Numerical model of air pollutant emitted from an area source of primary pollutant with chemical reaction

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ABSTRACT

A two dimensional advection-diffusion mathematical model of primary and secondary pollutants of an area source with chemical reaction and gravitational settling is presented. 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 for more realistic atmospheric conditions. 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 wind velocity and eddy diffusivity profiles are functions of vertical height, frictional velocity, terrain categories, geostrophic wind, Monin Obhukov stability length parameter and several stability dependent meteorological parameters. Consistency, stability and convergence criteria for this technique have been analysed. The variation of ground level concentration of primary and secondary pollutants with the downwind distance and the height for stable and neutral atmospheric conditions is analysed extensively.

Key words: Air pollution model; Chemical reaction; Crank-Nicolson implicit scheme; Eddy diffusivity; Settling velocity; Variable wind velocity.

1. INTRODUCTION

Rapid industrialization and urbanization have posed a serious threat to the human life and its environment in recent years. Continuous emission of air pollutants like CO, NO, SO2 by the combustion of hydrocarbon fuels in residential area, vehicular exhausts due to traffic flow and several other major or minor sources pollute a part or whole area of an urban environment. Pollution from an area source not only affect people and environment within this area, but also the people staying in adjacent rural non-polluted area, as pollutants are diffused and advected downwind. An important atmospheric phenomenon that requires attention in mathematical modeling is the conversion of air pollutants from gaseous to particulate form. Study of such conversion processes in which sulphur dioxide is converted to particulate sulphate, nitrogen oxide to particulate nitrate, and hydrocarbons to particulate organic material would reveal a lot on urban plume characteristics. Also, the study of secondary pollutant is very important as the life period of secondary pollutant is longer than primary pollutant and it is more hazardous to the human life and environment. Experimental measurements have been carried out for the downwind of large urban complexes to obtain material balances on gaseous and particulate pollutants [1]-[2]. Above models are analytical in nature they deal with specialized forms of wind velocity and eddy diffusivity profiles. In this context study of air pollution model-through numerical scheme is highly important.

There are a few numerical models for area source to include the general forms of wind velocity and eddy diffusivity profiles. In particular, the two-dimensional multi-box model is quite reasonable [3]. This model considers eddy diffusivity and velocity profiles as functions of z, stability parameter and frictional velocity. In this model the geostrophic wind, the net heat flux, the surface roughness, the mixing height of the atmosphere and the emission rate of the source are specified and the steady state pollutant concentration is determined. Conservation of mass equations for an array of boxes (or nodes) are solved simultaneously by an implicit finite difference scheme for different atmospheric conditions. This two-dimensional atmospheric numerical model deals with only chemically inactive atmospheric pollutants. A generalized urban air pollution model based on numerical integration is developed for the study of air pollutant distribution over an urban area [4].
The most interesting and somewhat realistic model for SO$_2$ pollution from the point of view of eddy diffusivity is presented [5]. This quasi-steady β-mesoscale Lagrangian model incorporates the diurnal variability of planetary boundary layer (PBL) structure and of the parameters governing the chemical conversion and ground removal of SO$_2$. The vertical non-homogeneity of atmospheric dispersion is simulated by the use of vertical height and stability dependent profile of eddy diffusivity is defined as $K_z = \frac{\kappa u_z z}{\phi(z/L)}$ for surface layer, where $\phi(z/L)$ the stability correction factor and $L$ is the stability length parameter [25].

The following empirical expressions for the stability correction factor $\phi$ as [5]-[6].

$$
\phi = \begin{cases} 
0.74 & \text{neutral } L \to \infty \\
0.74 + 4.7z / L & \text{stable } L > 0 \\
0.74(1 - 9z / L)^{1/2} & \text{unstable } L < 0 
\end{cases}
$$

For the region above surface layer Gillani used the expressions for $K_z$ suggested by O’Brien [7] in stable condition and that of Deardorff [8] in unstable condition. These expressions depend on stability length $L$ and vertical height $z$. This model also takes into account the first order time-dependent chemical conversion rate of SO$_2$. However, in order to apply Taylor’s hypothesis $t = x/\bar{U}$ where $\bar{U}$ is the mean wind velocity, this model considers steady wind speed over the mixing layer and does not deal with the secondary pollutant which is formed from SO$_2$ by means of chemical reaction.

