TEST Engineering & Management

January - February 2020
ISSN: 0193 - 4120 Page No. 9764 - 9772

Numercal Model for Airpollutnt Emitted from an Area and Point Source in an Urban Area with Chemical Reaction and Removal Mechanisms

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Article Info
Volume 82
Page Number: 9764 - 9772
Publication Issue:
January-February 2020

Article History
Article Received*: 18 May 2019*
Revised*: 14 July 2019*
Accepted*: 22 December 2019*
Publication*: 14 February 2020*

Abstract

An inclusive numerical mathematical model of primary pollutants is presented. This model allows the estimation of the pollutants dispersionradiated from area and point source in city region. Theeddy diffusivity and realistic wind velocity profiles are taken in current model. The intricate problem is simplified numerically with Crank-Nicolson finite difference technique. In stable and neutral atmospheric conditions pollutant concentration is maximum on the boundary of point sourceand as well asat bottom surface.

Keywords; *Mathematical model, Point source, Area source, chemical reaction, Finite difference method.*

I. INTRODUCTION

Air pollution is most important problem among the worldwide and it is becoming more dangerous as it causes on living organisms and its surroundings. Due to drastic enhance of industries and motor vehicles flying on the road, these effects of pollutants are shown on the grown cities [1]. For instance, in Indian capital city new Delhi in the month of November 2017 fog is enclosed complete city due to this so many vehicles crash one another and could not able to find things 10m apart . With these effects the government planned use of vehicles in odd days to control the emission of pollutants from vehicular traffic. In 2017Test match Sri Lanka versus India,Srilankan players came to the field with protection of mask to avoid the pollution.This is the first time in cricket history that cricketers covering masks and playing, due to this some Sri Lankanplayers struggled with bad health conditions. The rising occurrence of Asthma is associated with a rapid growth of industries and fuel vehicles [2]. Volatile organic compounds [vocs] are the particles normallycomprising 1-18 carbon particleswhich are freely volatize from liquidor solid state are the keysources of indoor air pollution and due to many adverse effects including irritation and infection of lungs,allergic skin reaction, irritation to eyes, bronchitis and dyspnea [3],[4],[5].

An atmospheric diffusion numerical model for an air pollutant radiant from area and point source at origin is presented.Emission source is in the form of area source which is circulated with down distance.Initially we use the basic methods to calculate the concentration of air

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pollution in the nonexistence of removal mechanism at the point source is Gaussian plume model ([6],[7],[8]). Pasquill published his rates of dispersion over open level terrain than usage of Gaussian plume model started to obtain the fame [9].Gifford and Hilsmeier[10] explains these estimations marginally more suitable, although accurately samewhich is known as Pasquill–Gofford system and used extensively ever since to estimate the dispersion. Sardei and Runca presented a point source time dependent air pollution numerical model [11]. For their study point source condition are in the form of delta function which can be estimated by single step function having source width Δz_k. Arora [12] formed point source Gaussian distribution, but this model containing point source at the center of vertical grid spacing and uniformed on left side of the city boundary. There is a chance to miss the grid points at source since source is accumulated at random point. To overwhelm this we can consider one of subsequent ways. First technique is pollutant source of Gaussian distribution at the initial line which is corresponding to the above point source and second technique is allocating the point source to its adjacent two grid points on the boundary of the city. In this model we considered second technique procedure the source at its adjacent two grid points on the city boundary. The importance of forming a dispersion model of area source is puton conservation of mass for a specific contaminant being released from an area source with suitable boundary conditions. Venkatachalappa et al give a numerical model for area source due to primary and secondary pollutants [13]. In this model does not give point source effect. Lakshminarayanachari et al developed numerical model of area and point source with primary and secondary pollutants [14]. In their study they have not considered the mesoscale wind effect.

Thus in this paper we are developing a two-dimensional mathematical model of primary pollutants the removal by the chemically reactive nature of pollutants and the effect of mesoscale wind with large scale wind on the pollutants dispersion of area and point source emission. The realistic forms of variable profiles of wind velocity and eddy diffusivity are used here. We employ the finite difference technique by Crank-Nicolson to solve the problem numerically. Here the solution describes the concentration of area and point source pollutants downwind and infinite crosswind on the ground.

