, in order to connect the stability length L to the Pasquill stability categories, it is necessary to quantify the net radiation index. The following values of H_f (Table I) for urban area [18].

Table I: Net heat flux H_f ($langley \text{ min}^{-1}$)

Net radiating index	:	4.0	3.0	2.0	1.0	0.0	-1.0	-2.0
Net heat flux H_f	:	0.24	0.18	0.12	0.06	0.0	-0.03	-0.06

3.1 Eddy diffusivity profiles

Following gradient transfer hypothesis and dimensional analysis, the eddy viscosity, K_M , is defined as

$$K_M = \frac{u_*^2}{\partial U / \partial z}. \tag{14}$$

Using similarity theory [16], the velocity gradient may be written as

$$\frac{\partial U}{\partial z} = \frac{u_* \phi_M}{\kappa z}. \tag{15}$$

Substituting this in the equation (14), we have

$$K_M = \frac{\kappa u_* z}{\phi_M}. \tag{16}$$

The function ϕ_M depends on z/L , where L is Monin-Obukhov stability length parameter. It is assumed that the surface layer terminates at $z = 0.1\kappa \frac{u_*}{f}$ for neutral stability. For stable conditions, surface layer extends to $z = 6L$.

For the neutral stability condition with $z < 0.1\kappa \frac{u_*}{f}$ (within surface layer) we have

$$\phi_M = 1 \quad \text{and} \quad K_M = \kappa u_* z. \quad (17)$$

For the stable atmospheric flow with $0 < z/L < 1$ we get

$$\phi_M = 1 + \frac{\alpha}{L} z \quad (18)$$

and

$$K_M = \frac{\kappa u_* z}{1 + \frac{\alpha}{L} z}. \quad (19)$$

For the stable atmospheric flow with $1 < z/L < 6$ we get

$$\phi_M = 1 + \alpha \quad \text{and} \quad K_M = \frac{\kappa u_* z}{1 + \alpha}. \quad (20)$$

It has been shown that $\alpha = 5.2$ [23]. In the PBL (planetary boundary layer), where z/L is greater than the limits considered above and $z > 0.1\kappa \frac{u_*}{f}$, we have, the following expressions for K_M .

For the neutral atmospheric stability condition with $z > 0.1\kappa \frac{u_*}{f}$ we get

$$K_M = 0.1\kappa^2 \frac{u_*^2}{f}. \quad (21)$$

For the stable atmospheric flow with $z > 6L$, upto H , the mixing height we have

$$K_M = \frac{6\kappa u_* L}{1 + \alpha}. \quad (22)$$

Equations (16) to (22) give the eddy viscosity for the conditions needed for the model.

The common characteristics of K_z 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. An expression based on theoretical analysis of neutral boundary layer in the following form [19].

$$K_z = 0.4u_* z e^{-4z/H}, \quad (23)$$

where H is the mixing height.

For stable condition, the following form of eddy-diffusivity are used [20].

$$K_z = \frac{\kappa u_* z}{0.74 + 4.7 z/L} \exp(-b\eta), \quad (24)$$

$$b = 0.9L, \quad \eta = z/(L\sqrt{\mu}), \quad \mu = u_* / |fL|.$$

The above form of K_z 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 equation (23) and (24) have been used in this model developed for neutral and stable atmospheric conditions.

3.2 Wind Velocity Profiles

In order to incorporate some what realistic form of velocity profile in our model which depends on Coriolis force, surface friction, geostrophic wind, stability characterizing parameter L and vertical height z , we integrate equation (15) from z_0 to $z + z_0$ for neutral and stable conditions. So we obtain the following expressions for wind velocity.

