Journal of Mines, Metals and Fuels, *71(12A) : 355-369; 2023. DOI: 10.18311/jmmf/2023/43606*

Print ISSN : 0022-2755

Journal of Mines, Metals and Fuels

Contents available at: *www.informaticsjournals.com/index.php/jmmf*

Effect of Dry Deposition and Gravitational Settling Velocity on Primary and Secondary Pollutants Emitted from an Area Source in the Presence of Mesoscale Wind

Vanita R. Raikar[1,2*], K. Lakshminarayanachari[1,2], C. Bhaskar[1,2] and K. Bharathi[3]

[1]Department of Mathematics, Sai Vidya Institute of Technology, Bengaluru - 560064, Karnataka, India; vanitarraikar@gmail.com

[2]Visvesvaraya Technological University, Belagavi - 590018, Karnataka, India

[3]Department of Mathematics, UBDT College of Engineering, Davanagere - 577004, Karnataka, India

Abstract

The most crucial atmospheric phenomenon is the change of atmospheric pollutant from gaseous status into the particle shape. To study about advection and diffusion of environmental air pollutants emitted by an area resource in an urban region, a numerical model is being framed in the present article. The numerical solution of outlining differential equations is carried out using Crank-Nicolson implicit technique. The examination of results being done for the dispersion of pollutant in an urban region for atmospheric stable state as well as neutral state in presence and absence of mesoscale wind in various meteorological conditions.

Keywords: Area Source, Dry Deposition, Eddy Diffusivity, Gravitational Settling Velocity, Heat Island, Mesoscale Wind, Wet Deposition.

1.0 Introduction

Rapid growth of industry and urban development of many countries in world have created a very serious menace to the life of human beings and the surrounding atmosphere in recent years. Atmospheric contaminants namely carbon monoxide, nitric oxide, sulfur dioxide are being released continuously by the burning of fuels for domestic needs, exhausts by vehicles owing towards heavy traffic movement in urban areas, industrial wastes and several other sources pollute a part or entire urban region. Pollution aroused from an area source will affect people as well as atmosphere surrounded by the region and the people living in neighboring unpolluted rural region, as contaminants being diffused and adverted through downwind. Janice Kim *et al.*,[1] stated about contaminants emitted by vehicular traffic which are in particulate matter form, black carbon, oxides of nitrogen (NO_x) etc., have been associated with respirational symptoms, intensification of asthma and decrements in functioning of lungs in children. Small discrepancies in functioning of lung, greater risk of prolonged respiratory disease as well as augmented death rates have been connected with exposure towards particulate atmospheric pollution[2].

*Author for correspondence

Short and long-term exposure to ambient particulate matter increased the risk of cardiovascular functions evident by epidemiological studies[3]. Volatile Organic Compounds (VOCs) remain the major cause of indoor air contamination which are being responsible for various health issues comprising infection and also irritation of respirational tract, Irritation in eyes, allergies found in skin, bronchitis as well as dyspnea[4,5]. The fast-growing population among the metropolises has managed to worsen the air quality in surrounding atmosphere of the metropolitan cities. To be more specific, urban air contamination is an important aspect for changing the weather condition of the metropolises. Main metropolitan features which have reflective influence upon metropolitan weather in forming heat islands, lowering average wind speed, rise in fog frequency, creation of mesoscale circulation. In the current article a numerical representation designed for advection and diffusion of air contaminant emitting by an area source in existence of mesoscale wind is being discussed.

Most mining activities are carried out underground and above-ground. In particular particulate matters and methane gas emanations in open as well as underground mining constitute a huge part of the air contamination in mining zones. The dust resulting from the blast action in surface mining some gases being released into the atmosphere because of chemical reaction that take place due to the usage of explosives on the mining sites. These are carbon dioxide, water, nitrogen, carbon monoxide, sulphur dioxide and oxides of nitrogen. It is assessed that persons working in the mining industry are more likely to get work-related diseases due to their exposed contaminants. Mining activities contribute to the problem of air pollution directly or indirectly. The most important emissions during coal mining and through active mine fires are particulate matter, sulfur dioxide, nitrogen dioxide also heavy metals. These air pollutants worsen air quality and affect the human health, flora as well as fauna in and around coal mining regions.

Gaussian plume representation is fundamental technique in use to compute concentrations of air pollution starting from point resource[6]. Hilsmeir and Gifford articulated this estimation into additional suitable way, and this has been called as Pasquill - Gifford scheme designed for dispersal estimate and some have been extensively in use ever since[7]. The fundamental approach to develop a diffusion model for area sources is to apply conservation of mass for a definite pollutant being emitted by an area resource under appropriate boundary conditions. Venkatachalappa *et al*., gave a numerical representation for an area source due to both primary as well as secondary contaminants[8], where in point source effect being not discussed. A numerical model of atmospheric primary and secondary pollutants emitted from point source in presence of mesoscale wind along with removal mechanism, wet deposition[9]. A numerical model of pollutants emitted from an area source with chemical reaction and gravitational settling in addition with point source on the boundary presented by [10,11]. An analytical model for air pollution emitted from an elevated point source with mesoscale wind and a numerical representation for primary and secondary air contaminants released from area source and point resource with chemical reaction and elimination mechanisms[12,13].

In the present paper we have developed a model to analyze the properties of mesoscale winds on the diffusion of contaminants in an urban region using gravitational settling. For large urban areas, urban heat sources generate their own mesoscale winds. As pointed out by Griffiths[14], knowledge of large-scale winds is insufficient in order to forecast the air pollution among metropolitan areas. Griffiths has mentioned a definite incident occurred at Chicago town, where in the mesoscale occurrences played a very crucial part in determining the city contamination pattern. The present numerical model, we have discussed about primary and secondary atmospheric contaminants with large-scale airstream velocity, mesoscale airstream velocity, eddy diffusivity contours by means of different removal mechanisms like dry deposition, wet deposition also gravitational settling. The influence of mesoscale airstream is being examined for primary pollutants as well as secondary for stable and the neutral condition of atmosphere. Prevailing equations partial differentials of the representation have been deciphered by Crank–Nicolson implicit scheme. Pollutant concentrations are calculated by plotting different contours and also results being analyzed by means of mesoscale wind for different climatological parameters.

2.0 Model Development

As the course of dispersion being influenced by the prevailing flow and topographic circumstance, the physical nature as well as chemical behavior of the atmospheric pollutants will also affect the course of dispersion. The general equation used to calculate concentration of air pollutants is,

$$\frac{\partial c}{\partial t}+U\frac{\partial c}{\partial x}+V\frac{\partial c}{\partial y}+W\frac{\partial c}{\partial z} =$$

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right)-RC \qquad (1)$$

Here C refers to the pollutants concentration present in the atmosphere at any position (x, y, z) at time t. K_x, K_y and K_z be eddy diffusivity coefficients along x, y and z directions respectively. U, V and W, velocity components of wind along x, y and z direction correspondingly, R is coefficient of rate of chemical transformation. Physical problem comprises an area resource spread above the surface around metropolitan area through finite downwind distance as well as infinite cross wind dimensions. Here it's being assumed that the pollutants are emitted from area source at a constant rate and are spread within the mixing layer where in mixing takes place due to the turbulence and also convective movement of pollutants. The mixing layer ranges upwards starting from the ground surface towards a height where turbulent flux divergence dropped to zero resulting due to surface action. We have taken the region of source around the metropolitan center extending from the starting position of the origin towards a distance of l along downwind x-direction $(0 \le x \le l)$ with l=6000m. We propose to work out the concentration allotment together inside the source region and the region free from source till the preferred space X_o=12000m within the downwind where X_o being the desired distance for computing concentration distribution. A center of heat island is considered with the length $x=l/2$ at the city center. We have also considered pollutants to be chemically more reactive and get converted to secondary contaminants by first order chemical conversion. It's being assumed as removal mechanisms taking place about atmospheric pollutants namely dry settling (deposition) and wet (rain out) deposition. A schematic diagram of physical layout of current model is being depicted below by Figure 1.

2.1 Primary Pollutants

Certain assumptions made for the pollutant's dispersion in the atmosphere given below.