There is an interesting Lagrangian finite difference model, which has been developed by using fractional step method to compute time dependent advection of air pollutants [9]. Here, the Eulerian grid used for the diffusion part of the pollutant transport equation remains unchanged. The finite difference scheme used in the model avoids numerical pseudo-diffusion and it is unconditionally stable. The numerical solution obtained is compared with the corresponding analytical solutions of steady state case and reasonable agreement has been found. This paper gives a brief discussion of related numerical schemes like particle-in-cell methods [10] puff-in-cell methods [11] conservation of momentum model [12] and combination of all these methods [13]. However, this paper does not deal with any kind of removal processes and also the secondary pollutant.

A two-dimensional analytical model for turbulent dispersion of pollutants in stable atmospheric layer with a quadratic exchange co-efficient and linear velocity profile is presented [14]. But it fails light on any removal mechanism. A numerical model for dispersion with chemical reaction and dry deposition from area source, which is steady state in nature is presented [15]. All these area source models deal with only primary inert air pollutants. Subsequently, presented a time-dependent numerical model for both primary and secondary pollutants in order to obtain time dependent contours of pollutant concentration in urban area [16]. This model has been solved by using fractional step method taking into account the specified functional form of vertical eddy diffusivity ($K_z = z$) and velocity $U(z) = z^{0.2}$ profiles. A time dependent area source mathematical model of chemically reactive air pollutants and their byproduct in a protected zone above the source layer with rainout/washout and settling [17]. But, the horizontal homogeneity of pollutants and constant eddy diffusivity are assumed in this model. Acid precipitation can occur when particles and gases are removed from the atmosphere by both wet deposition and dry deposition. In order to justify controls on emissions of acid precursors, the relationship between a source and the deposition pattern that it produces needs to be understood [18]-[20]. A time dependent two dimensional air pollutant model for both primary pollutant (time dependent emission) and the secondary pollutant with instantaneous (dry deposition) and delayed (chemical conversion, rainout/washout and settling) removals [21]. However, this model being analytical, deals with the uniform velocity and eddy diffusivity profiles. An advection-diffusion numerical model is presented for air pollutants with chemical reaction and dry deposition [22]. However this model does not take into account of secondary pollutant.

Hence, in the present paper we develop a mathematical model of area source for both primary (steady emission) and secondary pollutants with more realistic variable wind velocity and eddy-diffusivity profiles. In this model the most acceptable general assumption is made, “the secondary pollutants are formed by means of first order chemical conversion of primary pollutant”. Both primary and secondary pollutants are removed from atmosphere by dry deposition on terrain. Upwind difference scheme is employed to discretise the advection term of the governing equation and is solved by using Crank-Nicolson implicit finite difference technique. Consistency, Stability and convergence criteria are tested for the numerical scheme used in this model. Concentration contours are plotted and results are analysed for the primary as well as secondary pollutants in stable and neutral atmospheric situations for various meteorological parameters, terrain categories and removal and transformation processes.
2. MODEL DEVELOPMENT

The physical problem consists of an area source, which is spread over the surface of the city with a finite downwind distance and infinite cross wind dimensions. We assume that the pollutants are emitted at a constant rate from an 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 upward from the surface to a height where all turbulent flux-divergences resulting from surface action have virtually fallen to zero. We have considered the source region within the urban centre which extends from the origin to a distance l in the downwind x direction (0 ≤ x ≤ l) and the source free region (l < x ≤ Xf) beyond l, where Xf is the desired distance for computing concentration distribution. Assuming the homogeneity of urban terrain, the mean concentration of pollutant is considered to be constant along the crosswind direction and pollutant concentration does not vary in cross wind direction. 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 Xf=12000 meters in the downwind. We have taken the primary source strength Q=1 µgm⁻²s⁻¹ at ground level from an area source and the mixing height is selected as 624 meters. We assume that the pollutants undergo the removal mechanisms, such as dry deposition and gravitational settling. The pollutants are considered to be chemically reactive to form secondary pollutants by means of first order chemical conversion.

