Time dependent advection diffusion model of air pollutants with removal mechanisms

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ABSTRACT
In this paper, we study a time dependent advection diffusion model for computation of the ambient air concentration of pollutants emitted from an area source. This model deals the dispersion of both primary and secondary pollutants emitted from an area with mesoscale wind along with large scale wind. The model takes into account the removal of pollutants through chemical reaction and gravitational settling. The obtained partial differential equation is solved using Crank-Nicolson implicit finite difference scheme under stability dependent meteorological parameters involved in wind velocities and eddy diffusivity profiles.

Key words: Atmospheric dispersion, Gaseous pollutant, Area source, urban heat island, diffusion coefficient.

1. Introduction
The purpose of this article is to describe a model for the atmospheric dispersion of an air pollutant emitted from an area source. An area source is an emission source which is spread out over a finite surface, as opposed to a point source or line source. The emitted species is assumed to undergo chemical reactions in the atmosphere. The emphasis is on long-term air quality. Atmospheric parameters which are taken into account include variable wind speed, atmospheric stability, surface roughness, mixing height and diffusivity. The model discussed here is two-dimensional downwind distance and vertical distance. A two-dimensional analysis is appropriate when the net lateral flux of pollutants is small. The fundamental approach to develope 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. Mathematical models are of fundamental importance in describing and understanding the dispersion of air pollutants in the atmosphere, since all the parameters are expressed in mathematical forms and therefore the influence of individual parameters on pollutant concentration can be easily examined. The effect of urban heat islands on pollution pattern through the use of mathematical models has been investigated in some studies. Chandler (1968) found that the winds produced by urban heat island effects tend to sharpen pollution gradients between urban and rural areas. Later on, Griffiths (1970) in his study pointed out that the knowledge of large-scale wind is not sufficient for air pollution forecasts in urban
areas because the mesoscale wind also plays an important role in shaping urban air pollution pattern.

Dilley and Yen (1971) studied the effect of mesoscale wind on the pollutant distribution from an infinite line source and found analytical solution to the two-dimensional transport and diffusion equation. But unfortunately, apart from the above some studies, not so much work has been done to find the effect of urban heat island generated mesoscale winds on urban air pollution pattern through mathematical models. Realizing this fact, an attempt in this direction is being made and we, therefore, present here a steady state two-dimensional mathematical model which studies the dispersion of air pollutants in the urban atmosphere under the cumulative effect of large-scale and mesoscale winds. The mesoscale wind is chosen to represent a local wind produced by urban heat island effect. The proposed model takes into account the realistic vertical height dependent power law profiles for the large-scale wind and eddy diffusivity, while the mesoscale wind is parameterized in the power law forms suggested by Dilley and Yen (1971). It may be noted that the topographical effects are not taken into account in such profiles. Solutions of the advection diffusion equation, with wind speed and vertical eddy diffusivity both as power function of vertical height, bounded by Atmospheric Boundary Layer (ABL) are well known for point and line sources (Arya, 1995). The advection diffusion equation has also solved with wind speed as function of height and eddy diffusivity as a function of downwind distance from the source (Sharan and Modani, 2006). Thus in general, the eddy diffusivity should be a function of both vertical as well as downwind distance (Mooney and Wilson, 1993). Recently (Sharan and Kumar, 2009) formulate the advection diffusion equation considering the wind speed as a function of vertical height and eddy diffusivity as a function of both vertical height and downwind distance applicable only for point source release in reflecting boundary condition. However, Dirichlet (total absorption), Neumann (total reflection) and mixed boundary conditions are also appropriate for calculating the actual ground-level concentration of air pollutants. In addition to these, the few studies have been made for the advection diffusion equation for area sources. Park and Baik (2008) have solved the advection diffusion equation for finite area source with wind speed and vertical eddy diffusivity as power function of vertical height in unbounded region.