1. Along the crosswind direction, the tangential flux of pollutants is understood to be small that is $V\frac{\partial c}{\partial y}$ and $\frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right)\to 0$, V being the speed along y-axis, K_y coefficient of vortex diffusivity along y –axis.
2. By means of gravitational settling speed pollutants get deposited on top of ground surface.
3. Advection along horizontal direction by the current of air is greater compared to the horizontal dispersion. i.e., $U\frac{\partial c}{\partial x}\gg \frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right)$ where U, wind speed along horizontal way K_x, coefficient of vortex diffusivity alongside of x-axis.
4. Vertical dispersion is greater as compared with vertical advection, due to vertical component of wind velocity.

Under above mentioned assumptions equation (1) reduces to,

$$\frac{\partial C_p}{\partial t} + U(x,z)\frac{\partial C_p}{\partial x} + W(z)\frac{\partial C_p}{\partial z} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)-\left(k+k_{wp}\right)C_p \qquad (2)$$

Where $C\equiv C(x,z,t)$ indicate pollutant group concentration. U, represents the speed of wind along horizontal direction. W, speed of wind in vertical way. k_{wp}, coefficient of wash out about primary pollutants, k is the first order co-efficient of rate of chemical reaction for the conversion. It is assumed that the area of concern is free from contamination in the beginning of the emission. Hence, during initial stage the conditions are,

$$C_p = 0 \text{ at } t=0,\quad 0\le x\le l \text{ and } 0\le z\le H \qquad (3)$$

Where l, preferred area length along wind direction, H height where mixing take place. It is also being assumed there is no background pollution of concentration entering at x=0 into the domain of interest. Thus, we have

$$C_p = 0 \text{ at } x=0,\quad 0\le z\le H \text{ and } \forall t>0 \qquad (4)$$

Here we assumed the reactive atmospheric contaminants being chemically released on steady rate starting through ground level, being removed by

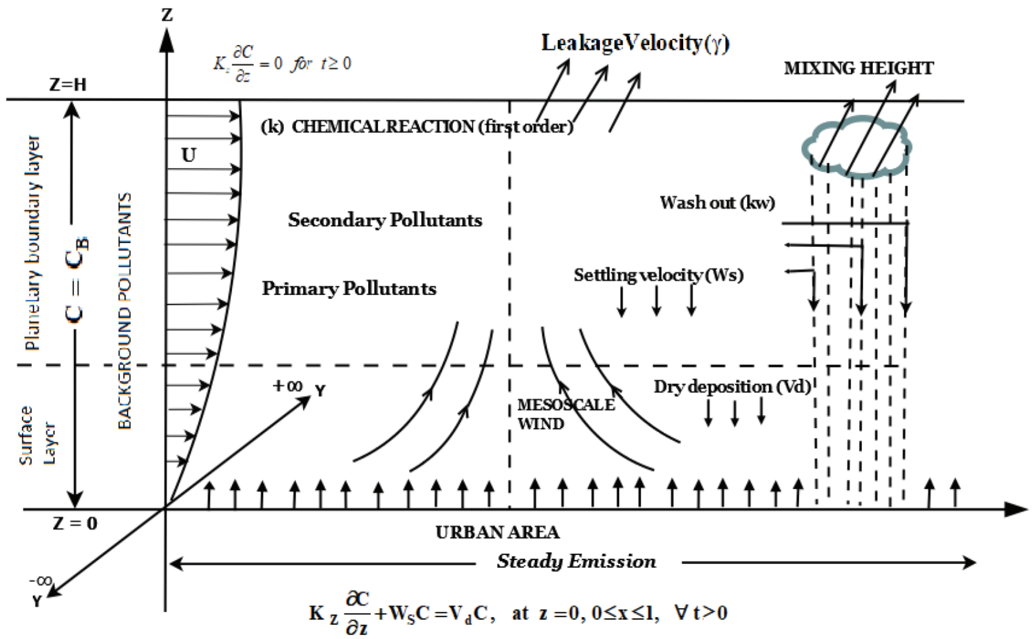

Figure 1. Physical layout of the model.

ground absorption. The resultant boundary conditions are, $K_z \frac{\partial C_p}{\partial z} + W_s C_p = V_{dp} C_p - Q$ when $z = 0, \quad 0 \leq z \leq l$, and $\forall t > 0$ (5)

With Q being emission speed of primary contaminant class, l is resource length along downwind path, V_{dp} being velocity of dry deposition for primary pollutant. Here z is considered as 20.5m. Pollutants have been restricted around mixing height, also no leakage of pollutants across upper boundary of the mixing layer. Then,

$$K_z \frac{\partial C_p}{\partial z} = 0 \text{ at } z = H, \quad x > 0 \ \forall \ t \qquad (6)$$

In equation (2), kC_p represents the transformation of pollutants in gaseous form into particulate form, with first-order chemical reaction. It's being assumed that the gaseous classes are being transformed to a particulate form.

2.2 Secondary Pollutants

The elementary governing equation meant for secondary pollutants C_s given by

$$\frac{\partial C_s}{\partial t} + U(x,z)\frac{\partial C_s}{\partial x} + W(z)\frac{\partial C_s}{\partial z} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_s}{\partial z}\right) + W_s \frac{\partial C_s}{\partial z} + V_g k C_p \qquad (7)$$

Here V_g denotes the mass ratio of secondary particulate species to primary gaseous species to which pollutants being get converted. In deriving the equation (2), the assumptions were considered as below.

1. Secondary air pollutants being formed by the first order chemical reaction rate.
2. These pollutants C_s are advected down wind and are being diffused vertically by turbulent eddies. Removal of secondary pollutants occur due to dry deposition taking place over the surface of earth via ground absorption through soil, plant life etc., gravitational settling velocity due to bigger size of contaminants.
3. By means of removal mechanism like wet deposition due to rainout or washout the elimination of secondary pollutants C_s takes place.
4. The contaminants being confined inside mixing height and hence no leakage take place across the topmost boundary of the mixing layer.
5. At the start of emission, we assume that the region of concern is considered to be free of pollution and

there exists certainly not background contamination inflowing on x=0 upon area of interest.

Under these assumptions, the initial as well as boundary conditions put on secondary pollutants C_s are as follows:

$$C_s = 0 \text{ when } t = 0,\ 0 \le x \le l \text{ and } 0 \le z \le H \tag{8}$$

$$C_s = 0 \text{ when } x = 0,\ 0 \le z \le H \text{ and } \forall t > 0 \tag{9}$$

It is well known fact that there is not any direct way for the production of secondary contaminants, then

$$K_z \frac{\partial C_s}{\partial z} + W_{gs} C_s = V_{ds} C_s \quad \text{at } z = 0,\quad 0 \le x \le l,\quad \text{and } \forall t > 0 \tag{10}$$

$$K_z \frac{\partial C_s}{\partial z} = 0,\ \text{at } z = H,\ x > 0\ \ \forall\ t > 0 \tag{11}$$

V_{ds}, is dry deposition velocity and W_{gs} gravitational settling velocity of secondary contaminants. To resolve equations (2) as well as (7) we need to use the same profiles of wind speed and vortex diffusivity for stable and also neutral conditions along with the other meteorological parameters.