II. DEVELOPMENT OF MODEL

This problem haspoint and area source on the ground with finite downwind distance and infinite crosswind dimension.It is assumed that the contaminants transported horizontallyin perpendicular direction by a large-scale windand both horizontally and vertically by a local wind which is generated by urban heat island called mesoscale wind effect. The center of the city i. e., $x = \frac{l}{2}$is considered as the center of heat island, where l is the length of the city. We have taken the city length in this problem as $l = 6\ km$ and the concentration of pollutants is calculated in the region $0 \leq x \leq l$. The point source of pollutants is kept on z- axis at $x = 0$ and z=20.5 meters that is at the beginning of the city and the industrial stack height respectively. The description of physical layout of this problem is as shown in the figure1.

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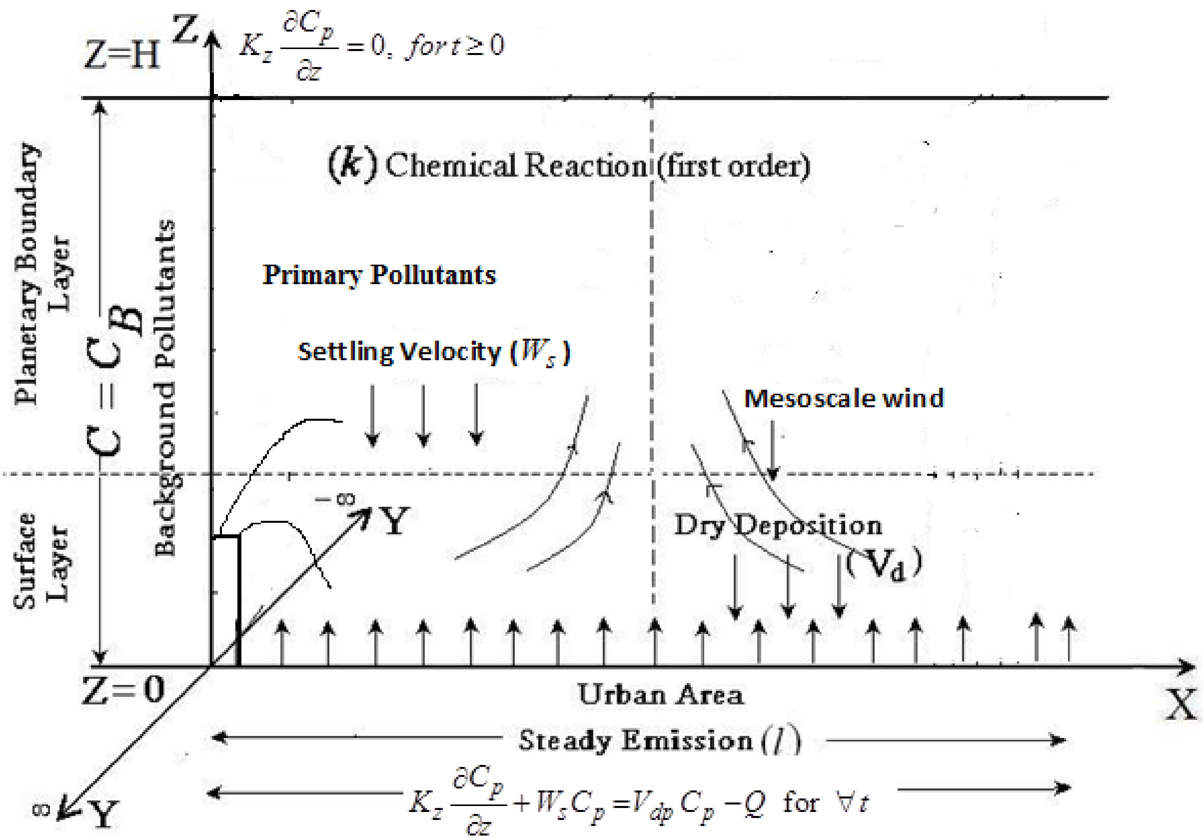

Figure 1: Physical layout of the model.

The general species diffusion equation for air pollution is

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial c}{\partial y} + W\frac{\partial c}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right) - kC \quad (1)$$

Where C is the concentration of pollutant, U, V and W are the components of velocity K_x, K_y and K_z are the coefficients of eddy – diffusivity along x, y and z directions respectively and k is the chemical reaction rate coefficient.

Now the following assumptions were formulated

- Pollutants are chemically reactive.
- The velocity of wind along the x direction is so large that the x direction diffusion is neglected.
- The pollutant lateral flux along cross wind direction is considered as small, thus $V\frac{\partial C}{\partial y} \to 0$ and $\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) \to 0$
.

