Mathematical Modelling of Air Pollutants Emitted from a Line Source with Chemical Reaction and Mesoscale Wind

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Abstract— A mathematical model for air pollutants emitted from a line source along with the mesoscale wind and chemical reaction is presented. The Crank-Nicolson finite difference scheme is employed to solve the model numerically. The realistic forms of large-scale, mesoscale wind velocities and eddy diffusivity profiles are used in the model. The results have been analysed for the dispersion of air pollutants for stable and neutral conditions of the atmosphere in the presence of mesoscale wind. The effect of mesoscale wind on pollutants is non-uniform over the simulated urban region and the effect of chemical reaction decreases the concentration of pollutants everywhere.

Index Terms— Mathematical model, Line Source, Mesoscale wind, Chemical reaction, Finite difference method.

1 Introduction

MATHEMATICAL modeling is a special tool through which one can infer about the solution of the real world problems. One among the major problems of the world today is air pollution. The effect of air pollution on human life and its environment has made it a major and serious threat globally. Numbers of studies have reported the association between the busy roads and a variety of adverse respiratory problems in children, including respiratory symptoms, asthma exacerbations and decrements in lung function. The traffic pollutants like particulate matter, black carbon, nitrogen oxides (NO_x) etc., have association with respiratory symptoms in children as reported by Janice J Kim et al. [1]. Thus the role of vehicular emissions to the atmosphere is remarkably high in modern days and the large highways have greater contribution to air pollution. A mathematical model gives a better option for monitoring air pollution problems.

W Koch [2] developed an analytical model of the two dimensional atmospheric diffusion equation of substances released from an infinite line source. In this model the height dependence of the wind velocity and the vertical diffusion coefficient is approximated by power function of height (z). P J Sullivan and H Yip [3] solved both analytically and numerically the steady state, two dimensional convective diffusion equation for a continuous elevated line source located at height h above impermeable plane at z=0. John M Stockie [4] studied the atmospheric dispersion modeling based on Gaussian plume approximations to the advection diffusion equation with a continuous point source. In the study he took a special case of continuous line source and gave a solution to line source emission. M Venkatachalappa, et al. [5] gave a time dependent mathematical model considering the variable wind velocity and eddy diffusivity along with the effect of chemical reaction for air pollutants which are emitted from an area source. Lakshminarayanachari K, et al. [6] constructed a two dimensional advection-diffusion numerical model of air pollutant emitted from a time dependent area source of primary and secondary pollutants with chemical reaction taking into account the realistic form of variable wind velocity and eddy diffusivity profiles. All these models have not considered the effect of mesoscale wind.

However Dilley and Yen [7] gave an analytical model for pollutant distributions from a line source considering the effect of mesoscale type wind. Mesoscale type wind is produced by urban heat island. M Agarwal and A Tandon [8] presented a two dimensional mathematical model including the effect of mesoscale type wind but for the pollutants emitted from an area source. These works does not include the chemically reactive pollutants.

Pandurangappa C et al. [9] developed a model considering the chemical reaction of the pollutants along with the effect of mesoscale wind for the pollutant distribution emitted from a line source. But this model is in analytical nature with simple form of wind velocity and eddy diffusivity under restrictive assumptions.

There are numerous models which includes the effect of mesoscale type wind, chemical reaction and stability dependent meteorological parameters involving variable wind velocity and eddy diffusivity profiles such as Lakshminarayanachari K, et al. [10] considered the dry deposition of pollutants and Pandurangappa C et al. [11] studied with gravitational settling velocity of pollutants. However these models considered the pollutants emission from an area source.

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In the present work we develop a mathematical model of air pollutants dispersion emitted from a line source with mesoscale wind, chemical reaction and realistic form of variable wind velocity and eddy diffusivity profiles. The problem is solved numerically by using Crank-Nicolson finite difference method. The solution describe the pollutants concentration downwind of an infinite crosswind line source on the ground under the influence of a horizontal large-scale wind and mesoscale wind generated by urban heat island with chemical reaction.