The dispersion of atmospheric contaminant has become a global problem in the recent years due to rapid industrialization and urbanization. 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 (Brook et al., 2004). Exposure to the fine airborne particulate matter is associated with cardiovascular functions and mortality in older and cardiac patients (Riediker et al., 2004). 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 (Arif and Shah, 2007, Oke, 1995). 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 (Pope et al., 1995).
For regulatory planning or risk assessment in urban areas, the estimation of pollutant distribution from area source is very useful. Pal and Sinha (1986) have found that area source can be regarded as the sum or integral of numerous small point sources across a broad area. Various investigations (Rudraiah et al. (1997), Lebedeff and Hameed (1975), Pal and Sinha (1990), Venkatachalappa, Khan and Kakamari (2003), Park & Baik (2008), Lakshminarayanachari et al., (2012)) have been made in the past to study the dispersion of air pollutants from area sources. However, these models do not take into account the mesoscale wind, so in this paper we have developed a numerical model for primary and secondary pollutants with more realistic large scale wind velocity, mesoscale wind velocity and eddy diffusivity profiles by considering the various removal mechanisms such as dry deposition and gravitational settling velocity. The secondary pollutants are formed by means of first order chemical reaction rate of primary pollutants. In this model, we have made general assumption that the secondary pollutants are formed by means of first order chemical conversion of primary pollutants. The model has been solved using Crank-Nicolson implicit finite difference technique. Concentration contours are plotted and results are analyzed for primary as well as secondary pollutants in stable and neutral atmospheric situations for various meteorological parameters, terrain categories, and removal mechanisms, transformation processes, with and without mesoscale winds. The effect of mesoscale wind is analyzed for both primary and secondary pollutants in stable and neutral atmospheric conditions.

2. Model development

The physical problem consists of an area source, which is spread out over the surface of a city with finite downwind distance and infinite cross wind dimensions. We assume that the pollutants are emitted at a constant rate from the area source and spread within the mixing layer adjacent to earth’s surface where mixing takes place as a result of turbulence and convective motion. This mixing layer extends upwards from the surface to a height where all turbulent flux-divergences resulting from surface action have virtually fallen to zero. The pollutants are transported horizontally by large scale wind which is a function of vertical height (z) and horizontally as well as vertically by local wind caused by urban heat source, called mesoscale wind. We have considered the centre of the heat island at a distance \( x = l/2 \) i.e. at the centre of the city. We have considered the source region within the urban area which extends to a distance \( l \) in the downwind \( x \) direction (\( 0 \leq x \leq l \)). In this model we have taken \( l = 6 \) km. Assuming the homogeneity of urban terrain, the mean concentration of pollutant is considered to be constant along the crosswind direction i.e., pollutants concentration does not vary in cross wind direction. Therefore, there is no \( y \)-dependence. Also lateral flux of pollutants is small and traverses the centre line of uniform area source. The physical description of the model is shown schematically in figure 1. We intend to compute the concentration distribution in the urban area. We assume that the pollutants undergo the removal mechanisms, such as dry deposition and gravitational settling.

2.1 Primary pollutant

The basic governing equation of primary pollutant can be written as

\[
\frac{\partial C_p}{\partial t} + U(x,z) \frac{\partial C_p}{\partial z} + W(z) \frac{\partial C_p}{\partial z} = \frac{\partial}{\partial z} \left( K_z(z) \frac{\partial C_p}{\partial z} \right) - k C_p
\]

(1)
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Figure 1: Physical layout of the model

The initial and boundary conditions on primary pollutant is as follows:

\[
C_p = 0 \quad \text{at} \quad t = 0, \quad 0 \leq x \leq l \quad \text{and} \quad 0 \leq z \leq H \quad (2)
\]
\[
C_p = 0 \quad \text{at} \quad x = 0, \quad 0 \leq z \leq H \quad \text{and} \quad \forall \ t > 0 \quad (3)
\]
\[
K_z \frac{\partial^2 C_p}{\partial z^2} = V_{dp} C_p - Q \quad \text{at} \quad z = 0, \quad 0 \leq x \leq l \quad \text{and} \quad \forall \ t > 0 \quad (4)
\]
\[
K_z \frac{\partial^2 C_p}{\partial z^2} = 0 \quad \text{at} \quad z = H, \quad 0 \leq x \leq l \quad \text{and} \quad \forall \ t > 0 \quad (5)
\]

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, \(W\) is the mean wind speed in \(z\)-direction, \(K_z\) is the turbulent eddy diffusivity in \(z\)-direction and \(k\) is the first order chemical reaction rate coefficient of primary pollutant \(C_p\), \(l\) is the source length in the downwind direction, \(H\) is the mixing height, \(Q\) is the emission rate of primary pollutant species and \(V_{dp}\) is the dry deposition velocity.