A. Primary Pollutant

The basic governing equation (1) under the above formulation for primary pollutant is given as

$$\frac{\partial C_p}{\partial t} + U(x,z)\frac{\partial C_p}{\partial x} + W(z)\frac{\partial C_p}{\partial z} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right) - kC_p \quad (2)$$

Where $C_p = C_p(x,z,t)$ represents primary pollutant species concentration, $U(x,z)$ denotes the velocity along horizontal direction and $W(z)$ denotes the velocity in the vertical direction because of the effect of mesoscale wind.

B. Initial and boundary conditions of Primary pollutants

We presume that the region considered is pollution free at the commencement of the emission. Hence we get initial condition as:

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

The point source boundary condition located at origin and $z = 20.5$ meters of strength Q_1 (in

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the z-direction which has an infinitesimally small extension) is as follows

$C_p = Q_1 \frac{\partial (z-h)}{U(x,z)}$,at $x = 0$, $z = h$and $\forall t > 0$ (4)

At the ground, we assume there is an emission of chemically reactive pollutants$Q$ at constant rate and they removed by settling velocity W_s and dry deposition velocity V_{dp}.

$K_z \frac{\partial C_p}{\partial z} + W_s C_p = V_{dp} C_p - Q$atz $= 0$, $0 \leq x \leq l, \forall t > 0$ (5)

The pollutants are restricted with in the mixing height and at the top of the boundary there is no leakage.Hence

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

III. METEOROLOGICAL PARAMETERS

The profiles of large-scale, mesoscale wind speeds and eddy diffusivity for a variety of atmospheric stability situations and for a variety of meteorological parameters such as surface roughness, friction velocity, stability length, heat flux etc. are considered in accordance with Pandurangappa C [15] are used to solve the equations (2).

It is considered for neutral atmospheric stability that the surface layer ends at$z = 0.1\kappa(\frac{u_*}{f})$ and for stable atmospheric condition of stability the surface layer extended up to $z = 6L$, where $\kappa = 0.4$ the Karman's constant, friction velocity is u_*, Coriolis parameter is$f$ and Monin-Obukhov stability length parameter is$L$.

For neutral atmospheric condition of stability the following wind velocity profiles are used

$U(x,z) = \left(\frac{u_*}{\kappa} - a(x - x_0)\right) \ln\left[\frac{z + z_0}{z_0}\right]$(7)

$W(z) = a\left[z \ln\left[\frac{z + z_0}{z_0}\right] - z + z_0 \ln(z + z_0)\right]$(8)

Where$z < 0.1\kappa(\frac{u_*}{f})$

For stable atmospheric stability condition the wind velocity profiles used are

$U(x,z) = \left(\frac{u_*}{\kappa} - a(x - x_0)\right)\left[ln\left(\frac{z + z_0}{z_0}\right) + \frac{\alpha}{L}z\right]$ (9) and

$W(z) = a\left[z \ln\left[\frac{z + z_0}{z_0}\right] - z + z_0 \ln(z + z_0) + \right.$ *α2Lz2* (10) for*0<zL<1* and for $1 < \frac{z}{L} < 6$ we have

$U(x,z) = \left(\frac{u_*}{\kappa} - a(x - x_0)\right)\left[ln\left(\frac{z + z_0}{z_0}\right) + 5.2\right]$ (11)and

$W(z) = a\left[z \ln\left[\frac{z + z_0}{z_0}\right] + z_0 \ln(z + z_0) + 4.2z\right]$ (12)

For both neutral$\left(z \geq 0.1\kappa(\frac{u_*}{f})\right)$ and stable $\left(\frac{z}{L} \geq 6\right)$ atmospheric condition of stability above the surface layer (planetary boundary layer) the wind profiles used are

$U(x,z) = \left[(u_g - u_{sl}) - a(x - x_0)\right]\left(\frac{z - z_{sl}}{H - z_{sl}}\right)^p + (1 - a(x - x_0))u_{sl}$ (13)

and

$W(z) = a\left[\left(\frac{z - z_{sl}}{p + 1}\right)\left(\frac{z - z_{sl}}{H - z_{sl}}\right)^p + zu_{sl}\right]$(14)

Here geostrophic wind velocityis u_g, upper surface layerisz_{sl} ,mixing heightis H,$u_{sl}$is wind at $z_{sl}$and an exponent$p$ hinge on the stability of atmosphere. Here p values are used as with Jones et al. [11]. All these wind velocity profiles from (7) to (14) are valid only for$x \leq \frac{u_*}{a\kappa} + x_0$

