CHAPTER - V

NUMERICAL MODEL OF ATMOSPHERIC POLLUTANTS FOR AN AREA SOURCE OF STEADY EMISSION WITH THE REMOVAL MECHANISMS, VARIABLE WIND VELOCITY AND EDDY-DIFFUSIVITY

5.1 INTRODUCTION

In this chapter, we study the effect of removal mechanisms such as dry deposition and gravitational settling on the total ambient pollutant burden. Ermak (1977), Rao (1981) and Lee (1985) have studied removal mechanisms by means of settling velocity but with $U$ and $K_z$ constant. Dhar et al (1991) have presented a time dependent mathematical model which takes care of settling of pollutants. Khan et al (1992 b) have studied a 3-dimensional analytical model of pollutant in a stable boundary layer by incorporating the removal mechanisms of pollutant from the atmosphere by means of ground absorption and settling of larger particles. We develop here a numerical model with these removal mechanisms and study their effects on concentration distribution in an urban area.

5.2 FORMULATION /MODEL DEVELOPMENT

The basic equation of conservation of species in the presence of turbulent diffusion, using K-theory approach, is given by
\[
\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial y} + W \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left( K_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial C}{\partial z} \right) + W \frac{\partial C}{\partial z} \quad (5.2.1)
\]

where, \( C \) is the mean pollutant concentration in the air at any location \((x,y,z)\) and time \( t \). \( U, V \) and \( W \) are the components of the mean wind velocity, the \( x \)-axis of the Cartesian coordinate system is aligned in the direction of actual wind near the ground surface (East), \( y \)-axis is oriented in the horizontal cross wind direction (North/South) and the \( z \)-axis is chosen vertically upwards where, \( K_x, K_y \) and \( K_z \) are eddy diffusivity coefficients in \( x, y, z \) directions respectively.

Physical problem consists of an area source at the ground level which is spread out over the surface of the city with finite down wind and infinite cross wind dimensions. Minor sources within the area are added up and the total is assumed to be distributed evenly over the area, i.e., uniform area source. The physical description of the model is shown in Fig.5.1. In this model we have incorporated dry deposition at ground level and gravitational settling of larger size pollutant particles which are shown schematically in Fig.5.1.

In addition to the assumptions made in the previous Chapter-III, we have also assumed that the pollutants undergo to removal mechanisms/processes. They are dry deposition due to adsorption by earth’s surface terrain and gravitational settling of larger-size particle pollutants.
Under the above assumptions, the governing partial differential equation becomes,

\[
\frac{\partial C}{\partial t} + U(z) \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left( K_z(z) \frac{\partial C}{\partial z} \right) + W_s \frac{\partial C}{\partial z} \quad (5.2.2)
\]

Where,

\[ C = C(x, z, t) \] is the ambient mean concentration of pollutant species

\[ U \] - mean wind speed in x-direction

\[ K_z \] - Turbulent eddy diffusivity in z-direction

\[ Q \] - Emission rate of the pollutant species

\[ l \] - Source length/extension

\[ L \] - Desired domain/length of interest

\[ H \] - mixing height.

\[ W_s \] - Gravitational settling velocity

We assume that the region of interest is not polluted before the emission. Thus, the initial condition is

\[ C = 0 \] At \( t = 0, 0 \leq x \leq L \) and \( 0 \leq z \leq H \).

If \( C_B \) is the background concentration of the pollutant species, then

\[ C = C_B \] At \( x = 0, \ 0 \leq z \leq H \) and \( \forall t > 0 \).
Here $C_B$ is the concentration in the surrounding suburbs and/or rural area.