![Figure 1. Physical layout of the model.](image)

2.1 PRIMARY POLLUTANT

The basic governing equation of primary pollutant can be written as:

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

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 \( kC_p \) 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 gaseous species is converted into particulate matter. Eq. 1 is derived under the following assumptions:

a. The lateral flux of pollutants along crosswind direction is assumed to be small

i.e., \( V \frac{\partial C_p}{\partial y} \) and \( \frac{\partial}{\partial y} \left( K_y \frac{\partial C_p}{\partial y} \right) \rightarrow 0 \), where \( V \) and \( K_y \) represent the velocity and eddy-diffusivity coefficient in the y direction respectively.

b. 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.,\( U(z) \frac{\partial C_s}{\partial x} \gg \frac{\partial}{\partial z} \left( K'_s(z) \frac{\partial C_s}{\partial z} \right) \), where \( U \) and \( K_s \) are the horizontal wind velocity and horizontal eddy diffusivity along \( x \) direction respectively.

c. Vertical diffusion is greater than vertical advection since the vertical advection is usually negligible compared to diffusion owing to the small vertical component of the wind velocity.

We assume that the region of interest is free from pollution at the beginning of the emission. Thus, the initial condition is:
\[ C_p = 0 \quad \text{at} \quad t = 0, \quad 0 \leq x \leq X_0 \quad \text{and} \quad 0 \leq z \leq H, \]
(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 entering at \( x = 0 \) into the domain of interest. Thus 
\[ C_p = 0 \quad \text{at} \quad x = 0, \quad 0 \leq z \leq H \quad \text{and} \quad \forall \ t > 0. \]
(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. Hence the corresponding boundary condition takes the form:
\[ K_z \frac{\partial C_p}{\partial z} = \begin{cases} V_{dp} C_p - Q & \text{at} \quad z = 0, \quad 0 < x \leq l, \\ V_{dp} C_p & \text{at} \quad z = 0, \quad l < x \leq X_0, \end{cases}, \text{for} \ t > 0 \]
(4)

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

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

Sulphate represents an example of gas-to-particle conversion. The governing basic equation and the boundary conditions for the concentration of secondary pollutant \( C_s \), such as sulphate is described below.

### 2.2 SECONDARY POLLUTANTS

The basic governing equation for the secondary pollutant \( C_s \) is:
\[ \frac{\partial C_s}{\partial t} + U(z) \frac{\partial C_s}{\partial x} = \frac{\partial}{\partial z} \left( K'_s(z) \frac{\partial C_s}{\partial z} \right) + W_s \frac{\partial C_s}{\partial z} + V_g k C_p, \]
(6)

Eq. (6) is solved subject to initial and boundary conditions:
\[ C_s = 0 \quad \text{at} \quad t = 0, \quad \text{for} \quad 0 \leq x \leq X_0 \quad \text{and} \quad 0 \leq z \leq H, \]
(7)

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

Since there is no direct source for secondary pollutants, we have
\[ K_z \frac{\partial C_s}{\partial z} + W_s C_s = V_{ds} C_s \quad \text{at} \quad z = 0, \quad 0 \leq x \leq X_0, \quad \forall t > 0, \]
(9)

\[ K_z \frac{\partial C_s}{\partial z} + W_s C_s = 0 \quad \text{at} \quad z = H, \quad x > 0 \quad \text{and} \quad \forall t > 0, \]
(10)

where \( C_s \) is concentration of secondary pollutants \( W_s \) is the gravitational settling velocity, \( V_g \) is the mass ratio of the secondary particulate species to the primary gaseous species which is being converted and \( V_{ds} \) is the dry deposition velocity.