In case of neutral atmospheric stability condition with $z < 0.1\kappa \frac{u_*}{f}$ we get

$$U = \frac{u_*}{\kappa} \ln \left(\frac{z + z_0}{z_0} \right). \tag{25}$$

In case of stable atmospheric flow with $0 < \frac{z}{L} < 1$ we get

$$U = \frac{u_*}{\kappa} \left[\ln \left(\frac{z + z_0}{z_0} \right) + \frac{\alpha}{L} z \right]. \tag{26}$$

In case of stable atmospheric flow with $1 < \frac{z}{L} < 6$ we get

$$U = \frac{u_*}{\kappa} \left[\ln \left(\frac{z + z_0}{z_0} \right) + 5.2 \right]. \tag{27}$$

In the planetary boundary layer, above the surface layer, power law scheme has been employed.

$$U = (u_g - u_{sl}) \left(\frac{z - z_{sl}}{H - z_{sl}} \right)^p + u_{sl}, \tag{28}$$

where, u_g is the geostrophic wind, u_{sl} 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. The values for the exponent p , obtained from the measurements made from urban wind profiles are as follows [21].

$$p = \begin{cases} 0.2 & \text{for neutral conditions} \\ 0.35 & \text{for slightly stable flow} \\ 0.5 & \text{for stable flow} \end{cases}.$$

Wind velocity profiles given by equations (25) – (28) are used in this model [18].

4. Numerical Method

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 governing partial differential equation (1) is

$$\frac{\partial C_p}{\partial t} + U(z) \frac{\partial C_p}{\partial x} = \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) - (k + k_{vp}) C_p.$$

The spatial derivatives are replaced by the arithmetic average of its finite difference approximations at the n^{th} and $(n + 1)^{th}$ time steps and we replace the time derivative with a forward difference with time step $n + 1/2$. Then equation (1) at the grid points (i, j) and time step $n + 1/2$ can be written as

$$\begin{aligned} \frac{\partial C_p}{\partial t} \Big|_{ij}^{n+\frac{1}{2}} + \frac{1}{2} \left[U(z) \frac{\partial C_p}{\partial x} \Big|_{ij}^n + U(z) \frac{\partial C_p}{\partial x} \Big|_{ij}^{n+1} \right] &= \frac{1}{2} \left[\frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^n + \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^{n+1} \right] \\ - \frac{1}{2} (k + k_{vp}) (C_{pij}^n + C_{pij}^{n+1}), \quad i = 1, 2, \dots, \quad j = 1, 2, \dots \end{aligned} \tag{29}$$

Using

$$\frac{\partial C_p}{\partial t} \Big|_{ij}^{n+\frac{1}{2}} = \frac{C_{pij}^{n+1} - C_{pij}^n}{\Delta t}, \tag{30}$$

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

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

$$\frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^n = \frac{1}{2(\Delta z)^2} \left[(K_{j+1} + K_j)(C_{pij+1}^n - C_{pij}^n) - (K_j + K_{j-1})(C_{pij}^n - C_{pij-1}^n) \right] \quad (33)$$

Equation (29) can be written as

$$A_j C_{pi-i}^{n+1} + B_j C_{pij-1}^{n+1} + D_j C_{pij}^{n+1} + E_j C_{pij+1}^{n+1} = F_j C_{pi-i}^n + G_j C_{pij-1}^n + M_j C_{pij}^n + N_j C_{pij+1}^n, \quad (34)$$

for each $i = 2, 3, 4, \dots, i_{max} l \dots \dots i_{max} X_0$, $j = 2, 3, 4, \dots, j_{max} - 1$ and $n = 0, 1, 2, 3, \dots$

Here

$$A_j = -U_j \frac{\Delta t}{2\Delta x}, \quad F_j = U_j \frac{\Delta t}{2\Delta x}, \quad B_j = -\frac{\Delta t}{4\Delta z^2} (K_j + K_{j-1}), \quad G_j = \frac{\Delta t}{4\Delta z^2} (K_j + K_{j-1}),$$

$$E_j = -\frac{\Delta t}{4\Delta z^2} (K_j + K_{j+1}), \quad N_j = \frac{\Delta t}{4\Delta z^2} (K_{j+1} + K_j),$$

$$D_j = 1 + U_j \frac{\Delta t}{2\Delta x} + \frac{\Delta t}{4\Delta z^2} (K_{j+1} + 2K_j + K_{j-1}) + \frac{1}{2} (k + k_{wp}),$$

$$M_j = 1 - U_j \frac{\Delta t}{2\Delta x} - \frac{\Delta t}{4\Delta z^2} (K_{j+1} + 2K_j + K_{j-1}) - \frac{1}{2} (k + k_{wp}).$$

and $i_{max} l$ and $i_{max} X_0$ are the i values at $x = l$ and X_0 respectively and j_{max} is the value of j at $z = H$.