2 Model Development

The physical problem consists of an infinite crosswind line source on the ground with finite downwind distance and infinite crosswind dimension. We assume that the pollutants are transported horizontally in perpendicular direction by a large-scale wind which is a function of vertical height (z) and horizontally as well as vertically by a local wind called mesoscale wind produced by urban heat island which is a function of both height (z) and distance (x). We have considered the center of heat island at a distance $x = l/2$ that is at the center of the city, where l is the city length. In this problem we have taken $l = 6\,km$. We have computed the concentration of pollutants in the region $0 \le x \le l$. The line source is kept at $x = 0$, that is at the beginning of the city. Here we have considered chemically reactive pollutants and are converted into secondary pollutants by means of first order chemical reaction rate. The physical description of this mathematical model is as shown in the figure1.

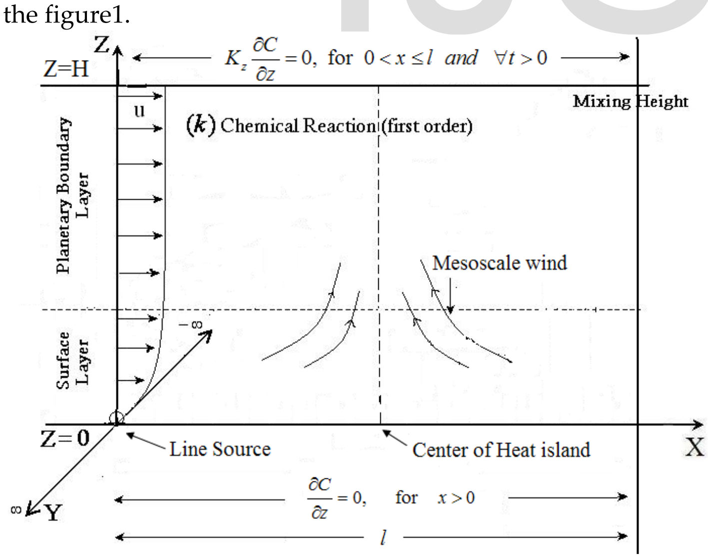

Figure 1. Physical layout of the model.

The general species advection 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 pollutant concentration at any location (x, y, z) and time t, K_x, K_y and K_z are the eddy – diffusivity coefficients along x, y and z directions respectively, U, V and W are the velocity components along x, y and z directions respectively and k is the chemical reaction rate coefficient.

Now we introduce the following assumptions

- Pollutants are chemically reactive.
- Wind velocity along the x direction is so large that the x direction diffusion is neglected.
- The lateral flux of pollutants along crosswind direction is assumed to be small i.e., $V\frac{\partial C}{\partial y} \to 0$ and $\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) \to 0$.

Therefore, the basic governing partial differential equation (1) under the above assumptions becomes,

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

where $U(x,z)$ denotes the velocity along both horizontal and vertical direction and $W(z)$ denotes the velocity in the vertical direction due to the effect of mesoscale wind.

2.1 Initial and Boundary Conditions

We assume that at the beginning of the emission, the region of interest is free from pollution.

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

We assume that no background pollution is entering the region of interest

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

For a continuous line source of strength Q located at origin (which has an infinitesimal small extension in the z-direction), we have the following boundary condition (W Koch [2]):

$$C = Q\frac{\delta(z)}{u(x,z)}, \text{ at } x = 0, \ z = 0 \text{ and } \forall t > 0 \quad (5)$$

We assume that there is no transfer or deposition of pollutants at the ground. Therefore there is no concentration gradient at the ground level i.e.,

$$\frac{\partial C}{\partial z} = 0, \quad \text{at} \quad z = 0, \quad x > 0 \quad (6)$$

The pollutants are confined within the mixing height and there is no leakage across the top boundary of the mixing layer. Thus

$$K_z \partial C/\partial z = 0, \text{ at } z = H, \ 0 < x \le l \text{ and } \forall t > 0 \quad (7)$$

2.2 Meteorological Parameters

The profiles of large-scale, mesoscale wind speeds and eddy diffusivity for various atmospheric stability conditions and for various meteorological parameters such as surface roughness, friction velocity, stability length, net heat flux etc., are used to solve the equation (2). These are considered in accordance with Pandurangappa C [12].

For neutral atmospheric stability condition it is assumed that the surface layer terminates at $z = 0.1k(u_* / f)$ and for stable atmospheric stability condition the surface layer extends up to $z = 6L$, where $k = 0.4$ is the Karman's constant, u_* is the friction velocity, f is the Coriolis parameter and L is the Monin-Obukhov stability length parameter.