2.2 Secondary pollutant

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

\[
\frac{\partial C_s}{\partial t} + U(x, z) \frac{\partial C_s}{\partial x} + W(z) \frac{\partial C_s}{\partial z} = \frac{\partial}{\partial z} \left( K_z(z) \frac{\partial C_s}{\partial z} \right) + W_z \frac{\partial C_s}{\partial z} + V_g k C_p 
\]

(6)

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

\[
C_s = 0 \quad \text{at} \quad t = 0, \quad \text{for} \quad 0 \leq x \leq l \quad \text{and} \quad 0 \leq z \leq H \quad (7)
\]
\[
C_s = 0 \quad \text{at} \quad x = 0, \quad \text{for} \quad 0 \leq z \leq H \quad \text{and} \quad \forall \ t > 0 \quad (8)
\]

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

\[
K_z \frac{\partial^2 C_s}{\partial z^2} + W_z C_s = V_{ds} C_s \quad \text{at} \quad z = 0, \quad 0 \leq x \leq l \quad \text{and} \quad \forall \ t > 0 \quad (9)
\]
\[
K_z \frac{\partial^2 C_s}{\partial z^2} + W_z C_s = 0 \quad \text{at} \quad z = H \quad \text{and} \quad \forall \ t > 0 \quad (10)
\]

where \(V_g\) is the mass ratio of the secondary particulate species to the primary gaseous species which is being converted, \(V_{ds}\) is the dry deposition velocity and \(W_z\) is the gravitational settling velocity of the secondary pollutant \(C_s\).
To solve the equations (1) and (6) we have used the profiles of large scale wind velocity, mesoscale wind velocity and eddy-diffusivity for stable and neutral conditions and other meteorological parameters which are discussed in the succeeding section.

3. Meteorological parameters

To solve Eq. (1) and Eq. (6) 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 $L$ (Monin and Obukhov 1954), which is also a function of net heat flux among several other meteorological parameters. $L$ is defined by

$$L = -\frac{u_* \rho c_p T}{\kappa g R_f},$$

where $u_*$ is the friction velocity, $H_f$ the net heat flux, $\rho$ the ambient air density, $c_p$ the specific heat at constant pressure, $T$ the ambient temperature near the surface, $g$ the gravitational acceleration and $\kappa$ the Karman’s constant $\approx 0.4$. $H_f < 0$ and consequently $L > 0$ represents stable atmosphere, $H_f > 0$ and $L < 0$ represent unstable atmosphere and $H_f = 0$ and $L \rightarrow x$ 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 $u_* = c_g u_g$, (12)

where $c_g$ is a function of the surface Rossby number $R_0 = \frac{u_*}{f z_0}$, where $f$ is the Coriolis parameter due to earth’s rotation and $z_0$ is the surface roughness length. Lettau (1959) derived the expression for $c_g$, the drag coefficient for a neutral atmosphere in the form

$$c_g = \frac{0.16}{\log_{10} (R_0) - 1.8}.\quad (13)$$

The effect of thermal stratification on the drag coefficient can be accounted through the relations:

$$c_{gsu} = 1.2 c_g$$ for unstable flow, (14)

$$c_{gs} = 0.8 c_g$$ for slightly stable flow and (15)

$$c_{gs} = 0.6 c_g$$ for stable flow. (16)

In order to evaluate the drag coefficient, the surface roughness length $z_0$ may be computed according to the relationship developed by Lettau (1970) i.e., $z_0 = \frac{R \alpha}{2 A}$, where $R$ is the effective height of roughness elements, $\alpha$ is the frontal area seen by the wind and $A$ 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. Ragland (1973) used the following values of $H_f$ (Table 1) for urban area.
Table 1: Net heat flux $H_f (langle y \ min^{-1})$

<table>
<thead>
<tr>
<th>Net radiating index</th>
<th>4.0</th>
<th>3.0</th>
<th>2.0</th>
<th>1.0</th>
<th>0.0</th>
<th>-1.0</th>
<th>-2.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Net heat flux $H_f$</td>
<td>0.24</td>
<td>0.18</td>
<td>0.12</td>
<td>0.06</td>
<td>0.0</td>
<td>-0.03</td>
<td>-0.06</td>
</tr>
</tbody>
</table>