The initial condition (2) can be written as

$$C_{pij}^0 = 0 \text{ for } j = 1, 2, 3, \dots, j_{max}, \quad i = 1, 2, 3, \dots, (i_{max})_l, \dots, (i_{max})_{X_0},$$

The condition (4) becomes

$$C_{pij}^{n+1} = 0 \text{ for } i = 1, \quad j = 1, 2, 3, \dots, j_{max}, \quad n = 0, 1, 2, 3, \dots,$$

$$\left(1 - V_d \frac{\Delta z}{K_j} \right) C_{pij}^{n+1} - C_{pij+1}^{n+1} = -\frac{Q\Delta z}{K_j}, \quad (35)$$

for $j = 1, i = 2, 3, 4, \dots, i_{max} l$ and $n = 0, 1, 2, 3, \dots$

$$\left(1 - V_d \frac{\Delta z}{K_j} \right) C_{pij}^{n+1} - C_{pij+1}^{n+1} = 0, \quad (36)$$

for $j = 1, i = i_{max} l + 1, \dots, i_{max} X_0$ and $n = 0, 1, 2, 3, \dots$

The boundary condition (5) can be written as

$$C_{pij_{max}-1}^{n+1} - \left(1 - \frac{\gamma_p \Delta z}{k_{j_{max}}} \right) C_{pij_{max}}^{n+1} = 0, \quad (37)$$

for $j = j_{max}, i = 2, 3, 4, \dots, i_{max} l, i_{max} X_0$.

The above system of equations (34)-(37) has a tridiagonal structure and is solved by Thomas Algorithm [22].

A similar procedure is adopted to obtain the finite difference equations for the secondary pollutant C_s for the partial differential equation (6) can be written as

$$A_j C_{s\ i-1\ j}^{n+1} + B_j C_{s\ ij-1}^{n+1} + D_j C_{s\ ij}^{n+1} + E_j C_{s\ ij+1}^{n+1} = F_j C_{s\ i-1\ j}^n + G_j C_{s\ ij-1}^n + M_j C_{s\ ij}^n + N_j C_{s\ ij+1}^n + V_g k C_{s\ ij}^n, \quad (38)$$

for $i = 2, 3, 4, \dots, i_{max} l, \dots, i_{max} X_0$, $j = 2, 3, 4, \dots, (j_{max} - 1)$.

The initial and boundary conditions on secondary pollutant C_s obtained from equations (7) to (10) are

$$C_{sij}^0 = 0 \text{ for } i = 1, 2, \dots, (i_{max})_l, \dots, (i_{max})_{X_0}, \quad j = 1, 2, \dots, j_{max},$$

$$C_{s1j}^{n+1} = 0 \text{ for } i = 1, \quad j = 1, 2, \dots, j_{max}, \quad n = 0, 1, 2, \dots,$$

$$\left(1 + (V_d + W_{gs}) \frac{\Delta z}{K_j} \right) C_{s\ ij}^{n+1} - C_{s\ ij+1}^{n+1} = 0, \quad j = 1, i = 2, 3, \dots, i_{max}, \dots, i_{max} X_0, \quad (39)$$

$$C_{s\ i\ j_{max}-1}^{n+1} - \left(1 - \frac{\gamma_s \Delta z}{k_{j_{max}}} \right) C_{s\ i\ j_{max}}^{n+1} = 0, \quad (40)$$