For neutral atmospheric stability condition the wind velocity profiles used are

$$U(x,z)=\left(\frac{u_*}{\kappa}-a(x-x_0)\right)\ln\left(\frac{z+z_0}{z_0}\right) \tag{8}$$

and $$W(z)=a\left[z\ln\left(\frac{z+z_0}{z_0}\right)-z+z_0\ln(z+z_0)\right] \tag{9}$$

where $z < 0.1k(u_* / f)$.

For stable atmospheric stability condition the wind velocity profiles are

$$U(x,z)=\left(\frac{u_*}{\kappa}-a(x-x_0)\right)\left[\ln\left(\frac{z+z_0}{z_0}\right)+\frac{\alpha}{L}z\right] \tag{10}$$

and $$W(z)=a\left[z\ln\left(\frac{z+z_0}{z_0}\right)-z+z_0\ln(z+z_0)+\frac{\alpha}{2L}z^2\right] \tag{11}$$

for $0<\frac{z}{L}<1$ and for $1<\frac{z}{L}<6$, we have

$$U(x,z)=\left(\frac{u_*}{\kappa}-a(x-x_0)\right)\left[\ln\left(\frac{z+z_0}{z_0}\right)+5.2\right] \tag{12}$$

and $$W(z)=a\left[z\ln\left(\frac{z+z_0}{z_0}\right)+z_0\ln(z+z_0)+4.2z\right]. \tag{13}$$

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

$$U(x,z)=\left[(u_g-u_{sl})-a(x-x_0)\right]\left(\frac{z-z_{sl}}{H-z_{sl}}\right)^p+(1-a(x-x_0))u_{sl} \tag{14}$$

and $$W(z)=a\left[\frac{(z-z_{sl})}{p+1}\left(\frac{z-z_{sl}}{H-z_{sl}}\right)^p+z\,u_{sl}\right] \tag{15}$$

where u_g is the geostrophic wind velocity, u_{sl} is wind at z_{sl}, H is the mixing height, z_{sl} is the top of the surface layer and p is an exponent which depends on the atmospheric stability. Here p values are used as with Jones et al. [13].

All the above wind velocity profiles (8) to (15) are valid only for $x \le \frac{u_*}{a\kappa}+x_0$ (Pandurangappa C [12]).

For both surface layer and planetary boundary layer (entire boundary layer) the eddy diffusivity profiles used are

$$K_z = 0.4u_* z e^{-4z/H}\text{, for neutral case (Shir [14])} \tag{16}$$

and $K_z = \frac{\kappa u_* z}{0.74+4.7\,z/L}\exp(-b\eta)$, for stable case (Ku et al. [15]) (17)

where $b = 0.91$, $\eta = z/(L\sqrt{\mu})$, $\mu = u_*/|fL|$ and $f = 10^{-4}$.

3 Method of Solution

Our aim is to study and analyse the effect of mesoscale wind on concentration of chemically reactive air pollutants emitted from a line source. For this we need to solve equation (2) along with the initial and boundary conditions (3) to (7). We note that due to the variable forms of wind speed and diffusivity, it is tedious to obtain the analytical solution of (2). Thus to obtain the solution we have used numerical method based on Crank-Nicolson finite difference scheme. Now to apply Crank-Nicolson finite difference scheme the continuum region of interest is subdivided into a set of equal rectangles of sides Δx and Δz, by equally spaced grid lines, parallel to z axis and x-axis, defined by $x_i = (i-1)\Delta x$, $i = 1,2,3,\ldots$ and $z_j = (j-1)\Delta z$, $j=1,2,3,\ldots$ respectively. Time is indexed as $t_n = n\Delta t$, $n = 0, 1, 2, 3\ldots$, where Δt is the time step. Now the equation (2) is replaced by the equation valid at time step $n+1/2$ and at the interior grid points (i, j)

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

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

$$i = 2,3,4,\ldots\ldots i\max,\quad j = 2,3,4,\ldots\ldots j\max-1,\ n = 0,1,2\ldots\ldots \tag{18}$$

Here the time derivative is replaced by a central difference with time step $n+1/2$ and the spatial derivatives are replaced by the arithmetic average of its finite difference approximations at the n^{th} and $(n+1)^{th}$ time steps.