For both surface and planetary boundary layer the eddy diffusivity profiles used are$k_z = 0.4\, u_* z e^{-4z/H}$, for neutral case (Shir [16]) (15)

And $k_z = \frac{k\ u_*\ z}{0.74 + 4.7\ z/L} e^{(-b\eta)}$, for stable case (Ku et al. [17]) (16)

Where$b = 0.91 \eta = {}^{z}/_{L\sqrt{\mu}}$ and$\mu = {}^{u_*}/_{|fL|}$ and $f = 10^{-4}$

IV. METHOD OF SOLUTION

Advection numerical model is meant to study and examine the concentration of chemically reactive primary air pollutants from area and point source with mesoscale type wind. For this we need to solve equation (2) with initial and boundary conditions (3) to (6). It is tedious to obtain the analytical solutions from (2) to (6) due to the variable wind speed and diffusivity forms. Thus we have used finite difference scheme of Crank-Nicolson based on numerical method to obtain the solutions of (2). Now to apply this scheme we

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take a set of equivalent rectangles of side Δx *and* Δz by subdividing the continuum region of interest,by equidistant grid lines parallelto $x$and$z$axis,given as$x_i = (i-1)\Delta x, i = 1,2,3,\ldots$..and$z_j = (j-1)\Delta z, j = 1,2,3,\ldots$..respectively.Time is indexed with time stepΔt as$t_n = n\Delta t, n = 0,1,2,3,\ldots$.. now replace the equation (2) by equation feasible at$\left(n+\frac{1}{2}\right)$th time step and at the interior grid points (i,j) takes the below form

$$\left.\frac{\partial C_p}{\partial t}\right|_{ij}^{n+\frac{1}{2}} + \frac{1}{2}\left[\left.U(x,z)\frac{\partial C_p}{\partial x}\right|_{ij}^{n} + \left.U(x,z)\frac{\partial C_p}{\partial x}\right|_{ij}^{n+1}\right] + \frac{1}{2}\left[\left.W(z)\frac{\partial C_p}{\partial z}\right|_{ij}^{n} + \left.W(z)\frac{\partial C_p}{\partial z}\right|_{ij}^{n+1}\right] = \frac{1}{2}\left[\left.\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)\right|_{ij}^{n} + \left.\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)\right|_{ij}^{n+1}\right] - \frac{1}{2}k\left(C_{pij}^{n} + C_{pij}^{n+1}\right)$$

For $i = 2,3,4,5,\cdots i\,max,\ j = 2,3,4 \cdots j\,max - 1\ and n = 0,1,2,\cdots$ (17)

Here the time derivative is substituted by a central difference with $\left(n+\frac{1}{2}\right)$time step and the spatial derivatives are converted by the arithmetic mean of its finite difference equations at the$n$and $\left(n+\frac{1}{2}\right)$ time steps.

$$\left.\frac{\partial C_p}{\partial t}\right|_{ij}^{n+\frac{1}{2}} = \frac{C_{pij}^{n+1} - C_{pij}^{n}}{\Delta t}, \quad (18)$$

$$U(x,z)\left.\frac{\partial C_p}{\partial x}\right|_{ij}^{n} = U_{ij}\left[\frac{C_{pij}^{n} - C_{pi-1j}^{n}}{\Delta x}\right], \quad (19)$$

$$U(x,z)\left.\frac{\partial C_p}{\partial x}\right|_{ij}^{n+1} = U_{ij}\left[\frac{C_{pij}^{n+1} - C_{pi-1j}^{n+1}}{\Delta x}\right], (20)$$

$$W(z)\left.\frac{\partial C_p}{\partial z}\right|_{ij}^{n} = W_j\left[\frac{C_{pij}^{n} - C_{pij-1}^{n}}{\Delta z}\right], (21)$$

$$W(z)\left.\frac{\partial C_p}{\partial z}\right|_{ij}^{n+1} = W_j\left[\frac{C_{pij}^{n+1} - C_{pij-1}^{n+1}}{\Delta z}\right], (22)$$

$$\left.\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)\right|_{ij}^{n} = \frac{1}{2(\Delta z)^2}\{(K_{j+1} +$$
KjCpij+1n−Cpijn−Kj+Kj−1Cpijn−Cpij−1n, (23)

$$\left.\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)\right|_{ij}^{n+1} = \frac{1}{2(\Delta z)^2}\{(K_{j+1} +$$
KjCpij+1n+1−Cpijn+1−Kj+Kj−1Cpijn+1−Cpij−1n+1 ,(24)