for $j = j_{max}, i = 2, 3, 4, \dots, i_{max}, \dots, i_{max} X_0$. Here

$$\begin{aligned} A_j &= -U_j \frac{\Delta t}{2\Delta x}, & F_j &= U_j \frac{\Delta t}{2\Delta x}, \\ B_j &= -\frac{\Delta t}{4\Delta z^2} (K_j + K_{j-1}), & G_j &= \frac{\Delta t}{4\Delta z^2} (K_j + K_{j-1} - W_s \frac{\Delta t}{2\Delta z}), \\ E_j &= -\frac{\Delta t}{4\Delta z^2} (K_{j+1} + K_j), & N_j &= \frac{\Delta t}{4\Delta z^2} (K_{j+1} + K_j + W_s \frac{\Delta t}{2\Delta z}), \\ M_j &= 1 - U_j \frac{\Delta t}{2\Delta x} - \frac{\Delta t}{4\Delta z^2} (K_{j+1} + 2K_j + K_{j-1}) - \frac{K_{ws}}{2}, \\ D_j &= 1 + U_j \frac{\Delta t}{2\Delta x} + \frac{\Delta t}{4\Delta z^2} (K_{j+1} + 2K_j + K_{j-1}) + \frac{k_{ws}}{2}. \end{aligned}$$

V_g is the mass ratio of the secondary particulate species to the primary gaseous species which is being converted and W_{gs} is the gravitational settling velocity of the secondary pollutant C_s .

The system of equations (38) to (40) also has tridiagonal structure but is coupled with equations (34) to (37). First, the system of equations (34) to (37) is solved for C_{pij}^n , which is independent of the system (38) to (40) at every time step n .

This result at every time step is used in equations (38) to (40). Then the system of equations (38) to (40) is solved for $(C_{s\ ij}^n)$ at the same time step n . Both the systems of equations are solved using Thomas algorithm. Thus, the solutions for primary and secondary pollutants concentrations are obtained.

5. Results and Discussions

In this numerical model, the effect of removal mechanism and transformation process of primary and secondary pollutants are analysed. Secondary pollutants are those which are formed through chemical reaction involving the primary pollutants, for example sulfate is formed when SO_2 is oxidized. The analysis of secondary pollutants is very essential because of longer life periods and much hazardous than the primary pollutants. Therefore to know the ambient air concentration one should know both the primary and secondary pollutants distribution in the urban area. We have considered source region extending upto $l=6$ km down wind from origin and source free region at the outskirts of the city. We have taken the primary source strength $Q=1\mu\text{gm}^{-2} \text{s}^{-1}$ at the ground level from an area source and the mixing height is selected as 624 meters.

The model has been solved using Crank-Nicolson finite difference technique, which is unconditionally stable. The concentration distribution is computed both in the source region and source free region till the desired distance X_0 . We have considered grid size 75 meters along x direction and 1 meter along z direction. Based on the grid independence study the solution is obtained using 160×624 grids. Concentration contours are plotted and results are analysed for primary and secondary pollutants in stable and neutral atmospheric situations for various meteorological parameters, terrain categories and removal mechanisms such as deposition velocity and gravitational settling velocity.

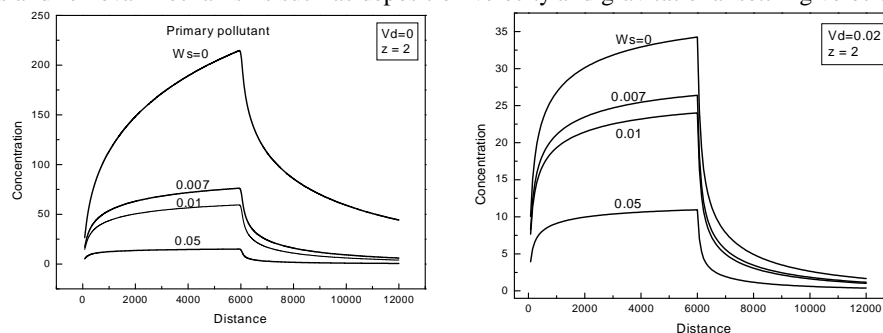


FIGURE 2. Ground level concentration versus distance of primary pollutants for various values of W_s (stable case).