3.0 Meteorological Parameters

To work out the equation (1), one should know (i) wind velocity (ii) vortex diffusivity at every grating position. The speed contour as well as vortex diffusivity depend essentially on the steadiness of the environment. The steadiness in the vicinity of ground depends mainly on net heat fluctuation. With boundary notation stability of atmosphere which is described by parameter[15]

L specified by the equation $L = \dfrac{\rho C_p T u_*^3}{\kappa g H_f}$ (12)

Where u_* velocity of the friction, H_f heat flux, C_p specific heat on fixed temperature, T being ambient temperature nearby surface, ρ density of air, κ Von Karman's constant ≈ 0.4, g is acceleration due to gravity. H_f<0 consequently L>0 signifies stable atmosphere, H_f>0, consequently L<0 represents unstable atmospheric condition and if H_f=0 and $L \to \infty$ denote the neutral state of the atmosphere. Friction velocity u_* well-defined by making use of geo-strophic coefficient of drag C_g with geo-strophic wind speed u_g as $u_*=C_g u_g$ (13)

The geo- strophic coefficient of drag C_g being function of Rossby number $R_0 = {u_g}/{z_0} f$ and L, with f as Coriolis constraint of the terrain and z_0 denote the length of surface roughness. C_g considered for neutral state of atmospheric stability by Lettau[16] suggested the empirical relationship

$$C_{gn} = \frac{0.16}{\left[\log_{10} R_0 - 1.8\right]} \tag{14}$$

The drag coefficient has been accounted the flows as:

$$C_{gus} = 1.2 C_{gn} \text{ for unstable} \tag{15}$$

$$C_{gss} = 0.8 C_{gn} \text{ for slightly stable} \tag{16}$$

$$C_{gs} = 0.6 C_{gn} \text{ for stable} \tag{17}$$

For evaluation of drag coefficient, length of surface roughness z_0 being calculated by using formula given by Lettau[17]; $z_0 = \dfrac{\bar{H} a}{2\bar{A}}$, here $\bar{H}$ refers to the effective height of roughness elements, a denotes frontal area and $\bar{A}$ being lot area which is the total area of region divided by the number of elements. Ragland[18] gave the values of heat flux H_f i.e., H_f=0 neutrally stable atmosphere; H_f=-0.06*ly/min* for stable atmosphere and H_f=-0.24*ly/min* for unstable atmosphere for urban area.

3.1 Vortex Diffusivity Profile

The eddy viscosity K_M is being defined as

$$K_M = \frac{\kappa u_* z}{\phi_M} \tag{18}$$

Here ϕ_M depends upon z/L, L being stability length parameter as given by Monin- Obukhov. Within surface layer for neutral stability condition at $< 0.1\kappa \dfrac{u_*}{f}$; $\phi_M = 1$

and $K_M = \kappa u_* z$ (19)

$\phi_M = 1 + \frac{\alpha}{L} z$ for stable atmospheric flow and $0 < \frac{z}{L} < 1$;

$$K_M = \frac{\kappa u_* z}{1 + \frac{\alpha}{L} z} \quad (20)$$

$\phi_M = 1 + \alpha$ and, $1 < \frac{z}{L} < 6$; $K_M = \frac{\kappa u_* z}{1 + \alpha}$; $\alpha = 5.2$ as shown by Webb[19] (21)

For the neutral atmospheric stability condition $z > 0.1\kappa \frac{u_*}{f}$; $K_M = 0.1\kappa^2 \frac{{u_*}^2}{f}$ (22)

For the stable atmospheric flow, z>6L till mixing height H; $K_M = \frac{6\kappa u_* L}{1 + \alpha}$ (23)

Equations from (18) - (23) give the vortex viscosity designed for the conditions required for present model. General character of k_z is linear variation in the vicinity of the ground, attains a stable value at middle assimilation deepness with declining tendency on crest once assimilation layer reached. On the basis of hypothetical study, the neutral boundary layer, Shir[20] furnished an expression of the form,

$$k_z = 0.4 u_* z e^{-4z/H} \quad (24)$$

The vortex diffusivity under stable condition by J Y Ku[21] is of the form.

$$k_z = \frac{k\ u_*\ z}{0.74 + 4.7\ z/L} e^{(-b\eta)} \quad b = 0.91 \quad \mu = z/L\sqrt{\mu}$$

$$\mu = u_*/|fL| \quad (25)$$

Vortex diffusivity profile given in equation (24) and (25) being made use of in current model, developed in support of neutral as well as stable atmospheric circumstance, H is mixing height.

3.2 Profiles of Wind Velocity

A distinguished truth is within a big metropolitan the generations of temperature cause the intensifying of air at the center of urban area and hence we can describe the urban area as a heat island. Rising air in the atmosphere creates air circulation; such flow gets over bigger height. But we are concerned barely about whatever is taking place on ground level.

Pollutant dispersion mechanisms recommend that topography of the site and meteorological situations strongly impact the concentrations of particulates. Greater concentrations of particulate matter during winter could be endorsed to low temperature and low wind speed, which leads in lowering mixing height and poor dispersion situations. During summer, particulate matter concentrations were found to be lesser than winter owing to enhanced dispersion initiated by high wind speed. The lowermost concentration was detected during monsoon, which may be credited to washout by rainfall also due to greater relative humidity which decreases re–suspension of dust particles.

To include practical structure toward velocity contour for the current representation based on Coriolis force, friction about surface, geostrophic wind stability factor z, vertical height. Integrate the velocity gradient $\frac{\partial U}{\partial z} = \frac{u_* \Phi_M}{kz}$ with lower limit z_0 to upper limit $z + z_0$ with stable state as well as neutral conditions of atmosphere to get the expression meant for wind velocity as below.

3.2.1 For Neutral Condition of Atmosphere

$$z < 0.1\kappa \frac{u_*}{f} \ ; \ u = \frac{u_*}{\kappa} \ln\left[\frac{z + z_0}{z_0}\right]$$

The Mesoscale wind W_e found by integrating continuity equation so we have

$u_e = -\left[a\left(x - x_0\right)\right]\ln\left[\frac{z + z_0}{z_0}\right]$, where **a** is a proportionality constant.

$$U\left(x,z\right) = u + u_e = \left(\frac{u_*}{\kappa} a(x - x_0)\right) \ln\left[\frac{z + z_0}{z_0}\right]$$

$$W\left(x,z\right) = W_e = a\left[z\ \ln\left[\frac{z + z_0}{z_0}\right] - \left(z + z_0\right)\ln\left(z + z_0\right)\right] \quad (26)$$

3.2.2 For Stable Condition of Atmosphere

$$0<\frac{z}{L}<1\ ;\ u=\frac{u_*}{k}\left[\ln\left(\frac{z+z_0}{z_0}\right)+\frac{a}{L}z\right]$$

$$u_e=-a\left(x-x_0\right)\ln\left[\left(\frac{z+z_0}{z_0}\right)+\frac{a}{L}z\right]$$

$$U\left(x,z\right)=u+u_e\ =\left(\frac{u_*}{\kappa}-a(x-x_0)\right)\left[\ln\frac{z+z_0}{z_0}+\frac{a}{L}z\right]$$

$$W\left(x,z\right)=W_e$$

$$=a\left[z\ln\left(\frac{z+z_0}{z_0}\right)-\left(z+z_0\right)ln\left(z+z_0\right)+\frac{a}{2L}z^2\right] \quad (27)$$

3.2.3 For Stable Condition of Atmosphere

$$1<\frac{z}{L}<6\ ;\ u=\frac{u_*}{k}\left[\ln\left(\frac{z+z_0}{z_0}\right)+5.2\right]$$

$$u_e=-a\left(x-x_0\right)ln\left[\left(\frac{z+z_0}{z_0}\right)+5.2\right]$$

$$U\left(x,z\right)=\ u+u_e$$

$$=\left(\frac{u_*}{\kappa}-a(x-x_0)\right)\ \ln\left[\frac{z+z_0}{z_0}+5.2\right]$$

$$W\left(\text{x},\text{z}\right)=W_e$$

$$=a\left[z\ln\left(\frac{z+z_0}{z_0}\right)+\left(z_0\right)\ ln\left(z+z_0\right)+4.2z\right] \quad (28)$$

In the planetary periphery layer on top of the surface layer we have employed power law system.

$$U=\left(u_g-u_{sl}\right)\left(\frac{z-z_{sl}}{H-z_{sl}}\right)^p+u_{sl} \quad (29)$$

Here u_g geo-strophic wind, u_{sl} refers wind at z_{sl}, z_{sl} denote top of surface layer, x_0 denote x- coordinate of middle of heat island, H being the mixing height and p depend on atmospheric stability. Jones[22] recommended values designed for p, obtained by measurements set on urban wind profiles like

$$\boldsymbol{p}=\begin{cases}0.2 & \textit{for neutral flow}\\ 0.35 & \textit{for slightly stable flow}\\ 0.5 & \textit{for stable flow}\end{cases}$$

3.3 Profiles of Mesoscale Wind Velocity

It is well known fact that in the metropolitan region generation of heat makes the mounting of air around the center of the metropolitan, is termed as heat island. Such rising of air creates wind circulations which get competed at longer height and are termed as mesoscale circulation. The mesoscale circulation in urban areas is schematically depicted in Figure 2. Wind velocity profiles given by the above expressions from (26) to (29) are considered here for the development of model due to Ragland[23]. Also, mesoscale wind constraint '**a**' is being taken $\boldsymbol{a}$=0.00004.