We assume that the pollutants are being emitted at a steady flux at the surface. The pollutant is removed across a layer at height $z = z_a$ through deposition with a deposition velocity $V_d$. The pollutant deposition on the ground surface occurs at a rate proportional to the local concentration. Thus,

$$K_z \frac{\partial C}{\partial z} - W_s C + V_d C = Q \quad \text{at } z = 0, \ 0 \leq x \leq l$$

$$K_z \frac{\partial C}{\partial z} - W_s C + V_d C = 0 \quad \text{at } z = 0, \ l \leq x \leq L$$

Where, $W_s$ is the gravitational settling velocity of larger size particle pollutant and $V_d$ is dry deposition velocity.

$$\frac{\partial C}{\partial z} = 0 \quad \text{At } z = H, x > 0 & \forall t.$$

Note that we have selected the lower boundary condition at $z_a$, the height at which a deposition velocity has been measured. A typical value of 1m is used for $z_a$. A deposition velocity ($V_d$) can be defined as an empirical function of the observed deposition rate ($W$) and concentration near the surface ($C_0$), $V_d = \frac{W}{C_0}$. The height at which $C_0$ is measured is typically about 1m. Once $V_d$ is known for a given set of conditions, the formula $W = V_d C_0$ can be used to predict dry deposition of gases and small particles, where $C_0$ would be obtained from advection-diffusion model. Particles with radii greater than about
$5 \mu m$ have significant gravitational settling speeds, here we have used $V_d = 0.01 m/sec$, independent of stability and wind speed and gravitational velocity $W_g = 10^{-2} m/sec$.

Many measurements of $V_d$ for gases have been reported by McMohan and Denisov (1979) and Sehmel (1980). Relatively inert gases, such as carbon monoxide, typically have nearly negligible deposition speeds varying from $10^{-3}$ to $10^{-4} cm/sec$. If the gas is chemically active, then, it will be of the order of 0.5 to 3 $cm/sec$. for $SO_2$, $V_d = 0.7 \ cm/sec$ in the cities, based on London data only.

### 5.3 METEOROLOGICAL PARAMETERS

To solve equation (5.2.2), it is essential to know the profiles of eddy diffusivity and wind speed for various atmospheric stability conditions and also for various meteorological parameters such as stability length, friction velocity, net heat flux, surface roughness etc. precisely. These are discussed in Chapter-III in detail and the same has been used in this model. To determine the wind speed and eddy diffusivity as accurate as possible, near the ground, two layers are considered: the surface layer and the planetary boundary layer. The surface layer extends up to 100m, sometimes much lower depending on the stability and roughness parameter, and the planetary boundary layer, which extends up to 1000m or so. It is assumed that the surface layer terminate at

$$z = 0.1k \frac{u_s}{f} \text{ For neutral stability condition,}$$

Where $k$ - Karman’s Constant $\approx 0.4$

$f$ - Carioles parameter
Friction velocity

For stable case, the surface layer extends up to \( z = 6L \), where \( L \) is the Monin-Obukhov parameter. The boundary layer extends up to mixing height, \( z = H \), for both the cases.

In the surface layer, logarithmic profiles are used for neutral stability with \( z < 0.1k \frac{u_*}{f} \)

\[
U = \frac{u_*}{k} \ln \left( \frac{z + z_0}{z_0} \right) \quad (\text{Within surface layer})
\]

For stable flow with \( 0 < \frac{z}{L} < 1 \),

\[
U = \frac{u_*}{k} \left[ \ln \left( \frac{z + z_0}{z_0} \right) + \frac{\alpha}{L} z \right]
\]

For stable flow with \( 0 < \frac{z}{L} < 6 \),

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

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

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

Where,

\( u_g \) - Geotropic wind
$z_{sl}$ - Top of the surface layer

$u_{sl}$ - wind at $z_{sl}$

$z_m$ - mixing height, H

$p$ - An exponent which depends upon the atmospheric stability.

Jones et al (1971) suggest the values for the exponent $p$, obtained from the measurements made from urban wind profiles, as follows:

- $p = 0.2$ for neutral condition
- $p = 0.35$ for slightly stable flow
- $p = 0.5$ for stable flow.