Substituting the equations (18) to (24) in (17) and simplifying and rearranging we attain concentration C_p of primary pollutant in the form of finite difference equation

$$A_{ij}C_{pi-1j}^{n+1} + B_jC_{pij-1}^{n+1} + D_{ij}C_{pij}^{n+1} + E_jC_{pij+1}^{n+1} = F_{ij}C_{pi-1j}^{n} + G_jC_{pij-1}^{n} + M_{ij}C_{pij}^{n} + N_jC_{pij+1}^{n} (25)$$

For each $i = 2,3,4,\cdots imax,\ j = 2,3,4,\cdots jmax - 1,$ and $n = 0,1,2,3,\cdots$

$A_{ij} = -U_{ij}\frac{\Delta t}{2\Delta x}$,$B_j = -\left[\left(K + K_{j-1}\right)\frac{\Delta t}{4(\Delta z)^2} + \right.$ *Δt2ΔzWj* , *Fij= UijΔt2Δx,*

$G_j = \left[\left(K_j + K_{j-1}\right)\frac{\Delta t}{4(\Delta z)^2} + \frac{\Delta t}{2\Delta z}W_j\right]$, $N_j = \left[\left(K_j + K_{j+1}\right)\frac{\Delta t}{4(\Delta z)^2}\right]$,$E_j = -\left[\left(K_j + \right.\right.$ *Kj+1Δt4Δz2,*

$D_{ij} = 1 + U_{ij}\frac{\Delta t}{2\Delta x} + W_j\frac{\Delta t}{2\Delta z} + \left(K_{j+1} + 2K_j + K_{j-1}\right)\frac{\Delta t}{4(\Delta z)^2} + k\frac{\Delta t}{2}$,

$M_{ij} = 1 - U_{ij}\frac{\Delta t}{2\Delta x} - W_j\frac{\Delta t}{2\Delta z} - \left(K_{j+1} + 2K_j + \right.$ *Kj−1Δt4Δz2−kΔt2* .

imax is value of i when $x = l$and jmax is value of j when$z = H$.

The initial condition (3) is written as

$C_{pij}^{0} = 0$ with$j = 1,2,\cdots\cdots jmax,\quad i = 1,2,\cdots\cdots imax$ (26)

The boundary conditions (4) to (6)

$C_{pij}^{n+1} = \frac{Q_1}{2u_{ij}}fori = 1,\ j = j_s, j_{s+1}$ and$n = 0,1,2,\cdots\cdots$ (27)

$C_{pij}^{n+1} = 0$ for$i = 1,\ j = 1,2,3,\ldots\ldots j_{s-1}, j_{s+2}\ldots\ldots jmax$ and $n = 0,1,2,\cdots\cdots$ (28)

$\left(1 + (V_{dp} + W_s)\frac{\Delta z}{K_j}\right)C_{pij+1}^{n+1} - C_{pij}^{n+1} = Q\frac{\Delta z}{K_j}$,for$j = 1,\ i = 1,2,3,\ldots imax$ and $n = 0,1,2,\cdots\cdots$(29)

$C_{pij-1}^{n+1} - C_{pij}^{n+1} = 0$ for$j = j\,max,\ i = 2,3,\ldots, imax$(30)

V. RESULTS AND DISCUSSION

A comprehensive two-dimensional mathematical model has been developed for calculating the primary air pollutants

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concentration from area and point source emission along downwind and vertical directions with mesoscale type wind, chemical reaction and undergoing gravitational settling of pollutants. The model developed here uses more realistic meteorological conditions for estimating the concentration distribution of pollutants. The unconditionally stable Crank-Nicolson finite difference method is applied to solve the model presented here with grid size$\Delta x = 75$meter and $\Delta z = 1$ meter. The first order back difference scheme is applied to approximate the advective terms and the diffusion terms are approximated by using the central difference scheme in the basic equations (2) and (6). Then we get a discretized algebraic equation in tri-diagonal matrix form and we solved this efficiently by using Thomas algorithm. The results of this mathematical model are described graphically in figures 2 - 5 to examine the dispersion of primary pollutants for stable and neutral conditions of atmosphere.