4.0 Solution by Numerical Method

To solve involved partial differential equations in the present model numerically we have used finite difference method**,** which is a simple and powerful method for solving various flow problems in regular geometries. The numerical technique that is being referred in this article is Crank-Nicolson finite difference scheme in order to solve discretized equation (2). Roache and Wendt[24] explained numerical methods in detail and the procedure adopted to solve equations (1) and (2) is given below. In this technic derivatives actuality expressed by taking averages of their finite difference approximation with n^{th} also $(n+1)^{th}$ time steps. Equation (2) can be rewritten at the grid point (i, j), and $\left(n+\frac{1}{2}\right)$ time step as,

$$\left.\frac{\partial C_p}{\partial t}\right|_{ij}^{n+\frac{1}{2}}+\frac{1}{2}\left[\left.U\left(x,z\right)\frac{\partial C_p}{\partial x}\right|_{ij}^{n}+\left.U\left(x,z\right)\frac{\partial C_p}{\partial x}\right|_{ij}^{n+1}\right]$$

$$+\frac{1}{2}\left[\left.W\left(x,z\right)\frac{\partial C_p}{\partial z}\right|_{ij}^{n}+\left.W\left(x,z\right)\frac{\partial C_p}{\partial z}\right|_{ij}^{n+1}\right]$$

$$= \frac{1}{2}\left[\frac{\partial}{\partial x}\left(K_z(z)\frac{\partial C_p}{\partial z}\Big|_{ij}^{n}\right)+\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\Big|_{ij}^{n+1}\right)\right] - \frac{1}{2}\left(k+k_{wp}\right)\left(C_{pij}^{n}+C_{pij}^{n+1}\right)$$

For $i=1,2,3,\cdots,\ j=1,2,3,\cdots and\ n=0,1,2,\cdots$ (30)

Using $\frac{\partial C_p}{\partial t}\Big|_{ij}^{n+\frac{1}{2}} = \frac{C_{ij}^{n+1}-C_{ij}^{n}}{\Delta t}$ (31)

$$U(x,z)\frac{\partial C_p}{\partial x}\Big|_{ij}^{n} = U_j\left[\frac{C_{ij}^{n} - C_{i-1,j}^{n}}{\Lambda x}\right] \quad (32)$$

$$U(x,z)\frac{\partial C_p}{\partial x}\Big|_{ij}^{n+1} = U_j\left[\frac{C_{ij}^{n+1} - C_{i-1,j}^{n+1}}{\Delta x}\right] \quad (33)$$

And

$$W(x,z)\frac{\partial C_p}{\partial z}\Big|_{ij}^{n} = W_j\left[\frac{C_{ij}^{n} - C_{ij-1}^{n}}{\Delta z}\right] \quad (34)$$

$$W(x,z)\frac{\partial C_p}{\partial x}\Big|_{ij}^{n+1} = W_j\left[\frac{C_{ij}^{n+1} - C_{ij-1}^{n+1}}{\Delta z}\right] \quad (35)$$

Also $kC_p\Big|_{ij}^{n+\frac{1}{2}} = k\left[\frac{C_{ij}^{n} + C_{ij}^{n+1}}{2}\right]$ (36)

$$k_{wp}C_p\Big|_{ij}^{n+\frac{1}{2}} = k_{wp}\left[\frac{C_{ij}^{n} + C_{ij}^{n+1}}{2}\right] \quad (37)$$

And second order central difference for

$$\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C}{\partial z}\right)\Big|_{ij}^{n} = \frac{1}{4(\Delta z)^2}\left\{\begin{matrix}(K_{j+1}+K_j)(C_{ij+1}^{n}-C_{ij}^{n})\\ -(K_j+K_{j-1})(C_{ij}^{n}-C_{ij-1}^{n})\end{matrix}\right\} \quad (38)$$

$$\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C}{\partial z}\right)\Big|_{ij}^{n+1} = \frac{1}{4(\Delta z)^2}\left\{\begin{matrix}(K_{j+1}+K_j)(C_{ij+1}^{n+1}-C_{ij}^{n+1})\\ -(K_j+K_{j-1})(C_{ij}^{n+1}-C_{ij-1}^{n+1})\end{matrix}\right\} \quad (39)$$

Equation (30) can be rewritten as

$$A_{ij}C_{pi-1,j}^{n+1}+B_jC_{pij-1}^{n+1}+D_{ij}C_{ij}^{n+1}+E_jC_{pij+1}^{n+1} = F_{ij}C_{i-1j}^{n}+G_jC_{pij-1}^{n}+M_{ij}C_{ij}^{n}+N_jC_{pij+1}^{n} \quad (40)$$

For each $i=1,2,3,\cdots imax$, for each $j=1,2,3,\cdots jmax-1$, and $n=0,1,2,3,\cdots$

Here, $A_{ij}=-\left[U_{ij}\frac{\Delta t}{2\Delta x}+W_{ij}\frac{\Delta t}{2\Delta z}\right]$:

$$B_j=-(k_j+k_{j-1})\frac{\Delta t}{4(\Delta z)^2}:$$

$$E_j=-(k_{j+1}+k_j)\frac{\Delta t}{4(\Delta z)^2}$$

$$F_{ij}=U_{ij}\frac{\Delta t}{2\Delta x}+W_{ij}\frac{\Delta t}{2\Delta z}:$$

$$G_{ij}=(k_j+k_{j-1})\frac{\Delta t}{4(\Delta z)^2}:$$

$$V_j=(k_{j+1}+k_j)\frac{\Delta t}{4(\Delta z)^2}$$

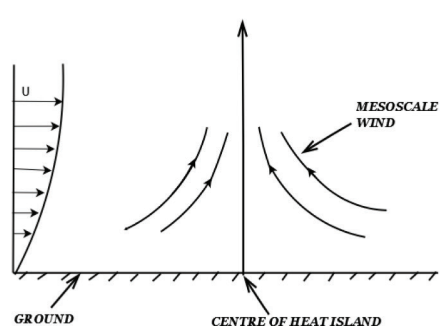

Figure 2. Urban mesoscale wind circulation.

$$D_{ij} = 1 + U_{ij}\frac{\Delta t}{2\Delta x} + W_{ij}\frac{\Delta t}{2\Delta z} + \left(k_{j+1} + 2k_j + k_{j-1}\right)\frac{\Delta t}{4\left(\Delta z\right)^2} + \left(k + k_{wp}\right)\frac{\Delta t}{2}$$

$$M_{ij} = 1 - U_{ij}\frac{\Delta t}{2\Delta x} + W_{ij}\frac{\Delta t}{2\Delta z} - \left(k_{j+1} + 2k_j + k_{j-1}\right)\frac{\Delta t}{4\left(\Delta z\right)^2} - \left(k + k_{wp}\right)\frac{\Delta t}{2}$$

*i*max is 'i' value about $x=l$ also *j* max is value of '*j*' at $z=H$.