Now consider

$$\left.\frac{\partial C}{\partial t}\right|_{ij}^{n+\frac{1}{2}}=\frac{C_{ij}^{n+1}-C_{ij}^{n}}{\Delta t}, \tag{19}$$

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

$$U(x,z)\left.\frac{\partial C}{\partial x}\right|_{ij}^{n+1} = U_{ij}\left[\frac{C_{ij}^{n+1}-C_{i-1\,j}^{n+1}}{\Delta x}\right], \tag{21}$$

$$W(z)\frac{\partial C}{\partial z}\Big|_{ij}^{n} = W_j\left[\frac{C_{ij}^{n} - C_{i\,j-1}^{n}}{\Delta z}\right], \qquad (22)$$

$$W(z)\frac{\partial C}{\partial z}\Big|_{ij}^{n+1} = W_j\left[\frac{C_{ij}^{n+1} - C_{i\,j-1}^{n+1}}{\Delta z}\right], \qquad (23)$$

$$\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C}{\partial z}\right)\Big|_{ij}^{n} = \frac{1}{2(\Delta z)^2}\left[\left(K_{j+1}+K_j\right)\left(C_{ij+1}^{n}-C_{ij}^{n}\right)-\left(K_j+K_{j-1}\right)\left(C_{ij}^{n}-C_{ij-1}^{n}\right)\right] \qquad (24)$$

$$\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C}{\partial z}\right)\Big|_{ij}^{n+1} = \frac{1}{2\Delta z^2}\left[\left(K_{j+1}+K_j\right)\left(C_{ij+1}^{n+1}-C_{ij}^{n+1}\right)-\left(K_j+K_{j-1}\right)\left(C_{ij}^{n+1}-C_{ij-1}^{n+1}\right)\right] \qquad (25)$$

Substituting Equations (19)-(25) in (18) and rearranging and simplifying we get finite difference equation for the pollutant concentration C in the form

$$B_jC_{ij-1}^{n+1}+D_{ij}C_{ij}^{n+1}+E_jC_{ij+1}^{n+1} = F_{ij}C_{i-ij}^{n}+G_jC_{ij-1}^{n}+M_{ij}C_{ij}^{n}+N_jC_{ij+1}^{n}-A_{ij}C_{i-ij}^{n+1}. \qquad (26)$$

for each i = *2,3,4,…..* $i\max$, for each *j=2,3,4,……jmax-1* and *n=0,1,2,3,…….*

Here $A_{ij} = -U_{ij}\frac{\Delta t}{2\Delta x}$, $F_{ij} = U_{ij}\frac{\Delta t}{2\Delta x}$,

$$B_j = -\left[\frac{\Delta t}{4\Delta z^2}(K_j+K_{j-1})+\frac{\Delta t}{2\Delta z}W_j\right],$$

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

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

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

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

and *imax* is the i value at $x = l$ and *jmax* is the value of j at $z = H$.

The initial condition (3) can be written as

$$C_{ij}^{0} = 0 \quad \text{for} \quad j = 1,2,\ldots\ldots\ldots j\max,\ i = 1,2,\ldots\ldots\ldots i\max. \qquad (27)$$

The boundary conditions (4) and (5) together can be written as

$$C_{ij}^{n+1} = \begin{cases} \dfrac{Q}{u_{ij}} & \text{for } i=1,\ j=2 \\ 0 & \text{for } i=1,\ j\neq 2 \end{cases} \qquad (28)$$

The boundary condition (6) can be written as

$$C_{ij+1}^{n+1} - C_{ij}^{n+1} = 0, \quad \text{for } j=1,\ i=2,3,\ldots\ldots,i\max \text{ and } n = 0,1,2,3,\ldots.. \qquad (29)$$

The boundary condition (7) can be written as

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

4 Results and Discussion

A two dimensional numerical model has been developed to compute the air pollutants concentration along downwind and vertical directions emitted from a line source with mesoscale type wind and chemical reaction. The model presented here allows the estimation of concentration distribution for more realistic meteorological conditions. The model has been solved by using Crank-Nicolson finite difference method which is unconditionally stable. We considered $\Delta x = 75$ meter and $\Delta z = 1$ meter as grid size. The discretized algebraic equations are in tri-diagonal matrix form and the Thomas algorithm is used to solve it efficiently. The results of this model have been presented graphically in figures 2 – 6 to analyse the effect of mesoscale wind and the dispersion of air pollutants for stable and neutral conditions of atmosphere.