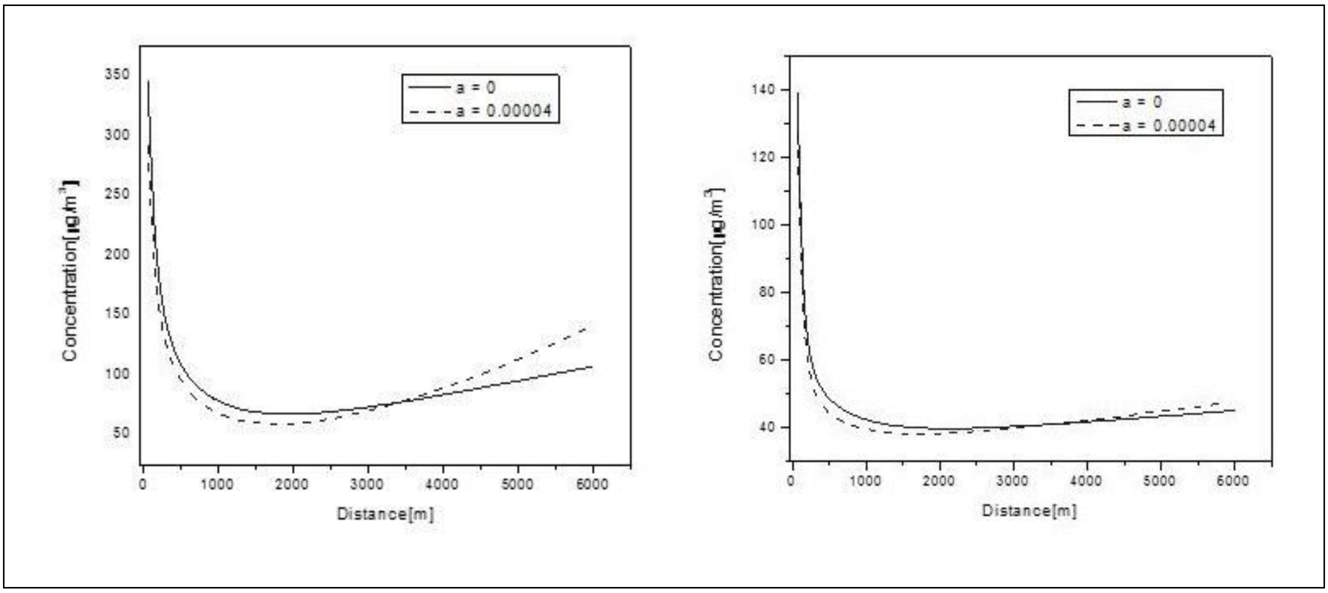

Figure 2: Concentration versus Distance with and without mesoscale wind for stable and neutral cases at z=20m

The Figure 2 demonstrates consequence ofthe mesoscale wind on pollutant concentration against distance in the nonexistence of removal mechanism in both atmospheric conditions isexamined. Theconcentration of pollutant is minimum in the existence of mesoscale wind (a=0.00004) associated to that in the nonexistence of mesoscale wind (a=0) at height z=20m. It happens due to mesoscale wind horizontal components are with large scale from left against to that with right side.

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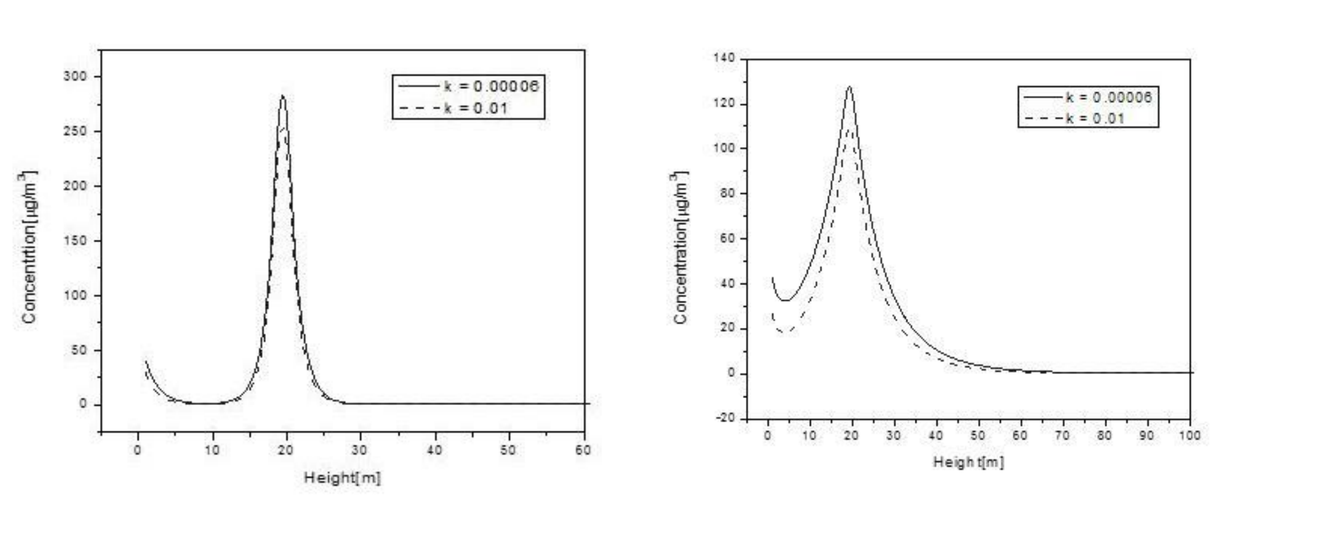