Condition (3) imply $C^{o}_{pij}=0$ for $j=1,2\cdots j_{max}$ and $i=1,2,\cdots (imax)_i\ldots\ldots (imax)_l$

Condition (4) imply $C^{n+1}_{pij}=0$ for $j=1,2\cdots jmax$, $i=1$ and $n=0,1,2,\cdots$. Condition (5) imply

$$\left(1+\left(V_d - W_s\right)\frac{\Delta z}{k_j}\right)C^{n+1}_{pij} - C^{n+1}_{pij+1} = Q\frac{\Delta z}{k_j} \text{ for } j=1,$$

$i = 2,3,\cdots imaxl,\ n = 0,1,2,\ldots.$

Boundary Condition (6) imply $C^{n+1}_{pijmax-1} - C^{n+1}_{pijmax} = 0$,

for $j = jmax,\ i = 2,3,\cdots,imaxl,\ n = 0,1,2,\cdots$

A similar technique is adopted to get the finite difference equations for the secondary contaminant C_s about the partial differential equation (7) which can be written as

$$\frac{\partial C_s}{\partial z}\Big|_{ij}^{n+\frac{1}{2}} + \frac{1}{2}\left[u(x,z)\frac{\partial C_s}{\partial x}\Big|_{ij}^{n} + u(x,z)\frac{\partial C_s}{\partial x}\Big|_{ij}^{n+1}\right] + \frac{1}{2}\left[w(x,z)\frac{\partial C_s}{\partial z}\Big|_{ij}^{n} + w(x,z)\frac{\partial C_s}{\partial z}\Big|_{ij}^{n+1}\right]$$
$$= \frac{1}{2}\left[\frac{\partial}{\partial x}\left(K_z(z)\frac{\partial C_s}{\partial z}\Big|_{ij}^{n}\right) + \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_s}{\partial z}\Big|_{ij}^{n+1}\right)\right] + \frac{1}{2}\left[W_s\frac{\partial C_s}{\partial z}\Big|_{ij}^{n} + W_s\frac{\partial C_s}{\partial x}\Big|_{ij}^{n+1}\right] + \frac{1}{2}\left[V_g k\left(C^n_{pij} + C^{n+1}_{pij}\right)\right]$$

$i = 2,3,4,\cdots,imax$, *for* each j

For each $= 2,3,4,\cdots, jmax - 1\, and\, n = 0,1,2,\cdots$ (41)

Equation (41) can be rewritten as,

$$\bar{A}_{ij}C^{n+1}_{si-1,j} + \bar{B}_j C^{n+1}_{si,j-1} + \bar{D}_{ij}C^{n+1}_{si,j} - \bar{E}_j C^{n+1}_{si,j+1} = \bar{F}_{ij}C^n_{i-1j} + \bar{G}_j C^n_{sij-1} + \bar{M}_{ij}C^n_{si,j} + \bar{N}_j C^n_{si,j+1} \quad (42)$$

For each $i = 1,2,3,\cdots imax$ and $j = 1,2,3,\cdots jmax - 1$ and $n = 0,1,2,3,\cdots$

imax is the '*i*' value about $x=l$ also *j* max is the value of '*j*' at $z=H$.

Here, $\bar{A}_{ij} = -\left[U_{ij}\frac{\Delta t}{2\Delta x} + \left(W_j - W_S\right)\frac{\Delta t}{2\Delta z}\right]$:

$$\bar{B}_j = -\left(k_j + k_{j-1}\right)\frac{\Delta t}{4\left(\Delta z\right)^2}:$$

$$\bar{E}_{ij} = -\left(k_{j+1} + k_j\right)\frac{\Delta t}{4\left(\Delta z\right)^2}$$

$$\bar{F}_{ij} = U_{ij}\frac{\Delta t}{2\Delta x} + \left(W_j - W_S\right)\frac{\Delta t}{2\Delta z}:$$

$$G_{ij} = \left(k_j + k_{j-1}\right)\frac{\Delta t}{4\left(\Delta z\right)^2}:$$

$$\bar{N}_j = \left(k_{j+1} + k_j\right)\frac{\Delta t}{4\left(\Delta z\right)^2}$$

$$\bar{D}_{ij} = 1 + U_{ij}\frac{\Delta t}{2\Delta x} + \left(W_{ij} - W_S\right)\frac{\Delta t}{2\Delta z} + \left(k_{j+1} + 2k_j + k_{j-1}\right)\frac{\Delta t}{4\left(\Delta z\right)^2} - \left(V_g k\right)\frac{\Delta t}{2}$$

$$M_{ij} = 1 - U_{ij}\frac{\Delta t}{2\Delta x} - \left(W_{ij} - W_S\right)\frac{\Delta t}{2\Delta z} - \left(k_{j+1} + 2k_j + k_{j-1}\right)\frac{\Delta t}{4\left(\Delta z\right)^2} + \left(V_g k\right)\frac{\Delta t}{2}$$

The initial condition and boundary conditions for secondary contaminant C_S : The condition (8) imply $C^0_{sij}=0$ for $j=1,2,3,\ldots j_{max}$; $i=1,2,3,\ldots,(imax)_{i\ldots}(imax)_P$, $n=0,1,2,\ldots$

Condition (9) imply $C^{n+1}_{sij}=0$ for $i=1$, $j=1,2,\ldots j_{max}$ and $n = 0,1,2,\cdots$

Condition(10) imply

$$\left(1+\left(V_{ds}+W_{gs}\right)\frac{\Delta z}{k_j}\right)C_{sij}^{n+1}-C_{sij+1}^{n+1}=0 \quad \text{for}$$

$j=1, i=2,3,\cdots imax \cdots imaxl$

Boundary condition (11) imply $C_{sij-1}^{n+1}-C_{sij}^{n+1}=0$, for

$j=jmax$ and $i=2,3,...imax,...imaxl$

5.0 Results and Discussion

In computing the concentration of pollutants present about atmosphere along downwind also in the vertical direction released from an area resource through washout mechanisms with mesoscale wind as well as course of transformation, a numerical model has been presented in this document. The developed numerical mathematical model designed for primary as well as secondary pollutants in the atmosphere in an urban region comprises realistic wind velocity and also vortex diffusivity profile. The physical state of the problem contains an area resource, spread over the metropolitan through finite downwind distance along with infinite cross wind magnitudes. It's being assumed that the contaminants are released with constant speed from an area source and spread within the mixing layer adjacent to the earth's surface where mixing happens as a result of turbulence and convective motion. This mixing layer ranges upwards from the surface to a height where turbulent flux divergences resulting from surface action have been practically fallen to zero. The model is being solved by using Crank-Nicolson technique, which is unconditionally stable. The concentration distribution is calculated both in the source area and source free area till the preferred distance X_0. Here we have taken grid size 75meters along x-direction and 1meter along z- direction. Based on the grid independence study the solution is obtained using 160×624 grids.

Concentration contours are plotted, and results are analyzed for primary and secondary contaminants in stable and neutral atmospheric states for a number of meteorological parameters, terrain categories and also removal mechanisms namely deposition velocity and gravitational settling velocity. The pollutants are assumed to be released at a constant speed from a uniformly spread area source over a busy urban region. We have considered the source area extending up to $l=6km$ downwind starting from the origin and source free region at the outskirts of the city ($x>l$). We have computed concentration of the pollutants till the desired downwind distance $X_0=12km$. Appropriate boundary conditions have been employed to take into account the impact of ground level area source several removal mechanisms. Here the primary resource strength $Q=1\mu gm^{-2}s^{-1}$ on ground by an area resource with mixing height considered to be 624 meters.

Figure 3 depicts the variation of the concentration against distance and height for primary and secondary pollutants under stable atmospheric condition. Here we studied the consequence of dry deposition V_d on the contaminants against distance and height. It is being noticed that whenever deposition rate increases, then concentration of contaminants starts decreasing. When $V_d=0$, the primary contaminant's concentration rises upto $250\mu gm^{-3}$and as V_d assumes the values from 0 to 0.01 the concentration decreases rapidly with the downwind distance designed for gravitational settling $W_s=0$. Same kind of effect being noticed in secondary pollutants. Similarly for $W_s=0$ the concentration of pollutants with respect to height also studied. The primary pollutant's concentration decreases with increase in the velocity of dry deposition. For $V_d=0$ the concentration reaches a peak value of $160\mu gm^{-3}$ and decreases as V_d increases. But incase of secondary pollutants the concentration is very very less.

Figure 4 depicts the dry deposition effect on pollutants against distance and height in neutral state is being studied. We notice that deposition velocity increases from $V_d=0$ to $V_d=0.01$ then there will be decreases in the concentration of primary contaminants from $225\mu gm^{-3}$ to $185\mu gm^{-3}$ that is as deposition speed increases then concentration decreases quickly with downwind distance. Same kind of result is seen in case of secondary pollutants.