Figures 2 and 4 demonstrate the effect of gravitational settling velocity W_s on primary pollutant and secondary pollutant along downwind distance for stable case. From the graphs we notice that the effect of increasing the values of gravitational settling velocity W_s is to decrease the ground level concentration of primary pollutants and secondary pollutants significantly for $V_d=0$ and $V_d=0.02$. This is quite consistent with the fact that settling velocity occurs due to larger size of the particles and dry deposition occurs due to the absorption of pollutants by surface terrain. We have considered gravitational settling velocity on the boundary condition of primary pollutant as well as secondary pollutant equations in this model. Therefore we studied the effect of gravitational settling velocity extensively on primary and secondary pollutant along with leakage velocity at the top of the boundary.

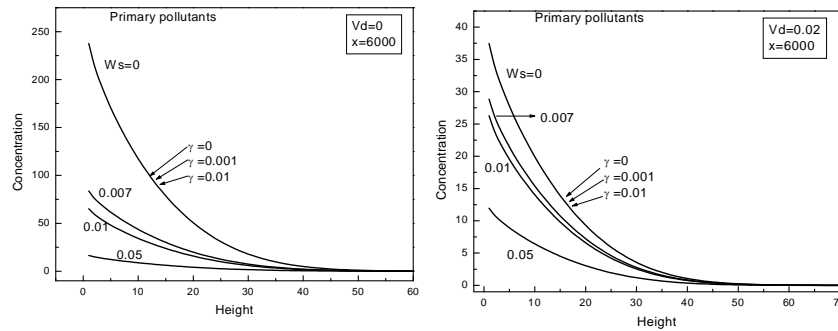


FIGURE 3. Concentration versus height of primary pollutants for various values of W_s and leakage velocity γ (stable case).

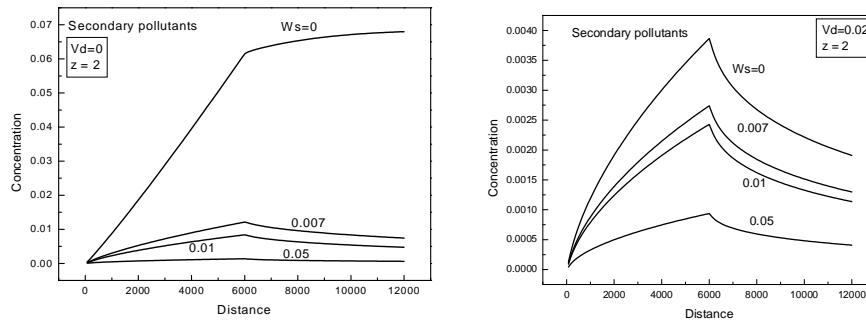


FIGURE 4. Ground level concentration versus distance of secondary pollutants for various values of W_s (stable case).

The effect of settling velocity on primary pollutant and secondary pollutants concentrations with respect to height is noticed from figures 3 and 5. We have analysed for deposition velocity $V_d=0$ and $V_d=0.02$. It is noticed that the effect of increasing the values W_s of is to reduce the concentration level of primary pollutant and secondary pollutant along height. This is in conformity with the fact that settling occurs due to the gravitational acceleration of larger particles.

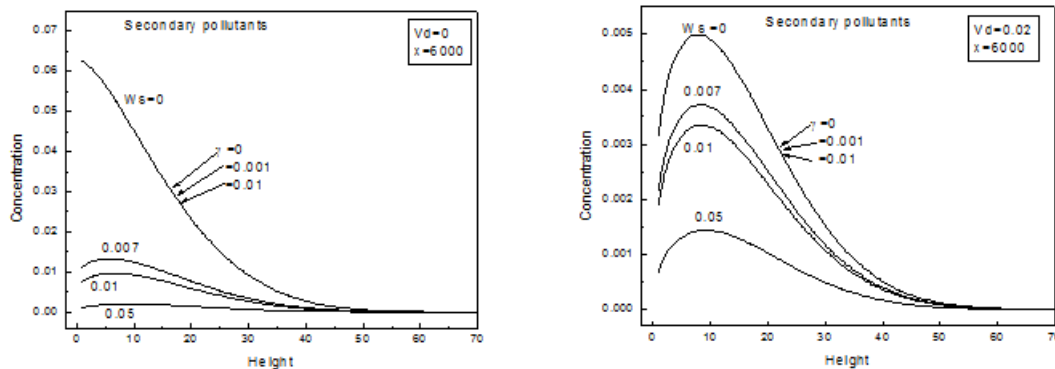


FIGURE 5. Concentration versus height of secondary pollutants for various values of W_s and leakage velocity γ (stable case).