Our objective is to analyze the conversion of gaseous species to secondary particulate matter in the air shed. Therefore, we need to know the important mechanisms of gas-to-particle conversion in urban atmosphere and the values of reaction rate constant. The important examples of gas-to-particle conversion are:

i. Sulphate formation from SO\(_2\).

ii. Particulate organic formation from certain gaseous hydrocarbons.

iii. Nitrate formation from NO\(_X\) (NO, NO\(_2\)).

Parameters used in SO\(_2\)/Sulphate and NO\(_X\)/Nitrate simulation are given in the Table 1.

| Table 1: The values of parameters used in the analysis of the model |
The profiles of wind velocity, eddy diffusivity and other meteorological parameters, used to solve the Eqs. 1 and 6 are discussed in the next section for stable and neutral stability conditions.

3. METEOROLOGICAL PARAMETERS

The treatment of Eq. 1 mainly depends on the proper estimation of diffusivity coefficient and velocity profile of the wind near the ground/or lower layers of the atmosphere. The meteorological parameters influencing eddy diffusivity and velocity profile are dependent on the intensity of turbulence, which is influenced by the atmospheric stability.

3.1 EDDY DIFFUSIVITY PROFILES

The common characteristics 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 [23] gave such an expression, based on theoretical analysis of neutral boundary layer, in the form:

$$K_z = 0.4u_* z \eta / H$$

For stable condition, Ku et al., [24] used the following form of eddy-diffusivity:

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

where $b = 0.91$, $\eta = z / (L\sqrt{\mu})$, $\mu = u_* / |fL|$. (12)

where $H$ is the mixing height, $u_*$ is the friction velocity, $L$ is Monin-Obukhov [25] stability length parameter and $\kappa$ is the Karman’s constant $\approx 0.4$.

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 Eqs. 11 and 12 are used in this model developed for neutral and stable atmospheric conditions.

3.2 WIND VELOCITY PROFILES

In order to incorporate more 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 the velocity gradient 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 stability with $z < 0.1\kappa u_* / f$,

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

(13)

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

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

(14)

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

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

(15)

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

<table>
<thead>
<tr>
<th>Parameter</th>
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<th>NO$_x$/ nitrate</th>
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<td>$V_{dp}$ (cm/sec)</td>
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</tr>
<tr>
<td>$k$ (hour$^{-1}$)</td>
<td>0.08</td>
<td>0.03</td>
</tr>
<tr>
<td>$V_{d0}$ (cm/sec)</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
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<td>0.03</td>
<td>0.03</td>
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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.

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

where, \( u_g \) is the geostrophic wind \( z_{sl} \), \( u_{sl} \) is the wind at the top of the surface layer, \( H \) the mixing height and \( p \) is an exponent which depends upon the atmospheric stability. Jones et al., [26] suggested the values for the exponent \( p \), from the measurements made from urban wind profiles, as follows:

- \( 0.2 \) for neutral condition
- \( 0.35 \) for slightly stable flow and
- \( 0.5 \) for stable flow.

Wind velocity profiles given by Eqs. 13 to 16 due to Ragland [3] are used in this model.

4. NUMERICAL SOLUTION

We note that it is difficult to obtain the analytical solution for Eqs. 1 and 6 because of the complicated form of wind speed and eddy diffusivity profiles considered in this model. Hence, we use numerical method based on Crank-Nicolson finite difference scheme to obtain the solution. 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 grid points, the finite difference solution of the variable \( C_p \) is defined. The dependent variable \( C_p(x, z, t) \) is denoted by \( C_{p(i,j)} = C_p(x_i, z_j, t_n) \), 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 implicit Crank-Nicolson scheme to discretize the Eq. 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 Eq. 1 at the grid points \((i, j)\) and time step \(n+1/2\) can be written as:

\[
\frac{\partial C_{p}}{\partial t} \bigg|_{ij}^{n+1/2} + \frac{1}{2} \left[ U(z) \frac{\partial C_{p}}{\partial x} \bigg|_{ij}^{n+1/2} + U(z) \frac{\partial C_{p}}{\partial x} \bigg|_{ij}^{n} \right] + \frac{1}{2} \left[ \frac{\partial}{\partial z} \left( K_{z}(z) \frac{\partial C_{p}}{\partial z} \bigg|_{ij}^{n} \right) + \frac{\partial}{\partial z} \left( K_{z}(z) \frac{\partial C_{p}}{\partial z} \bigg|_{ij}^{n+1} \right) \right] \bigg|_{ij}^{n+1/2} = 0
\]