It has been observed that the effect of dry deposition on the primary pollutants is to the left of centre of heat island where the effect of mesoscale wind is less. Due to the presence of mesoscale wind at the centre of heat island the reduction in the concentration of secondary pollutants, which is clear from the Figure that at distance $x=450m$ the decrease in the concentration of secondary pollutants is noticed. The effect of dry deposition on the concentration of pollutants with respect to height indicates that as V_d increases the concentration of pollutants decreases. For primary pollutants the peak value of $160m$ is attained and is gradually redused to zero when height $h=2m$ is reached. In the case of secondary pollutants the peak value is attained at $h=3.5m$ with concentration being very very less. From Figure 3 and Figure 4 it is observed that the magnitude of

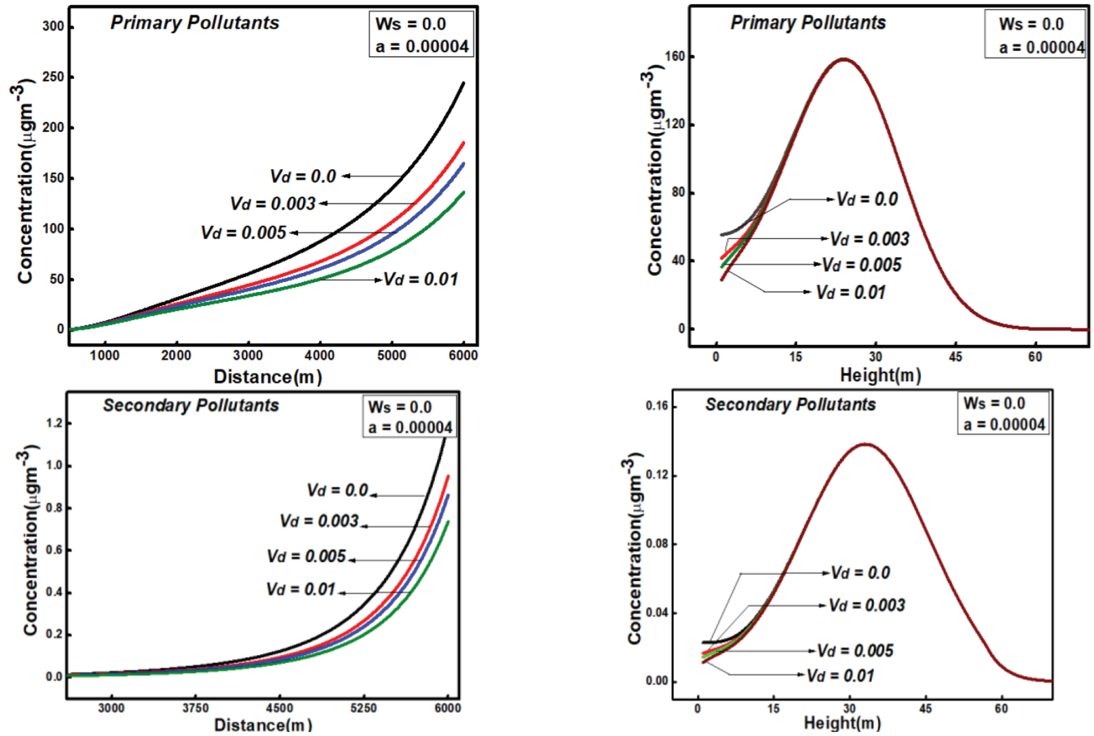

Figure 3. Ground-level concentration versus distance and height for stable atmospheric condition.

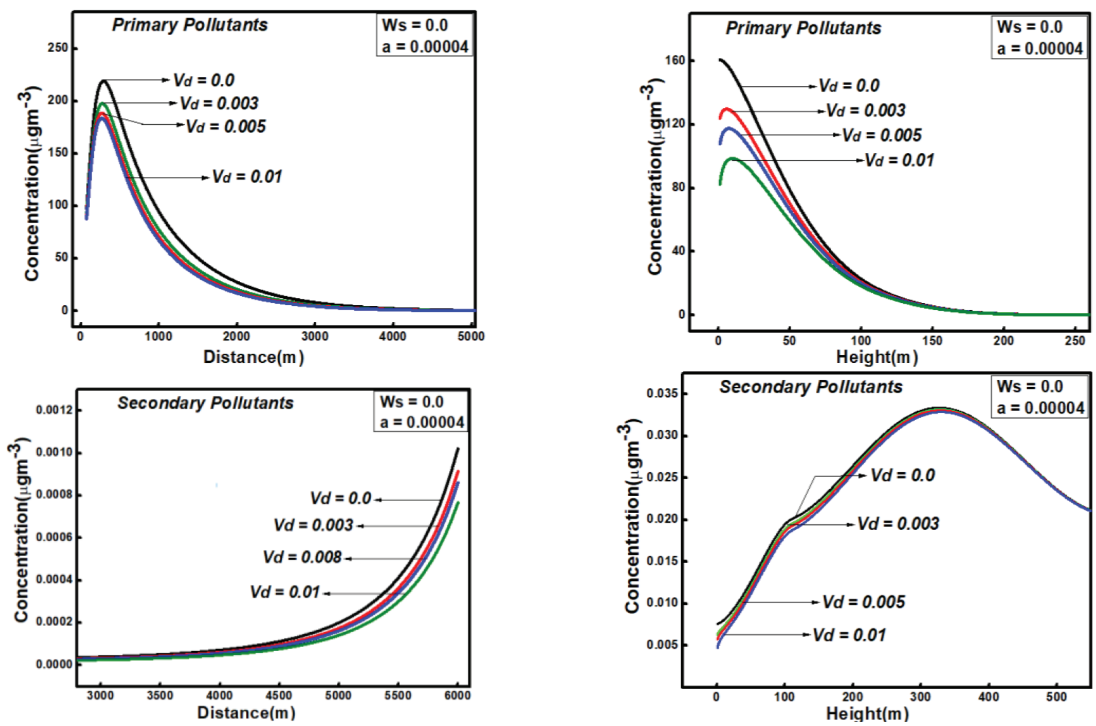

Figure 4. Ground-level concentration versus distance and height for neutral atmospheric condition.

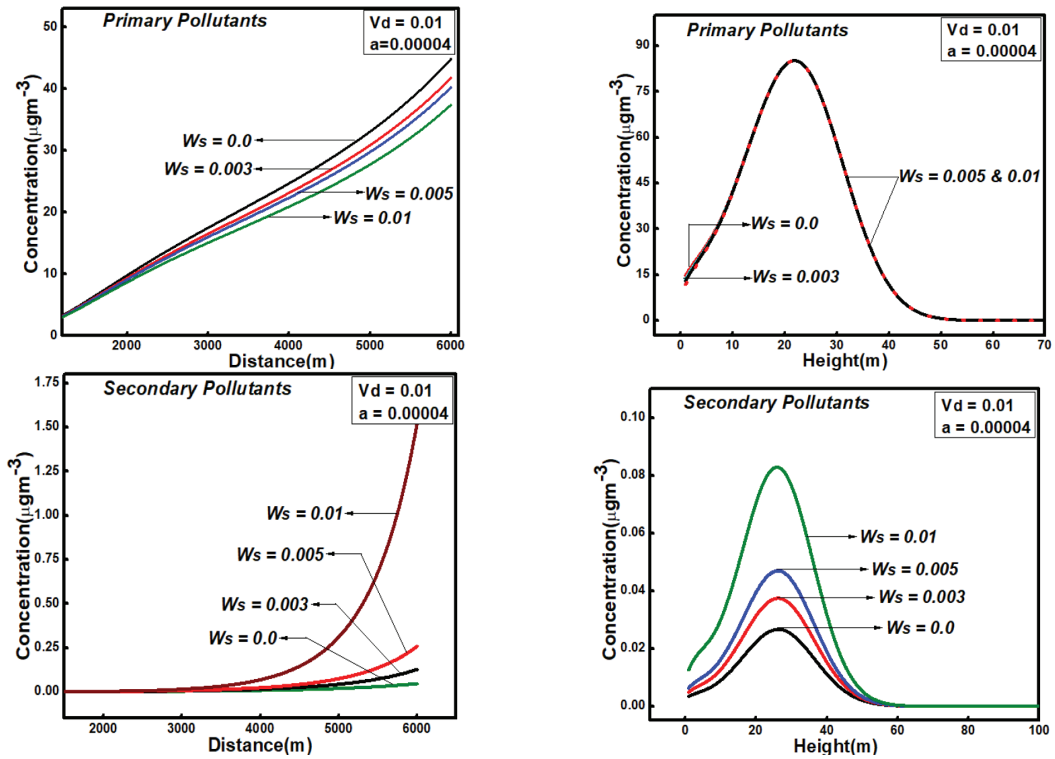

Figure 5. Ground-level concentration versus Distance and Height for stable atmospheric condition.