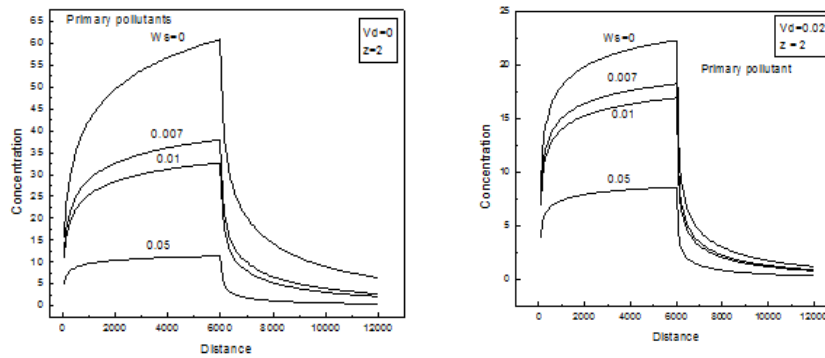


FIGURE 6. Ground level concentration versus distance of primary pollutants for various values of W_s (neutral case).

Figure 6 depicts ground level concentration versus distance in neutral atmospheric condition for various values of removal mechanisms with deposition velocity $V_d=0$ and $V_d=0.02$. Figure 7 demonstrates the concentration of primary pollutant versus height in neutral atmosphere for various removal mechanisms with deposition velocity $V_d=0$ and $V_d=0.02$. Comparison of these figures with the corresponding figures 2 and 3 in the case of stable atmospheric condition reveals that the concentration of primary pollutant is lower in neutral atmospheric situations. This is due to the fact that in neutral atmospheric condition pollutants will be diffused with higher rate than in stable atmospheric condition. Hence concentration level will be less in neutral atmospheric condition in comparison with the stable atmospheric conditions.

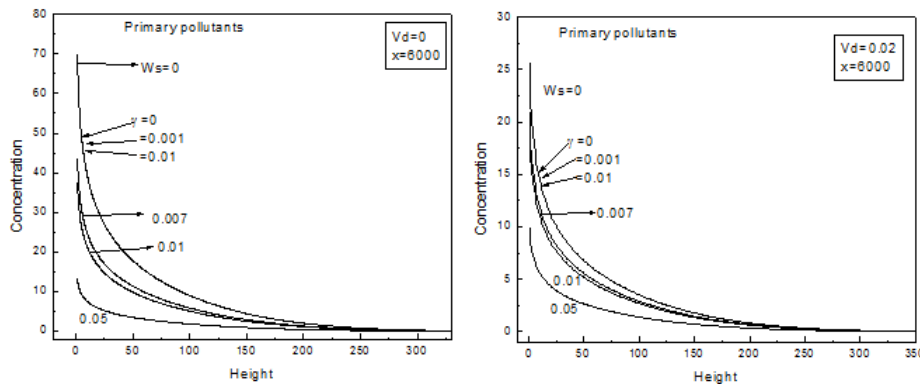


FIGURE 7. Concentration versus height of primary pollutants for various values of W_s and leakage velocity γ (neutral case).

Figures 8 and 9 depicts ground level concentration versus distance of secondary pollutants for various values of W_s and leakage velocity γ with dry deposition velocity $V_d=0$ and $V_d=0.02$ in neutral case. For the removal mechanisms $W_s=0$ and $V_d=0$ the concentration of secondary pollutants is maximum for neutral atmospheric condition. If we take $W_s=0$ and $V_d=0.02$ the concentration of secondary pollutants decreases when compare to $W_s=0$ and $V_d=0$.