3.1 EddyDiffusivity Profiles

Following gradient transfer hypothesis and dimensional analysis, the eddy viscosity $K_M$ is defined as
\[
K_M = \frac{\nu^2}{\partial u/\partial z}.
\]
(17)
Using similarity theory of Monin and Obukhov(1954) the velocity gradient may be written as
\[
\frac{\partial u}{\partial z} = \frac{\nu \cdot \phi_M}{\kappa z}.
\]
(18)
Substituting equation (18) in the equation (17), we have
\[
K_M = \frac{\kappa u_z}{\phi_M}.
\]
(19)
The function $\phi_M$ depends on, $z/L$ where $L$ is Monin-Obukhov stability length parameter. It is assumed that the surface layer terminates at $z = 0.1\kappa \frac{u_z}{f}$ for neutral stability. For stable conditions, surface layer extends to $z = 6L$.

For neutral stability with $z < 0.1\kappa \frac{u_z}{f}$ (within surface layer)
\[
\phi_M = 1 \quad \text{and} \quad K_M = \kappa u_z z
\]
(20)
For stable flow with $0 < \frac{z}{L} < 1$
\[
\phi_M = 1 + \frac{\alpha}{L} z
\]
\[
K_M = \frac{\kappa u_z z}{1 + \alpha}
\]
(21)
(22)
For stable flow with $1 < \frac{z}{L} < 6$
\[
\phi_M = 1 + \alpha \quad \text{and} \quad K_M = \frac{\kappa u_z z}{1 + \alpha}
\]
(23)
Webb (1970) has been shown that $\alpha = 5.2$. In the PBL (planetary boundary layer), where $z/L$ is greater than the limits considered above and $z > 0.1\kappa \frac{u_z}{f}$, we have, the following expressions for $K_M$:

For neutral stability $z > 0.1\kappa \frac{u_z}{f}$,
\[
K_M = 0.1\kappa^2 \frac{u_z^2}{f}
\]
(24)
For stable flow with $z > 6L$, up to $H$, the mixing height,
\[
K_M = \frac{5\kappa u_z L}{1 + \alpha}
\]
(25)
Equations (19) to (25) give the eddy viscosity for the conditions needed for the model.
The common characteristic of $K_z$ is that it has a 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 (1973) gave an expression based on theoretical analysis of neutral boundary layer in the form:
\[
K_z = 0.4u_z z e^{-z/H}
\]
(26)
where $H$ is the mixing height.

For stable condition, Ku et al.,(1987) used the following form of eddy-diffusivity.

$$K_z = \frac{\kappa u_* z}{0.74 + 0.7z/L} e^{-\left(b \eta \right)}$$

$$b = 0.91, \quad \eta = \frac{x}{L \sqrt{\mu}}, \quad \mu = \frac{u_*}{|f| L}$$

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 equations (26) and (27) have been used in this model developed for neutral and stable atmospheric conditions.

### 3.2 Large Scale and Mesoscale wind velocity profiles

It is known that in an urban city the heat generation causes the vertical flow of air with maximum velocity (rising of air) at the centre of the city. Hence the city can be called as heat island. This rising air forms an air circulation and this circulation is completed at larger heights. This is called mesoscale circulation. In order to incorporate more realistic form of velocity profile in the models, we integrate equation \( \frac{\partial U}{\partial z} = \frac{u_* \phi_M}{\kappa z} \) from $z_o$ to $z + z_o$ for stable and neutral conditions which depends on Coriolis force, surface friction, geostrophic wind, stability characteristic parameter $L$ and vertical height $z$. But large urban areas generate an additional circulation called Mesoscale circulation. Therefore, to take into account the mesoscale wind over the urban areas, for realistic form of velocity profiles, it is necessary to modify the wind velocity profiles. So we obtain the following expressions for large and mesoscale wind velocities.

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

$$u = \frac{u_*}{\kappa} \ln \left( \frac{z + z_o}{z_o} \right)$$

(28)

It is assumed that the horizontal mesoscale wind varies in the same vertical manner as $U$.