And the following eddy-diffusivity profiles are used for the entire boundary layer (surface layer and planetary boundary layer)

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

For neutral case

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

$$K_z = \frac{ku_* z}{0.74 + 4.7 z/l} \exp(-b\eta).$$

$b = 0.91, \quad \eta = z/(L \sqrt{\mu}), \quad \mu = u_* / |fL|$ and $f = 10^{-4}$, carioles parameter.
5.4 NUMERICAL SOLUTION AND VALIDATION

We have used Crank-Nicolson implicit finite difference method for the solution of the equation (5.2.2), which has been discussed in detail in chapter-II.

The governing partial differential equation (5.2.2) is

\[
\frac{\partial c}{\partial t} + U(z) \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left( K_z(z) \frac{\partial C}{\partial z} \right) + W_s \frac{\partial C}{\partial z}
\]

This can be approximated as,

\[
\frac{\partial c}{\partial t} n \mid_{ij}^{n+1/2} + U(z) \frac{\partial C}{\partial x} n \mid_{ij}^{n+1/2} = \frac{\partial}{\partial z} \left( K_z(z) \frac{\partial C}{\partial z} \right) n \mid_{ij}^{n+1/2} + W_s \frac{\partial C}{\partial z} n \mid_{ij}^{n+1/2}
\]

Using, \( \frac{\partial c}{\partial t} n \mid_{ij}^{n+1/2} = \frac{C_{ij}^{n+1} - C_{ij}^{n}}{\Delta t} \), \( U(z) \frac{\partial C}{\partial x} n \mid_{ij}^{n} = U_j \left[ \frac{C_{ij}^{n} - C_{ij}^{n-1}}{\Delta x} \right] \),

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

\[
W_s \frac{\partial C}{\partial z} n \mid_{ij}^{n} = \frac{C_{ij}^{n+1} - C_{ij}^{n}}{\Delta z},
\]

Substituting all these equations in the equation (5.4.1) and rearranging we get,
\[ A_{j} C_{i-1,j}^{n+1} + B_{j} C_{i,j}^{n+1} + D_{j} C_{i,j-1}^{n+1} + E_{j} C_{i,j+1}^{n+1} = F_{j} C_{i-1,j}^{n} + G_{j} C_{i,j-1}^{n} + M_{j} C_{i,j}^{n} + N_{j} C_{i,j+1}^{n} \]

Where,

\[ A_{j} = -\frac{U_{j} \Delta t}{2 \Delta x} ; \]
\[ F_{j} = \frac{U_{j} \Delta t}{2 \Delta x} ; \]
\[ B_{j} = -\frac{\Delta t}{4 \Delta z^{2}} (K_{j} + K_{j-1}) ; \]
\[ G_{j} = \frac{\Delta t}{4 \Delta z^{2}} (K_{j} + K_{j-1}) ; \]
\[ D_{j} = \left\{ 1 + U_{j} \frac{\Delta t}{2 \Delta x} + \frac{\Delta t}{4 \Delta z^{2}} (K_{j+1} + 2 K_{j} + K_{j-1}) + \frac{W_{j}}{2} \Delta t \right\} ; \]
\[ M_{j} = \left\{ 1 - U_{j} \frac{\Delta t}{2 \Delta x} - \frac{\Delta t}{4 \Delta z^{2}} (K_{j+1} + 2 K_{j} + K_{j-1}) - \frac{W_{j}}{2} \Delta t \right\} ; \]
\[ E_{j} = -\frac{\Delta t}{4 \Delta z^{2}} (K_{j+1} + K_{j}) ; \]
\[ N_{j} = \frac{\Delta t}{4 \Delta z^{2}} (K_{j+1} + K_{j}) ; \]

And for \( j = 1 \) and \( j = j_{\text{max}} \) and \( n = 0,1,2,3,...... \)(lower and upper boundary Conditions)

equations are,

\[ \left( 1 - W_{s} \frac{\Delta z}{K_{j}} + V_{d} \frac{\Delta z}{K_{j}} \right) C_{i,j}^{n+1} - C_{i,j+1}^{n+1} = -\frac{Q \Delta z}{K_{j}} \quad \text{For } j = 1, \ i = 2,3,4,......(i_{\text{max}})_{j}, n = 0,1,2,3,...... \]