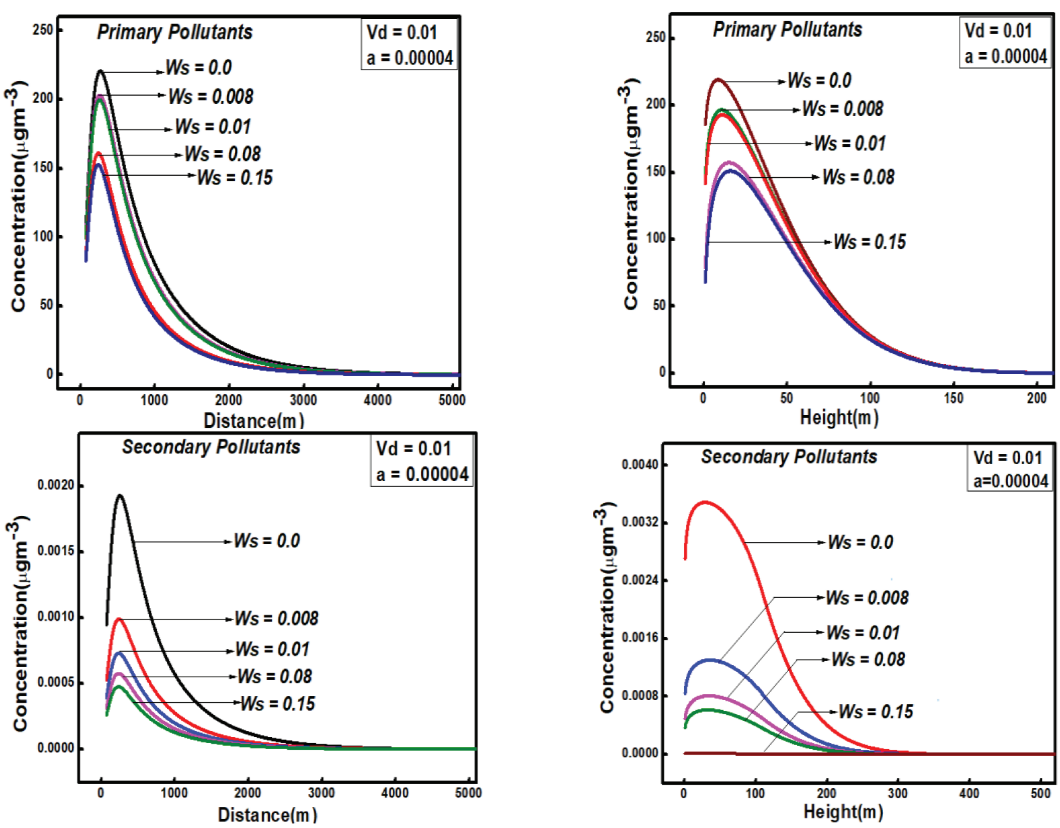

Figure 6. Ground-level concentration versus Distance and Height for neutral atmospheric condition.

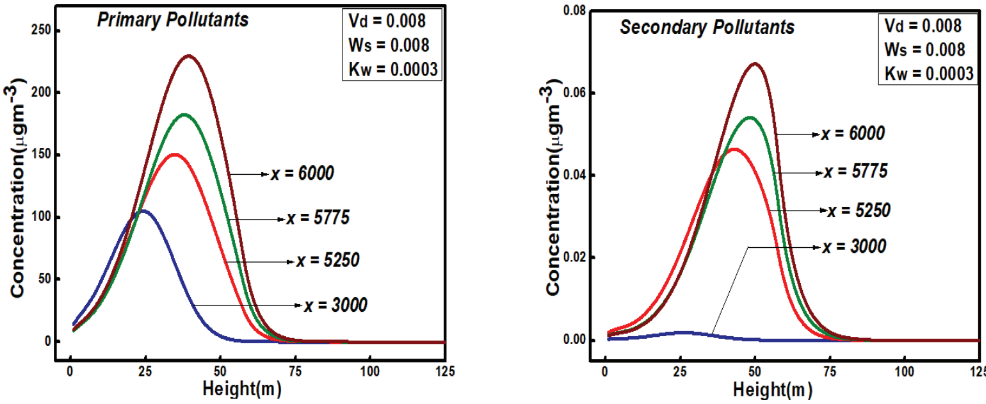

Figure 7. Ground-level concentration versus Height for stable atmospheric condition for different values of x with constant removal mechanisms.

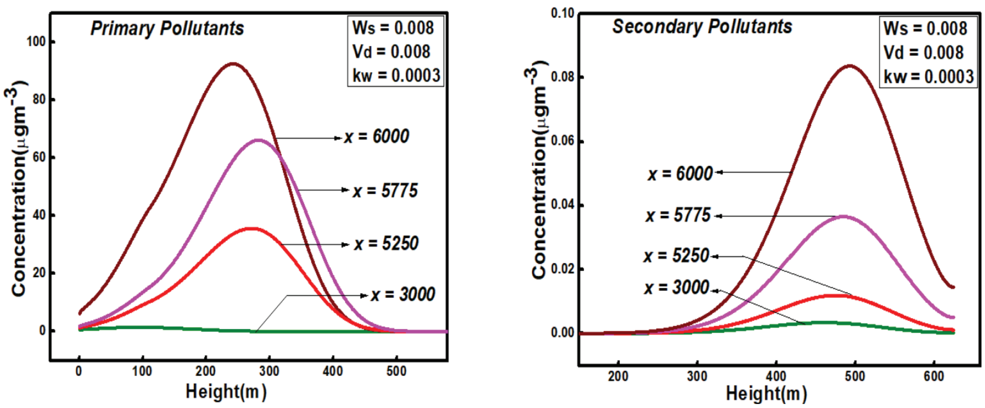

Figure 8. Ground-level concentration versus Height for neutral atmospheric condition for different values of x with constant removal mechanisms.

primary pollutant's concentration in stable case is greater than neutral case.

Figure 5 shows the ground level concentration of both primary contaminants as well as secondary contaminants for not same values of W_s with V_d=0.01 for stable atmospheric condition with downwind distance and height is studied. We observed that the concentration of both pollutants decrease as the value of gravitational settling velocity W_s increase. Also it is clear from the Figure that the concentration of secondarypollutants decreases as the distance reaches x=3500m and it becomesalmost zero when x=6000m, city area limit which indicates that existence of mesoscale wind causes the reduction in magnitude of concentration of pollutants in the urban city. Similarly the variation of concentration against height shows the magnitude of concentration touches a peak value 80 μgm^{-3} for primary pollutants. And for secondary pollutants the magnitude of concentrations very very less as compared to primary pollutants. When height reaches 50m the graph of concentration of pollutants against height becomes straight line maens concentration is zero.

Figure 6 depicts the concenration for primary as well as secondary pollutants for various values of gravitational setteling velocity W_s, for dry deposition velocity V_d=0.01 under neutral atmospheric condition with downwind distance and height is being studied. The effect noticed in neutral state is same as stable atmosphric state but secondary contaminant's concentration comes to zero when height reaches 325m and 210m for primary pollutants.

From Figures 5 and 6 the increase of dry deposition velocity has significant role because the concentration of pollutant decreases almost zero for larger values of deposition velocity. Thus deposition velocity is dominant when compared to settling velocity.