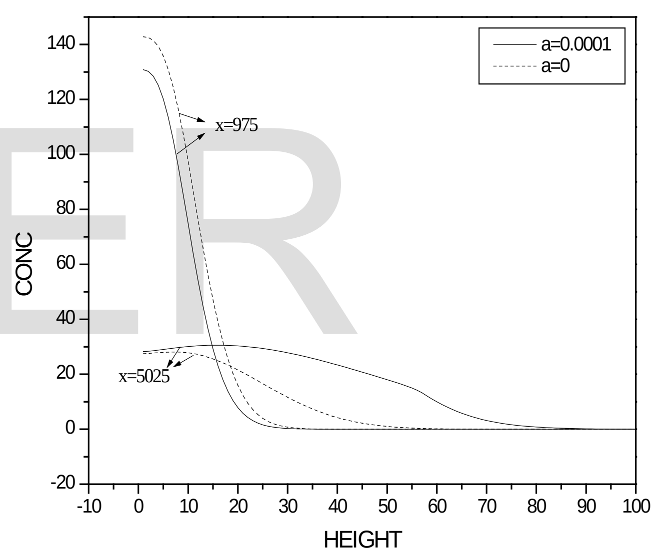

Fig. 2a. Concentration versus Height for Stable case

In figure 2(a &b) the effect of mesoscale wind on pollutants concentration with respect to height is studied for stable and neutral case. The pollutant concentration is less in the presence of mesoscale wind compared to that in the absence of mesoscale wind at the distance x=975 meter, whereas the concentration is more in the presence of mesoscale wind compared to that in the absence of mesoscale wind at the distance x=5025 meter for both stable and neutral case. This is because in the upwind side of center of heat island the mesoscale wind increases the velocity of large-scale wind and decreases the velocity of large-scale wind in the downwind side of center of heat island. Therefore in the upwind side of the centre of heat island the mesoscale wind reduces the concentration of pollutants and increases the concentration in the downwind side of the center of heat island. Compared to the stable case, the neutral case carries pollutants concentration to greater heights. But the magnitude of the pollutant concentration is more for stable case compared to that of neutral case.