\[ \left( 1 - W_{s} \frac{\Delta z}{K_{j}} + V_{d} \frac{\Delta z}{K_{j}} \right) C_{i,j}^{n+1} - C_{i,j-1}^{n+1} = 0 \quad \text{For } j = 1, i = (i_{\text{max}})_{j} + 1......(i_{\text{max}})_{L} \text{ and } n = 0,1,2,3,...... \]

\[ C_{i,j+1}^{n+1} - C_{i,j}^{n} = 0 \quad \text{For } j = j_{\text{max}}, i = 2,3(i_{\text{max}})_{j} + 1......(i_{\text{max}})_{L} \text{ and } n = 0,1,2,3,...... \]
The above system of equations gives a tridiagonal structure and has been solved by Thomas algorithm.

The verification of the code is ensured by as in chapter III, Section 3.5

i) Using consistent and stable numerical scheme, and

ii) Performing convergence study through residue fall and mesh-dependency analysis.

The result of the present model has been compared with the results of Ragland (1973) and chapter III and a good agreement are found.

5.5 RESULTS AND DISCUSSIONS

The results of this model are presented graphically in Figs.5.2 -5.6. The ground level concentration profiles have been plotted for stable and neutral conditions.

Fig.5.2 shows that GLC distribution for stable case with and without the removal mechanisms. The maximum concentration is observed in the presence of removal mechanisms. This is because the pollutant will be deposited to the ground by the surface terrain and settles down due to gravitation of larger size pollutant particles. As expected the concentration increases with downwind till the city limit, where the pollutant is emitted at constant rate and decreases afterwards. The variation of concentration with height is depicted in Fig 5.3 with and without removal mechanisms. At the ground level, more pollutant concentration is observed when both the removal mechanism are present and as we move upwards the concentration of pollutants will remain the same
irrespective of the presence of the removal mechanisms. This is because most of the pollutants are either absorbed or settled near the ground. The distribution of GLC and variation of pollutant concentration with heights for neutral case is shown in Figs.5.4 and 5.5. As in the case of stable atmospheric condition, the maximum concentration of pollutant is observed at ground level with the removal mechanisms for the neutral condition also. But the magnitude of concentration in the neutral condition is comparatively less than that of the stable atmospheric condition.

The effects of dry deposition and gravitational settling are depicted in Figs.5.6 for stable and neutral cases. For a fixed value of gravitational settling and increase in the dry deposition the pollutant concentration decreases rapidly (see Fig.5.5). By increasing the value of gravitational settling, the concentration profiles do not change substantially. This is due to the fact that the dry deposition possesses more dominant removal mechanism than the gravitational settling. A similar phenomenon is also observed for the variation of concentration with height (Fig.5.6). It is interesting to note that in the neutral case the effects of pollutant are felt at greater heights compared to the stable case and hence it can be concluded that the effect of removal mechanisms does not play a significant role in the neutral case than in the stable case.
Fig. 5.1: Physical Layout of the Model
GLC for neutral case ($W_S = 0.0, V_d = 0.0$)

GLC for stable case ($W_S = 0.0, V_d = 0.0$)

**Fig. 5.2:** GLC for Neutral and Stable cases
Fig. 5.3: Effect of Dry Deposition on GLC for Neutral and Stable cases

GLC for neutral case \((W_S = 0.0, V_d = 0.01)\)

GLC for stable case \((W_S = 0.0, V_d = 0.01)\)
**Fig. 5.4:** Effects of Gravitational Settling and Dry Deposition on GLC for Neutral and Stable cases

GLC for neutral case \((W_S = 0.01, V_d = 0.01)\)

GLC for stable case \((W_S = 0.01, V_d = 0.01)\)
Fig. 5.5: Effect of $W_S$ and $V_d$ increasing on GLC for Neutral and Stable cases
**Fig. 5.6:** Effect of $W_S$ and $V_d$ increasing on GLC for Neutral and Stable cases

GLC for neutral case ($W_S = 0.03, V_d = 0.03$)

GLC for stable case ($W_S = 0.03, V_d = 0.03$)