Figures 7 and 8 depict the ground level concentration against height for four different distances for constant values in removable mechanisms namely W_s=0.008, V_d=0.008 and k_w=0.0003 under stable atmospheric condition and neutral atmospheric condition. In the case of stable state, the primary pollutants reach the peak value 230 μgm^{-3} of concentration is attained when height h=45m, where as for secondary pollutants the peak value is reached when h=50m and concentration becomes zero for the height h=75m both for primary and secondary pollutants. Also, it is being noticed that as the distance rises along with height the concentration of contaminants will also be rises, but the magnitude of secondary pollutant is very low.

Similar effect is observed for neutral atmospheric condition, but peak values are observed at much higher heights. The concentration of contaminants presents in a smaller amount as compared with atmospheric stable condition. This indicates neutral case enhances the vertical diffusion of pollutants. Also we observe that concentration of pollutants is less at the center of heat island which is due to the presence of mesoscale circulation at the center of the urban city.

6.0 Conclusions

A numerical two-dimensional representation being designed for atmospheric pollutants released by an area resource using mesoscale as well as large scale wind by gravitational settling and dry deposition is being presented. The article is concerned about realistic form of variable wind profiles as well as eddy diffusivity profiles. Analysis of this article gives concentration of atmospheric primary contaminant which achieves peak rate at the downwind end of resource region but above source free area it drops quickly towards a constant value. Here more emphasis is put on the consequences of gravitational settling velocity, dry deposition and wet deposition on both primary and secondary pollutants over an urban city. The results have been examined for stable and neutral condition of atmospheric air in an urban region. The effect of gravitational settling, dry deposition and wet deposition on primary and secondary pollutants is such that the amount of contamination decline in an urban city as the wet deposition enhance through height and also atmospheric state. We noticed enrichment of vertical dispersion of primary contaminants as well as secondary contaminants in neutral state in the presence of mesoscale winds.

The combined effect of wet deposition of primary pollutant and settling of larger sized particles at larger distances is to reduce the concentration roughly any values of settling velocity as well as rate of wet deposition. Such results would help in order to know more about the problems related with acid rains. It is observed that the amount of concentration of contaminants is much more in stable state than in the neutral state of atmosphere. From air pollution point of view, it can be concluded that stable condition of atmosphere is unfavorable and neutral atmospheric condition is being favorable for survival of animals, human beings and plants in urban area.

It is possible to lessen the factors which cause air contamination in the mining sector to a certain suitable level. Hence constant measurement should be employed depending on the emission resource, Particulate matter releases/factors must be ascertained according to the source, and dust lessening techniques must be applied depending on the kind of the activity. To safeguard workers from inevitable exposure to dust, it is essential to identify and examine risks by making many measurements as far as possible. Thanks to advancing sensor technology, it is easy to screen air quality levels at each production phase. It is being possible to create the working as well as environmental circumstances of the enterprises healthy and safe by inspecting the ecological effects of mining undertakings with cloud-backed uninterrupted measurement systems.

7.0 References

1. Kim JJ, Smorodinsky S, Lipsett M, Singer BC, Hodgson AT, Ostro B. Traffic related air pollution near busy roads-the east bay children's respiratory health study. Am J Respir Crit Care Med. 2004; 170:520-6. https://doi.org/10.1164/rccm.200403-281OC
2. Pope ICA, Dockery DW, Schwartz J, Routledge. Review of epidemiological evidence of health effects of particulate air pollution. Inhalation Toxicology. 1995; 7:1-18
3. Brook RD, Franklin B, Cascio W, Hong Y, Howard G, Lipsett M, Luepker R, Mittleman M, Samet J, Smith Jr SC, Tager I. Air pollution and cardiovascular disease: A statement for healthcare professionals from the expert panel on population and prevention. Sci Amer Heart Assoc. 2004; 109:2655-71. https://doi.org/10.1161/01.CIR.0000128587.30041.C8
4. Oke TR. Boundary layer climates. Inhalation Toxicology. 1995; 7:1-18.
5. Molders N, Olson MA. Impact of urban effects on precipitation in high latitudes. Journal Hydrometeorology. 2004; 5:409-

29. https://doi.org/10.1175/1525-7541(2004)005<0409:IOUEOP>2.0.CO;2

6. Morgenstern P, Morgenstern L, Chang KM, Barrett DH, Mears C. Modeling analysis of power plants for compliance extensions in 51 air quality control. J Air Pollut Control Ass. 1975; 25(3):287–91. https://doi.org/10.1080/00022470.1975.10470087
7. Hilsmeir W, Gifford F. Graphs for estimating atmospheric dispersion. USAEC, Division of Technical Information. 1962; ORD-549.
8. enkatachalappa M, Khan SK, Kakamari KAG. Time dependent mathematical model of air pollution due to area source with variable wind velocity and eddy diffusivity and chemical reaction. Proceedings of the Indian National Science Academy. 2003; 69(A6):745-58.
9. Raikar VR, Pandurangappa C, Lakshminarayanachari K. Point source numerical model of primary and secondary pollutants emitted from the point source in the presence of mesoscale wind and wet deposition. Materials Today: Proceedings. https://doi.org/10.1016/j.matpr.2020.10.665
10. Pandurangappa C, Lakshminarayanachari K. Mathematical Model for an area source and the point source in an urban area. IJRET. 2012; 20–8.
11. Lakshminarayanachari K, Sudheer Pai KL, Siddalinga Prasad M, Pandurangappa C. A two-dimensional numerical model of primary pollutant emitted from an urban area source with mesoscale wind, dry deposition and chemical reaction. Atmospheric Pollution Research. 2013; 4:106-16. https://doi.org/10.5094/APR.2013.011
12. Bhaskar C, Lakshminarayanachari K, Pandurangappa C. Analytical approach for air pollution emitted from an elevated point source with mesoscale wind. Journal of Computational and Theoretical Nano Science, American Scientific Publishers. 2018; 15:3553-7. https://doi.org/10.1166/jctn.2018.7662
13. Bhaskar C, Lakshminarayanachari K. Numerical model for primary and secondary air pollutants emitted from an area source and point source in an urban area with chemical reaction and removal mechanisms. Materials Today: Proceedings. https://doi.org/10.1016/j.matpr.2020.08.706
14. Griffiths JF. Problems in urban air pollution, in: AIAA 8th Aerospace Science Meeting. AIAA, Paper No.70-112, New York.
15. Monin AS, Obukhov AM. Basic laws of turbulent mixing in the ground layer of the Atmosphere. Dokl Akad, SSSR. 1970; 151:163.
16. Lettau HH. Wind profile, surface stress and geostrophic drag coefficients in the atmospheric surface layer. Advances in Geophysics. 1959; 6:241-57. https://doi.org/10.1016/S0065-2687(08)60111-9
17. Lettau HH. Physical and meteorological basis for mathematical models of urban diffusion processes. Proceedings of symposium on Multiple Source Urban Diffusion models, USEPA Publication AP-86; 1970.
18. Ragland KW. Multiple box model for dispersion of air pollutants from area sources. Atmospheric Environment. 1973; 7:1071. https://doi.org/10.1016/0004-6981(73)90213-8
19. Webb EK. Profile relationships: the long-linear range and extension to strong stability. Quart JR Met Soc. 1970; 9667.
20. Shir C. A preliminary numerical study of atmospheric turbulent flows in the idealized planetary Boundary layer. Atmospheric Science. 1973; 30.
21. Ku JY, Rao ST, Rao KS. Numerical simulation of air pollution in urban areas; model development. Atmospheric Environment. 1987; 21(1):201-14. https://doi.org/10.1016/0004-6981(87)90287-3
22. Jones PM, Larrinaga MAB, Wilson CB. The urban wind velocity profile. Atmospheric Environment. 1971; 5:89-102. https://doi.org/10.1016/0004-6981(71)90164-8
23. Ragland KW, Dennis RL. Point source atmospheric diffusion model with variable and diffusivity profiles. Atmospheric Environment. 1975; 9:175. https://doi.org/10.1016/0004-6981(75)90066-9
24. Roache PJ. Computational fluid dynamics. Hermosa publications; 1976.
25. Raikar VR, Pandurangappa C, Lakshminarayanachari K, Bharathi K. Effect of gravitational settling velocity on primary and secondary pollutants emitted from the point source in the presence of mesoscale wind-communicated with journal.