We use backward differences for advective term for this problem. Therefore we use:

\[
U(z) \frac{\partial C_{p}}{\partial x} \bigg|_{ij}^{n} = U_j \frac{C_{pj}^{n+1} - C_{pj}^{n-1}}{\Delta x}, \tag{18}
\]

and

\[
U(z) \frac{\partial C_{p}}{\partial x} \bigg|_{ij}^{n+1} = U_j \left[ \frac{C_{pj}^{n+1} - C_{pj}^{n-1}}{\Delta x} \right]. \tag{19}
\]

Also, for the diffusion term, we have used the second order central difference scheme:

\[
\frac{\partial}{\partial z} \left( K_{z}(z) \frac{\partial C_{p}}{\partial z} \bigg|_{ij}^{n} \right) = \left( K_{z}(z) \frac{\partial C_{p}}{\partial z} \bigg|_{ij}^{n} \right)_{1/2} = \frac{1}{\Delta z} \left[ K_{z}(z) \frac{C_{pj+1}^{n} - C_{pj}^{n}}{2\Delta z} - K_{z}(z) \frac{C_{pj}^{n} - C_{pj-1}^{n}}{2\Delta z} \right]. \tag{20}
\]

Hence, \( \frac{\partial}{\partial z} \left( K_{z}(z) \frac{\partial C_{p}}{\partial z} \bigg|_{ij}^{n} \right) \) can be written as:

\[
\frac{1}{2(\Delta z)^2} \left[ \left( K_{z}(z) \frac{C_{pj+1}^{n} - C_{pj}^{n}}{2\Delta z} - K_{z}(z) \frac{C_{pj}^{n} - C_{pj-1}^{n}}{2\Delta z} \right) \right].
\]
Similarly, \( \frac{\partial}{\partial z} \left( K(z) \frac{\partial C_p}{\partial z} \right) \) is given by \( \frac{1}{2(\Delta z)} \left[ (K_{j+1} + K_j) \left( C_{p_{ij+1}}^{n+1} - C_{p_{ij}}^{n+1} \right) - (K_j + K_{j-1}) \left( C_{p_{ij}}^{n+1} - C_{p_{ij-1}}^{n+1} \right) \right] \) \( (21) \)

Substituting Eqs. 18 to 21 in Eq. 17 and rearranging the terms we get the finite difference equations for the primary pollutant \( C_p \) in the form:

\[
A_j C_{p_{ij}}^{n+1} + B_j C_{p_{ij}}^{n+1} + D_j C_{p_{ij}}^{n+1} + E_j C_{p_{ij}}^{n+1} = F_j C_{p_{ij-1}}^{n} + G_j C_{p_{ij}}^{n} + M_j C_{p_{ij}}^{n-1} + N_j C_{p_{ij}}^{n},
\]

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

Here,\[
A_j = B_j = -U_j \Delta t / 2 \Delta x, \quad B_j = -\frac{\Delta t}{4 \Delta z} (K_j + K_{j-1}), \quad G_j = \frac{\Delta t}{4 \Delta z} (K_j + K_{j-1}), \quad D_j = 1 + U_j \Delta t / 2 \Delta x + \frac{\Delta t}{4 \Delta z} (K_{j+1} + 2K_j + K_{j-1}) + \frac{\Delta t}{2}, \quad M_j = 1 - U_j \Delta t / 2 \Delta x - \frac{\Delta t}{4 \Delta z} (K_{j+1} + 2K_j + K_{j-1}) - \frac{\Delta t}{2},
\]