The vertical mesoscale wind $W_s$ can then be found by integrating the continuity equation and we obtain in the form

$$u_e = -\alpha (x - x_o) \ln \left( \frac{z + z_o}{z_o} \right)$$

(29)

where $\alpha$ is proportionality constant. Thus we have

$$U(x, z) = u + u_e = \left( \frac{u_*}{\kappa} - \alpha (x - x_o) \right) \ln \left( \frac{z + z_o}{z_o} \right)$$

(30)

$$W(z) = w_e = \alpha \left[ z \ln \left( \frac{z + z_o}{z_o} \right) - z + z_o \ln(z + z_o) \right]$$

(31)

In case of stable flow with $0 < z/L < 1$, we get

$$u = \frac{u_*}{\kappa} \left[ \ln \left( \frac{z + z_o}{z_o} \right) + \frac{\alpha}{L} z \right]$$

(32)

$$u_e = -\alpha (x - x_o) \left[ \ln \left( \frac{z + z_o}{z_o} \right) + \frac{\alpha}{L} z \right]$$

(33)

$$U(x, z) = u + u_e = \left( \frac{u_*}{\kappa} - \alpha (x - x_o) \right) \left[ \ln \left( \frac{z + z_o}{z_o} \right) + \frac{\alpha}{L} z \right]$$

(34)

$$W(z) = w_e = \alpha \left[ z \ln \left( \frac{z + z_o}{z_o} \right) - z + z_o \ln(z + z_o) + \frac{\alpha}{2L} z^2 \right]$$

(35)

In case of stable flow with $1 < z/L < 6$, we get

$$u = \frac{u_*}{\kappa} \left[ \ln \left( \frac{z + z_o}{z_o} \right) + 5.2 \right]$$

(36)

$$u_e = -\alpha (x - x_o) \left[ \ln \left( \frac{z + z_o}{z_o} \right) + 5.2 \right]$$

(37)
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In the planetary boundary layer, above the surface layer, power law scheme has been employed.

\[ u(x, z) = u + u_e = \left( \frac{u_g}{z} - \alpha(x - x_o) \right) \left[ \frac{z + z_0}{z_0} + 5.2 \right] \]  
(38)

\[ W(z) = w_e = \alpha \left[ z \ln \left( \frac{z + z_0}{z_0} \right) + z_0 \ln(z + z_0) + 4.2z \right] \]  
(39)

where, \( u_g \) is the geostrophic wind, \( u_{sl} \) the wind at \( z_{sl}, z_{sl} \) the top of the surface layer, \( x_0 \) is the \( x \) co-ordinate of centre of heat island, \( H \) the mixing height and \( P \) is an exponent which depends upon the atmospheric stability. Jones et al., (1971) suggested values for the exponent \( P \), obtained from the measurements made from urban wind profiles, as follows;

\[ P = \begin{cases} 
0.20 & \text{for neutral condition} \\
0.35 & \text{for slightly stable flow} \\
0.50 & \text{for stable flow} 
\end{cases} \]

Wind velocity profiles given by equations (28), (32), (36), (40) are due to (Ragland 1973) equations (234), (35), (38), (39), (42) and (43) are modified as per (Dilley-Yen 1971) are used in this model.

3.3 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 detailed numerical method and procedure to solve the partial differential equations (1) and (6) is described below (Roache 1976, Wendt 1992). 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 \( C_p(x_i, z_j, t_n) \) is denoted by \( C_p^{nij} = C_p(x_i, z_j, t_n) \), 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 the \( n^{th} \) 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
We use 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 \((x_{i+1/2}, z_j, t_{n+1/2})\). We use the backward differences for advective term for this model. Therefore we use

\[
U(x, z) \frac{\partial C_p}{\partial x} \bigg|_{ij}^n = U_{ij} \left[ \frac{C^n_{p_{ij+1}} - C^n_{p_{ij-1}}}{2\Delta x} \right] \quad (45)
\]

\[
W(z) \frac{\partial C_p}{\partial z} \bigg|_{ij}^n = W_{j} \left[ \frac{C^n_{p_{j+1}} - C^n_{p_{j-1}}}{2\Delta z} \right] \quad (46)
\]