Figure 3: Concentration versus Heightfor different values of K in stable and neutral cases at x=75m

It is evident from the figure 3 that the chemical reaction rate coefficients effect on concentration of primary pollutants in stable and neutral case are presented. Since we kept point source at x= 0 and at z=20.5, in both atmospheric conditions pollutants the concentration is high near 20.5 meter height. Initially pollutants concentration at bottom surface is approximately 40 $\mu g\ /m^3$ and then gently decrease .In stable condition pollutant concentration is zero near 10 meter height and then raises up to 20.5meters and again reaches zero near 30 meter height. In stable case as coefficient of chemical reaction rate raises there is no much effect on concentration of pollutants at the point source. This happens due to raising the chemical reaction coefficient value is much smaller when related with continuous emission of point source.The pollutantsconcentrationin neutral case attains zero at 75m height. This is due to the fact that neutral case supports and hence increases vertical diffusion at the higher altitude.

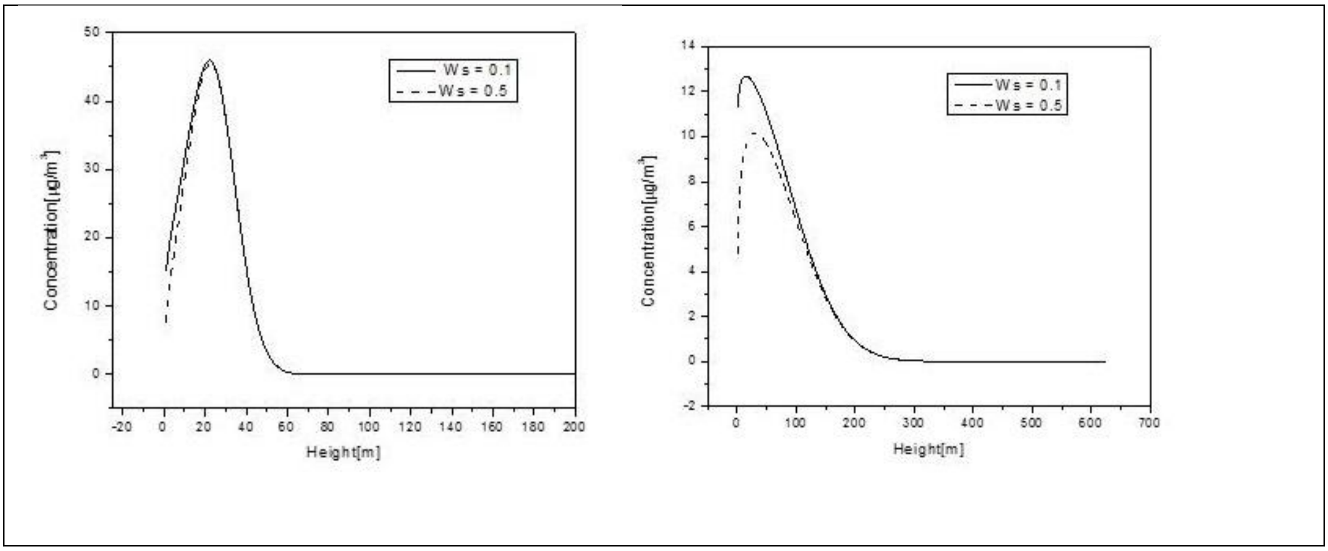

Figure 4: Concentration versus Height for different settling velocities in stable and neutral cases at x=2250.

It is evident that from figure 4 that the gravitational settling velocity effect on concentration for stable and neutral cases are presented. Since we kept point source at x= 0 and at z=20.5, in both atmospheric conditions pollutants concentration is high near 20.5 meter height. As heightraises, thepollutant concentration reduces due to removal mechanism and diffusion. In stable atmospheric case near the bottom surface concentration is less and raising up to 20.5 meter

Published by: The Mattingley Publishing Co., Inc.