\( \Delta t / 2 \Delta x \) and \( \Delta t / 4 \Delta z \) are the values of \( i \) at \( x = l \) and \( 0 \) respectively and \( \Delta t / 2 \) is the value of \( j \) at \( z = H \). The discretized form of Eqs. 2 to 5 are:

\[
C_{p_{ij}}^{n+1} = \frac{1}{k} \left[ 1 - V_d \frac{\Delta x}{K_j} \right] C_{p_{ij}}^{n+1} - \frac{Q \Delta z}{K_j}, \quad \text{for} \quad j = 1, 2, 3, \ldots \text{imax} \text{ and } n = 0, 1, 2, \ldots \text{ (22b)}
\]

\[
C_{p_{ij}}^{n+1} = 0, \quad \text{for} \quad j = 1, 2, 3, 4, \ldots \text{imax}, \quad n = 0, 1, 2, \ldots \text{ (22c)}
\]

\[
C_{p_{ij}}^{n+1} - C_{p_{ij}}^{n-1} = 0, \quad \text{for} \quad j = \text{imax}, \quad i = 2, 3, 4, 5, \ldots \text{imax}, \quad n = 0, 1, 2, \ldots \text{ (22d)}
\]

Eq. 22a is true for the interior grid points and Eqs. (22b) – (22d) at the boundary grid points.

The system of Eqs. 20 has a tridiagonal structure and is solved by Thomas Algorithm [27]. The ambient air concentration of primary pollutants (gaseous) is obtained for various atmospheric conditions and values of dry deposition and chemical reaction rate coefficient.

Similarly, the finite difference equations for the secondary pollutant \( C_s \) can be written as:

\[
A_j C_{s_{ij}}^{n+1} + B_j C_{s_{ij}}^{n+1} + D_j C_{s_{ij}}^{n+1} + e_j C_{s_{ij}}^{n+1} = F_j C_{s_{ij-1}}^{n} + G_j C_{s_{ij}}^{n} + M_j C_{s_{ij}}^{n-1} + N_j C_{s_{ij}}^{n} + V_k C_{v_{ij}}^{n}, \quad i = 2, 3, 4, \ldots \text{imax}, \quad j = 2, 3, 4, \ldots \text{imax} \text{-1a}
\]

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

\[
C_{s_{ij}}^{n+1} = 0, \quad \text{for} \quad i = 1, 2, 3, \ldots \text{imax}, \quad j = 1, 2, 3, \ldots \text{max} \text{ and } n = 0, 1, 2, \ldots \text{ (23a)}
\]

\[
C_{s_{ij}}^{n+1} = 0, \quad \text{for} \quad i = 1, 2, 3, \ldots \text{max}, \quad j = 2, 3, 4, \ldots \text{imax} \text{ and } n = 0, 1, 2, \ldots \text{ (23b)}
\]

\[
C_{s_{ij}}^{n+1} = 0, \quad \text{for} \quad j = \text{imax}, \quad i = 2, 3, 4, \ldots \text{imax}, \quad n = 0, 1, 2, \ldots \text{ (23c)}
\]

where,

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

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

$V_s$ is the mass ratio of the secondary particulate species to the primary gaseous species which is being converted and $W_s$ is the gravitational settling velocity of the secondary pollutant $C_s$.

The system of Eqs. 23 also has tridiagonal structure but is coupled with Eqs. 22. First, the system of Eqs. 22 is solved for $C^n_{pj}$, which is independent of the system 23 at each time step $n$. This result at every time step is used in Eqs. 23.

Then the system of Eqs. 23 is solved for $(C^n_{eq})$ at the same time step $n$. Both the system of Eqs. 22 and 23 are solved using Thomas algorithm. Thus, the solutions for primary and secondary pollutant concentrations are obtained.

We have analysed the above numerical scheme for consistency and stability. Consistency is investigated for the implicit discretization of the governing diffusion equation. The derivatives are replaced by the arithmetic average of its finite difference approximations at the $n^{th}$ and $(n+1)^{th}$ time steps. The resulting equation coincides with governing diffusion equation as $\Delta x$, $\Delta z$ and $\Delta t$ tend to zero. Hence the implicit finite difference scheme used for the solution of this model is consistent. We have used the Von Neumann’s method to study the stability analysis. Using Fourier mode analysis it is found that the employed numerical scheme is unconditionally stable. Therefore the whole scheme is unconditionally stable.