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

\[
\frac{\partial}{\partial z} \left( K_z(z) \frac{\partial C_p}{\partial z} \right)_{ij}^n = \frac{1}{2(\Delta z)^2} \left[ \frac{(K_{j+1} + K_j)(C^n_{p_{j+1}} - C^n_{p_{j-1}})}{2\Delta z} - \frac{(K_j + K_{j-1})(C^n_{p_{j}} - C^n_{p_{j-1}})}{2\Delta z} \right]
\]

Hence,

\[
\frac{\partial}{\partial z} \left( K_z(z) \frac{\partial C_p}{\partial z} \right)_{ij}^n = \frac{1}{2(\Delta z)^2} \left[ (K_{j+1} + K_j)(C^n_{p_{j+1}} - C^n_{p_{j-1}}) - (K_j + K_{j-1})(C^n_{p_{j}} - C^n_{p_{j-1}}) \right]
\]

Similarly,

\[
\frac{\partial}{\partial z} \left( K_z(z) \frac{\partial C_p}{\partial z} \right)_{ij}^{n+1} = \frac{1}{2(\Delta z)^2} \left[ (K_{j+1} + K_j)(C^{n+1}_{p_{j+1}} - C^{n+1}_{p_{j-1}}) - (K_j + K_{j-1})(C^{n+1}_{p_{j}} - C^{n+1}_{p_{j-1}}) \right]
\]

Substituting equations (45) to (50) in equation (44) and rearranging the terms we get the finite difference equations for the primary pollutant \(C_p\) in the form

\[
A_{ij} C^n_{p_{ij}} + B_j C^{n+1}_{p_{ij-1}} + D_j C^{n+1}_{p_{ij+1}} + E_j C^{n+1}_{p_{ij+1}} = F_j C^n_{p_{ij-1}} + G_j C^n_{p_{ij-1}} + M_j C^n_{p_{ij+1}} + N_j C^{n+1}_{p_{ij+1}}
\]

for each \(i = 2, 3, 4, ..., \max i\) and \(j = 2, 3, 4, ..., \max j\) and \(n = 0, 1, 2, 3, ...

where

\[
A_{ij} = -U_{ij} \frac{\Delta t}{2\Delta x}, \quad F_{ij} = U_{ij} \frac{\Delta t}{2\Delta x}
\]

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

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

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

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

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

\(t_{\text{max}}\) is the \(i\) value at \(x = i\) and \(j_{\text{max}}\) is the value of \(j\) at \(z = H\).
Equation (51) 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

\[ C_{pj}^0 = 0 \quad \text{for } j = 1, 2, \ldots, j_{max}, \quad i = 1, 2, \ldots, i_{max} \]
\[ C_{pij}^{n+1} = 0 \quad \text{for } i = 1 \text{ and } j = 1, 2, \ldots, j_{max}, \quad n = 0, 1, 2, \ldots \]  
(52)

\[ \left( 1 + V_{dp} \frac{\Delta z}{K_j} \right) C_{pij}^{n+1} - C_{pij+1}^{n+1} = \frac{Q_{in} \Delta x}{K_j} \quad \text{for } j = 1, \quad i = 2, 3, 4, \ldots, i_{max} \quad \text{and} \quad n = 0, 1, 2, 3, \ldots \]  
(53)

\[ C_{pj_{max}+1}^{n+1} - C_{pj_{max}}^{n+1} = 0 \quad \text{for } j = j_{max}, \quad i = 2, 3, 4, \ldots, i_{max} \]  
(54)

The above system of equations (51) to (54) has a tridiagonal structure and is solved by Thomas Algorithm. 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

\[ A_i C_{si_{j-1}}^n + B_i C_{si_{j-1}}^n + E_i C_{si_{j+1}}^n = F_i C_{si_{j-1}}^n + G_i C_{si_{j}}^n + N_i C_{si_{j+1}}^n + \frac{\Delta t}{2} \alpha_s \beta C_p^0 \]  
for \( i = 2, 3, 4, \ldots, i_{max} \), \( j = 2, 3, 4, \ldots, j_{max} - 1 \)  
(55)