January - February 2020
ISSN: 0193 - 4120 Page No. 9764 - 9772

height. The pollutant concentration decreases beyond 20.5m and attains zero near 70m height in stable case. In neutral case also we observed the same effect. But concentration of pollutants is zero around 300m height in neutral case. This is due to the fact that neutral case supports and hence increases vertical diffusion at the higher altitude. In stable condition, the primary pollutantsconcentration is more comparing to the neutral case for similar set of values of distance.

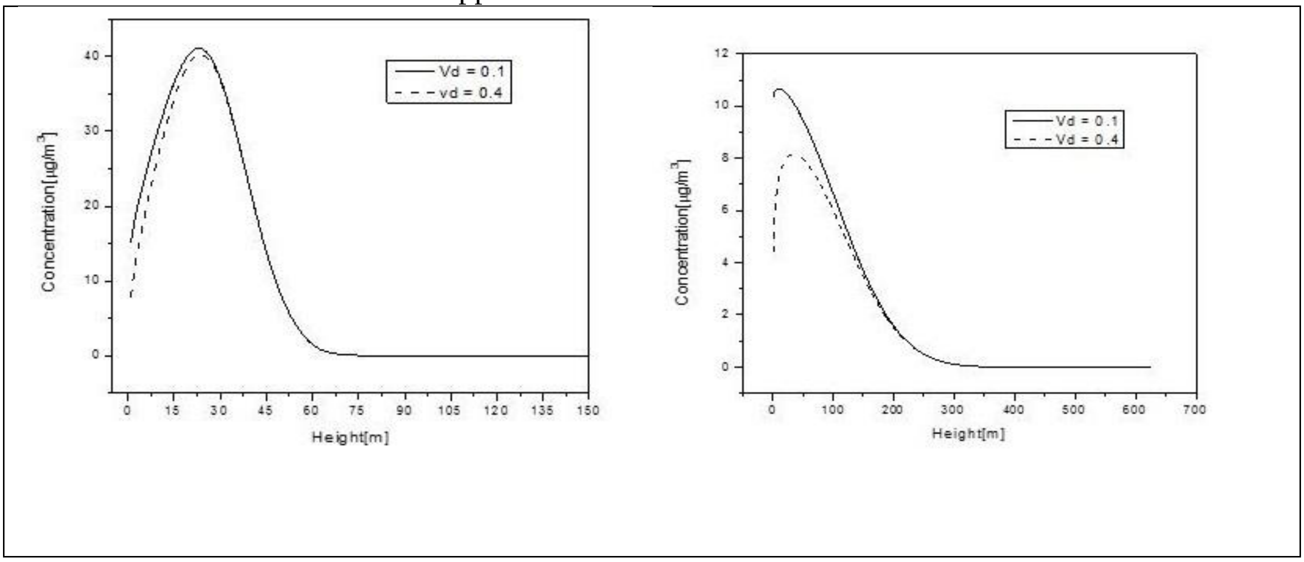

Figure 5: Concentration versus Height for different dry deposition in stable and neutral cases at x=3000m.

It is evident that from figure 5 that the dry deposition effect on concentration for both stable and neutral case are presented. Since we kept point source at x= 0 and at z=20.5,in both atmospheric conditions pollutants concentration is high near 20.5 meter height. In stable atmospheric case near the bottom surface concentration is less and raising up to 20.5meter height .The pollutant concentration decreases beyond 20.5m and attains zero near 70m height in stable case. In neutral case also we observed the same effect. But concentration of pollutants is zero around 350m height in neutral case. This is due to the fact that neutral case supports and hence increases vertical diffusion at the higher altitude.In stable condition, the primary pollutantsconcentration is more comparing to the neutral case for similar set of values of distance.

VI. CONCLUSION

A two-dimensional mathematical model to calculate the ambient concentration of air pollutants released by area and point source with the impact of mesoscale type wind,chemical reaction,gravitational settling and dry deposition has been presented in this paper. The results are examined in an urban area for the air pollutants dispersion in thevertical and downwind direction for neutral and stable atmospheric conditions. Primary pollutants concentration reaches its maximum value near the ground level at the downwind end of the source region. The impact of dry deposition velocity, gravitational settling velocity and chemical reaction rate coefficient near the point source are negligible. These removal mechanisms playscrucial role in decreasing the pollutant concentration inentire city region except near the point source. The level of concentration is more in stable case and less in neutral case. This study shows that the stable condition is an unfavorable condition for animals and plants from air pollution point of view.

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