5. RESIDUAL

The difference between the exact solution and the approximate solution is called the residual. We discuss the residual when the concentration of the pollutant reaches the steady state. When the system has reached the steady state, the time derivative of the physical quantity tends to zero. When the numerical solution obtained is not exactly steady, the time discrete derivatives will not be precisely zero. The non zero value is called residual. The magnitude of the residual indicates the accuracy of the method. When computational fluid dynamics experts are comparing the relative merits of different numerical schemes, the smallest value is usually looked upon most favorably.

In this problem we obtain the steady state residual to indicate the accuracy of the Crank – Nicolson method. The concept of residual can be understood from the following procedure.

Consider the governing equation:

$$\frac{\partial C_p}{\partial t} + U(z) \frac{\partial C_p}{\partial x} = \frac{\partial}{\partial z} \left( K_i(z) \frac{\partial C_p}{\partial z} \right) - kC_p$$

(25)

When an upwind version of the Crank – Nicolson method is applied to this equation, we get:

$$\left( \frac{\partial}{\partial t} \right)_{ij}^{+1/2} = \frac{1}{2\Delta x} (C^n_{p_{i+1}} - C^n_{p_{i-1}} + C^n_{p_{i+1}} - C^n_{p_{i-j}}) + \frac{1}{4(\Delta z)^2} (K_j + K_{j-1})(C^n_{p_{i+1}} + C^n_{p_{i-1}}) + \frac{1}{4(\Delta z)^2} (K_j + K_{j+1})(C^n_{p_{i+1}} + C^n_{p_{i+1}}) - \frac{k}{2} (C^n_{p_{i+1}} + C^n_{p_{i+1}})$$

When the steady state is reached the time derivative of the physical quantity should approach zero if the solution is exactly steady. Since the numerical values of the derivative are not precisely zero, the non zero value of the time derivative is called the residual. This is the left hand side of the Eq. 25 which is computed from:

$$\left( \frac{\partial}{\partial t} \right)_{ij}^{+1/2} = \frac{C^n_{p_{i+1}} - C^n_{p_{i-1}}}{\Delta t}$$

(26)

As time progress and as the steady state is approached, the time derivative (26) should approach zero. Since the numerical value of the left hand side of Eq. 25 are not precisely zero they are called residuals [18]. We have computed
the residuals obtained after every time step against the number of time steps and analyzed in Figure 2. It is seen that the residuals settle to around $10^{-6}$.

![Figure 2. Variation of residuals verses time](image)

6. RESULTS AND DISCUSSION

In this paper, we have developed a numerical model for the primary and secondary pollutants in an urban area with a more realistic wind velocity and eddy diffusivity profile with removal mechanisms such as gravitational settling and dry deposition. The concentration distribution is computed in the source region as well as source free region till the desired distance of $X = 12000$ meters. Concentration contours are plotted and results are analysed for primary and secondary pollutants in stable and neutral conditions. The results of this numerical model are presented graphically in Figures 3 to 10 to analyse the dispersion of air pollutants in the urban area with downwind and vertical direction for stable and neutral conditions of atmosphere. In Figure 3 the effect of dry deposition on primary and secondary pollutants with respect to distance for stable case is studied. As deposition velocity increases the concentration of primary and secondary pollutants decreases. If $V_d = 0$ the ground level concentration of primary pollutants increases up to 240 and as $V_d$ increases the ground level concentration decreases very rapidly with downwind distance. The ground level concentration of secondary pollutants is high if $V_d = 0$ and as $V_d$ increases the ground level concentration decreases with downwind distance for gravitational settling velocity $W_s = 0$.  

![Figure 3. Variation of Ground level concentration with respect to distance of primary and secondary pollutants for stable case.](image)

In Figure 4 the effect of dry deposition on primary and secondary pollutants with respect to the distance for neutral case is studied. As the deposition velocity increase the concentration of primary and secondary pollutants decreases. If $V_d = 0$, the ground level concentration of primary pollutants increases up to 65 and as $V_d$ increases the ground level concentration decreases very rapidly with downwind distance. Similar effect is observed for secondary pollutants with respect to downwind distance.