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

\[ C_{si_{j-1}}^0 = 0 \quad \text{for } j = 1, 2, 3, \ldots, j_{max}, \quad i = 1, 2, 3, \ldots, i_{max} \]  
(56)

\[ C_{si_{j+1}}^n = 0 \quad \text{for } i = 1, 2, \ldots, j_{max}, \quad j = 1, 2, \ldots, j_{max}, \quad n = 0, 1, 2, \ldots \]  
(57)

\[ C_{si_{j-1}}^{n+1} - C_{si_{j+1}}^{n+1} = 0 \quad \text{for } j = j_{max}, \quad i = 2, 3, 4, \ldots, i_{max} \]  
(58)

Where,

\[ B_i = -\left[ \frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j-1}) + W_{ij} \frac{\Delta t}{2 \Delta x} \right] \]
\[ G_j = \left[ \frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j-1}) + W_{ij} \frac{\Delta t}{2 \Delta x} \right] \]
\[ E_i = -\frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j+1}) \]
\[ N_i = \frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j+1}) \]
\[ D_{ij} = 1 + U_{ij} \frac{\Delta t}{2 \Delta x} + W_{ij} \frac{\Delta t}{2 \Delta z} + \frac{\Delta t}{4(\Delta z)^2} (K_{j+1} + 2K_j + K_{j-1}) \]
\[ M_{ij} = 1 - U_{ij} \frac{\Delta t}{2 \Delta x} - W_{ij} \frac{\Delta t}{2 \Delta z} - \frac{\Delta t}{4(\Delta z)^2} (K_{j+1} + 2K_j + K_{j-1}) \]

\( V_e \) is the mass ratio of the secondary particulate species to the primary gaseous species which is being converted and \( W_{di} \) is the gravitational settling velocity of the secondary pollutant \( C_s \).

The system of equations (51) to (54) has tridiagonal structure but is coupled with equations (55) to (58). First, the system of equations (51) to (54) is solved for \( C_{pi_{ij}}^n \), which is independent of the system (55) to (58) at every time step \( n \). This result at every time step is used in equations (55) to (58).

Then the system of equations (55) to (58) is solved for \( C_{si_{ij}}^n \) at the same time step \( n \). Both the systems of equations are solved using Thomas algorithm for tri-diagonal equations (51) to (54) and (55) to (58). Thus, the solutions for primary and secondary pollutant concentrations are obtained.
4. Results and discussion

A numerical model is developed to study the effect of mesoscale wind on the concentration of primary and secondary pollutants. The pollutants are emitted at a constant rate from an uniformly distributed area source. We have considered the source region within the urban city\((0 \leq x \leq l)\) which extends up to 6000 meters. We assume that the pollutants undergo through the removal mechanism dry deposition. The primary pollutant is considered to be chemically reactive to form secondary pollutant by means of first order chemical reaction. The results of this model have been presented graphically from figures 2 to 7.

In figure 2, the effect of mesoscale wind on the ground level concentration of primary pollutant for different values of dry deposition velocity with respect to distance for stable and neutral atmospheric conditions are analyzed. The concentration of primary pollutant decreases rapidly as the value of chemical reaction rate increases. The concentration of pollutant is less in upwind side of the centre of heat island and more in the downwind side of the centre of heat island in the presence of mesoscale wind \((a=0.00004)\) when compared to that of without mesoscale wind \((a=0)\). This behavior exists because horizontal component of mesoscale wind is along the large scale wind on the left and against it on the right side of the heat island. Thus in the presence of mesoscale wind, the advection is more on the left and less on the right side of the heat island. Therefore the concentration is less on the left and more on the right in the presence of mesoscale wind. In general, the concentration of primary pollutant increases in the downwind direction. Comparing figures (a) and (b), we find that the concentration of pollutant at given distance is much smaller in the neutral atmospheric condition than that in the stable atmospheric case. The maximum concentration of pollutant is around 250 in stable case and is near to 65 in neutral atmosphere at \(x=6000\) meters.

In figure 3, the effect of mesoscale wind on the ground level concentration of primary pollutant for different values of dry deposition velocity with respect to height for stable and neutral atmospheric conditions is studied. As dry deposition velocity increases, the concentration of primary pollutant decreases with respect to height. The similar effect is observed as in the case of figure 2. In stable case the magnitude of concentration reaches zero around 20 meters height and in neutral case the concentration is zero at 100 meters height from the ground level surface. Near the ground level the concentration of primary pollutant is around 130 in stable case whereas it is near to 50 in neutral atmospheric condition.