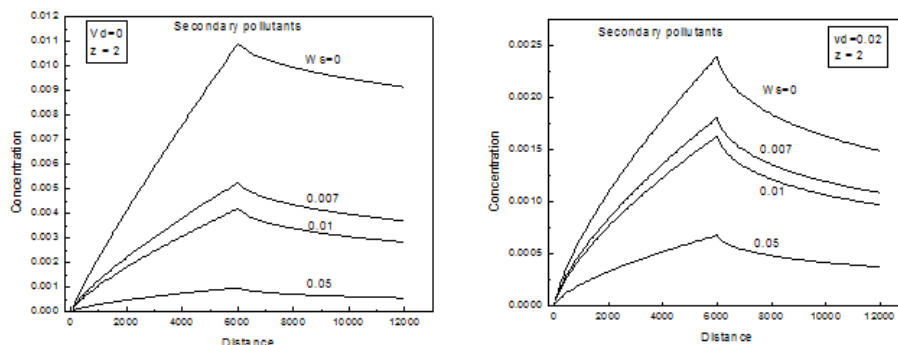


FIGURE 8. Ground level concentration versus distance of secondary pollutants for various values of W_s (neutral case).

Thus increasing the values of removal mechanisms the concentration of secondary pollutants decreases. We found that the concentration of primary and secondary pollutants is at the heights 350 m in neutral case. Therefore the leakage velocity on primary and secondary pollutants does not influence on the concentration distribution at 624 m. Thus there is no effect of leakage velocity on the concentration of primary and secondary pollutants.

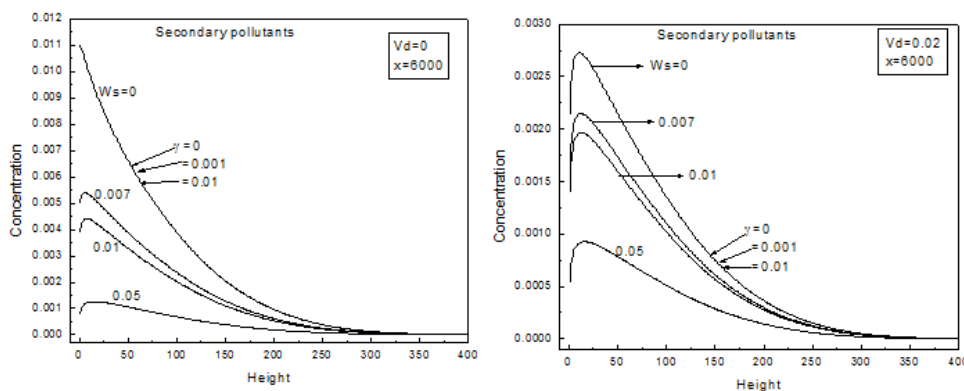


FIGURE 9. Concentration versus height of secondary pollutants for various values of W_s and V_d (neutral case).

6. Conclusions

A mathematical model is developed to study the effect of removal mechanisms namely leakage of pollutants through the top of the boundary layer, wet deposition due to rainout or washout, dry deposition and gravitational settling on the concentration distribution of primary and secondary pollutants. In this model we consider transformation of primary pollutant to secondary pollutants through first order chemical reaction. This model takes into account the more realistic form of variable wind and eddy diffusivity profiles. Concentration contours are plotted and results are analysed for primary and secondary pollutants in stable and neutral atmospheric situations.

From the graphs we conclude that the ground level concentration increases as the distance downwind within the source region, and then decreases rapidly in the source free region to an asymptotic value. This behaviour is because of the emission of pollutants and also the wind velocity in the direction along source region. The ground level concentration increases as the atmosphere becomes stable. We notice that the effect of various removal parameters on primary and secondary pollutants will reduce the concentration in the urban area. The magnitude of concentration is high in stable case and low in neutral case. The neutral condition enhances the vertical diffusion in the atmosphere. Thus the ground level concentration for primary as well as secondary pollutants is less in neutral atmospheric condition in comparison with the stable atmospheric condition. We find that the leakage velocity of primary and secondary pollutants, does not influence much on the concentration distribution due to the fact that the sources are at ground level and the top of the mixing layer where the pollutants are leaked is far away (624 meters) from the sources. Thus there is no effect of leakage on the pollutant concentration.

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