The concentration of primary and secondary pollutants attains the maximum values and steadily decreases as the removal mechanism $V_d$ increases. From Figures 3 and 4 it is found that the magnitude of the concentration of primary and secondary pollutants in stable case is higher when compared to the neutral case.
Figure 4. Variation of ground level concentration with respect to distance of primary and secondary pollutants for neutral case.

In Figure 5 the effect of dry deposition on primary and secondary pollutants at a distance 3000 meters with respect to height for stable case is studied. As the deposition velocity increases the concentration of primary and secondary pollutants decreases very rapidly with respect to height. The concentration of primary and secondary pollutants is zero around $z = 40$ meters height. The concentration of primary and secondary pollutants is high near the ground level. In Figure 6 the concentration of primary and secondary pollutants for different values of dry deposition with respect to height for neutral case is studied. Similar effect is observed in neutral case as in the case of stable atmosphere but the concentration of primary and secondary pollutants is zero around the height of $z = 225$ meters. This indicates that the neutral atmosphere case enhances the vertical diffusion of primary and secondary pollutants.

In Figure 7 the ground level concentration of secondary pollutants for different values of gravitational settling and dry deposition with downwind distance for stable case is studied. The concentration of secondary pollutants decreases as gravitational settling increases. The magnitude of secondary pollutants in the case of $V_d = 0$ is higher when compare to $V_d = 0.01$. The decrease of concentration of secondary pollutants is dominant as the deposition velocity increases.

Figure 5. Variation of ground level concentration with respect to height of primary and secondary pollutants for stable case.

Figure 6. Variation of ground level concentration with respect to height of primary and secondary pollutants for neutral case.
Figure 7. Variation of ground level concentration with respect to distance of secondary pollutants for stable case

In Figure 8 the ground level concentration of secondary pollutants for different values of gravitational settling and dry deposition with downwind distance for neutral case is studied. The concentration of secondary pollutants decreases for various values of gravitational settling and dry deposition. The magnitude of the concentration of secondary pollutants is very less in neutral case as compared to stable case in Figure 7.

In Figure 9 ground level concentration of secondary pollutants for various values of $V_s$ and $W_s$ with respect to height for stable case is studied. The increase of concentration of secondary pollutants attains maximum values and then decreases for different values of $W_s$ with respect to height. The concentration of secondary pollutant is high near the ground level around $z = 3$ meters. The concentration of secondary pollutant is zero around the height 35 meters.

Figure 8. Variation of ground level concentration with respect to distance of secondary pollutants for neutral case

Figure 9. Variation of ground level concentration with respect to height of secondary pollutants for stable case
Figure 10. Variation of ground level concentration with respect to height of secondary pollutants for neutral case

In Figure 10, the ground level concentration of secondary pollutants for various values of $V_g$ and $W_g$ with respect to height for neutral case is studied. Similar effect is observed in the neutral case as in the case of stable atmosphere as depicted in Figure 9, but the concentration of secondary pollutant is zero around the height $z = 200$ meters. This indicates that the neutral case enhances vertical diffusion of secondary pollutants.

7. CONCLUSION

A two dimensional advection-diffusion numerical model for air pollution in the presence of removal mechanisms and chemical reaction of primary and secondary pollutants due to area source in an urban area for stable and neutral conditions is presented in this paper. This model analysis gives that the ground level concentration of primary pollutants attains peak value at the downwind end of the city region and decreases rapidly to a constant value over the source free region. This is due to the fact that there is no emission beyond the city limit and hence the concentration decreases asymptotically to a constant value. The concentration of primary and secondary pollutants decreases as the removal mechanisms such as dry deposition and gravitational settling velocity increases for stable and neutral cases. The concentration of primary and secondary pollutants reaches more heights in neutral case when compared to the stable atmospheric condition. This indicates that neutral atmospheric condition enhances the vertical diffusion carrying the pollutants concentration to greater heights and thus the concentration is less at the surface region.

REFERENCES


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