![Figure 2: Variation of ground level concentration with respect to distance of primary pollutant for (a) Stable (b) Neutral case.](image-url)
Time dependent advection diffusion model of air pollutants with removal mechanisms

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Figure 3: Variation of ground level concentration with respect to height of primary pollutants for (a) Stable (b) Neutral case.

In figure 4, the effect of mesoscale wind on the ground level concentration of secondary pollutant for different values of gravitational settling velocity with respect to distance for stable and neutral atmospheric conditions is studied. As gravitational settling velocity increases, the concentration of secondary pollutant decreases. The magnitude of the pollutant is higher in the stable case and lower in the neutral case. The concentration of secondary pollutant increases as distance increases. We observe that the concentration of secondary pollutant is more at the ground level (z = 2 meter) and at the end of the city region.

In figure 5, the effect of mesoscale wind on the ground level concentration of secondary pollutant for different values of dry deposition velocity with respect to distance for stable and neutral atmospheric conditions are studied. As dry deposition velocity increases, the concentration of secondary pollutant decreases. The magnitude of the pollutant is higher in the stable case and lower in the neutral case. The concentration of secondary pollutant increases as distance increases. We observe that the concentration of secondary pollutant is more at the ground level (z = 2 meter) and at the end of the city region.

Figure 4: Variation of ground level concentration with respect to distance of secondary pollutants with various values of gravitational settling for (a) Stable (b) Neutral case.
**Figure 5:** Variation of ground level concentration with respect to distance of secondary pollutants with various values of dry deposition for (a) Stable (b) Neutral case.

In figure 6, the effect of mesoscale wind on the ground level concentration of secondary pollutant for different values of gravitational settling velocity with respect to height for stable and neutral atmospheric conditions is studied. As gravitational settling velocity increases, the concentration of secondary pollutant decreases. In the stable case near the ground level the concentration of secondary pollutant is more comparing to that in the neutral case. The concentration reaches zero around 25 meters height in stable case. But in neutral atmospheric condition the concentration is zero at 110 meters height.

In figure 7, the effect of mesoscale wind on the ground level concentration of secondary pollutant for different values of dry deposition velocity with respect to height for stable and neutral atmospheric conditions is studied. As dry deposition velocity increases, the concentration of secondary pollutant decreases. In the stable case near the ground level the concentration of secondary pollutant is more comparing to that in the neutral case. The concentration reaches zero around 25 meters height in stable case. But in neutral atmospheric condition the concentration is zero at 110 meters height. This effect is due to neutral atmospheric condition enhances the vertical diffusion of pollutants.

**Figure 6:** Variation of ground level concentration with respect to height of secondary pollutants with various values of gravitational settling for (a) Stable (b) Neutral case.
5. Conclusions

An atmospheric diffusion model considering heavy admixture’s concentration has been studied. It is found that the effect of settling of larger particles is to reduce concentration throughout the city region for large values of settling velocities. The results of this model gave the pathway for determining the accurate concentration distribution for the case when the effect of gravitational force on the larger size particles cannot be neglected. 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 the atmosphere. The concentration of secondary pollutants decreases as gravitational settling velocity increases in both stable and neutral cases. The concentration of primary and secondary pollutants is less on the upwind side of the center of heat island and more on the downwind side of the center of heat island in the case of mesoscale wind when compared in the absence of mesoscale wind, because the mesoscale wind increases the velocity in the upwind direction and decreases in the downwind direction of the center of heat island. The concentration of primary and secondary pollutants is less in magnitude for the neutral atmosphere when compared to the stable condition. The neutral atmospheric condition enhances vertical diffusion carrying the pollutant concentration to greater heights and thus the concentration is less at the surface region of the urban city.

The urban heat island effect generates their own mesoscale winds and consequently prevents the dispersal of pollutants which will result in an increase in pollution concentration in the atmosphere. The urban heat island adds to the development of hazehood of contaminated pollutants and also helps these pollutants to circulate in upward direction, thus making the pollution problem more severe. It should be understood that the reasons for the transformation of big cities into ‘urban heat islands’ is attributed to human factors, hence, collective efforts should be made in the process of reducing the urban heat island and for the creation of cooler and healthy city. The present study shows that the stable condition is an unfavorable condition for the animals and plants from air pollution point of view.

6. References


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