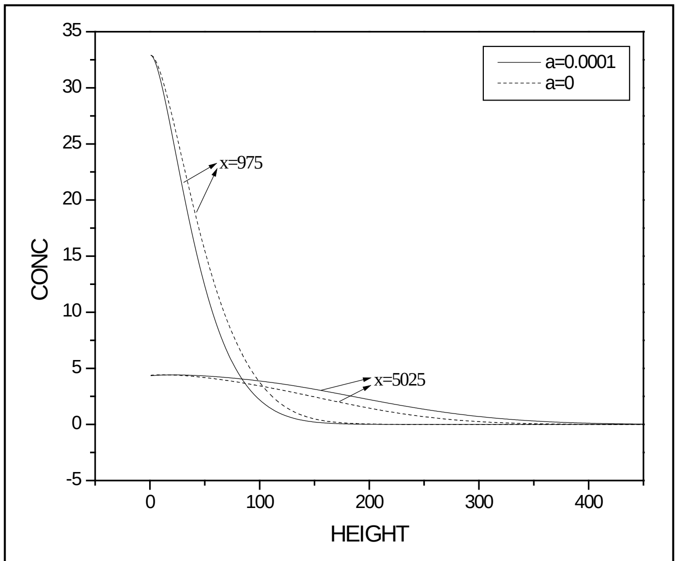

Fig. 2b. Concentration versus Height for Neutral case

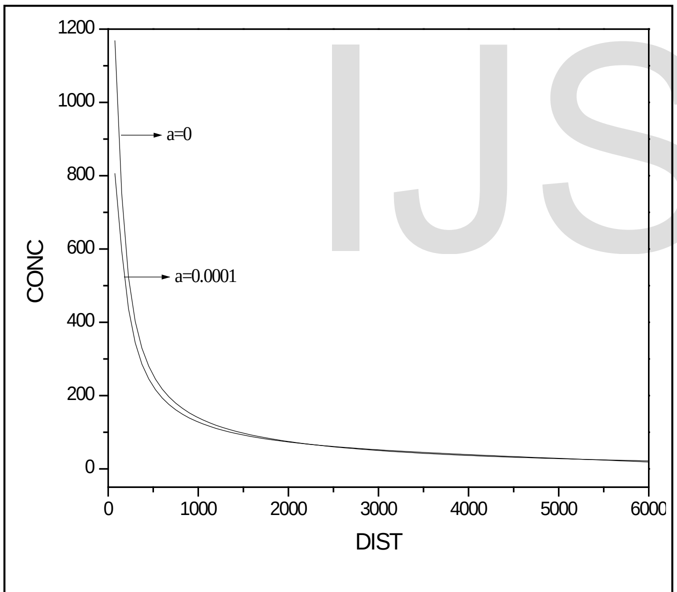

Fig. 3a. Concentration versus Distance for Stable case

In figure 3 the pollutant concentration with respect to distance is presented for different atmospheric stability conditions (figure 3 (a) for stable case and figure 3 (b) for neutral case). The concentration of pollutants is maximum in magnitude in the case of stable atmospheric condition compared to that of neutral atmospheric condition and the difference between the pollutants concentration in the presence and absence of mesoscale wind is very less in the case of neutral atmospheric condition when compared to stable atmospheric condition.

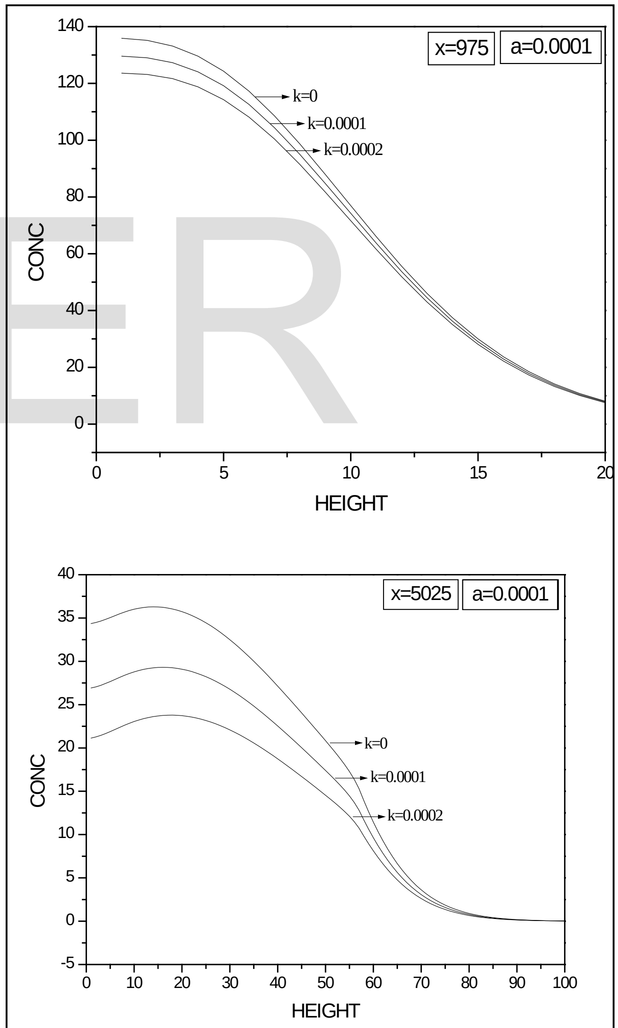

Fig. 4. Concentration versus Height for different chemical reaction rate coefficient for Stable case.

Figures 4 and 5 demonstrates the effect of chemical reaction on pollutant concentration with respect to height for

ISSN 2229-5518

stable and neutral atmospheric condition at the fixed distances x=975m and x=5025m. As the chemical reaction rate coefficient increases the concentration of pollutant decreases at both x=975m and x=5025m. This behavior is due to removal of air pollutants through chemical reaction. The magnitude of pollutant concentration is maximum for stable case compared to neutral case but the neutral case takes the pollutants to greater heights. This is due to the neutral case enhances vertical diffusion at the greater heights thus the concentration becomes less.

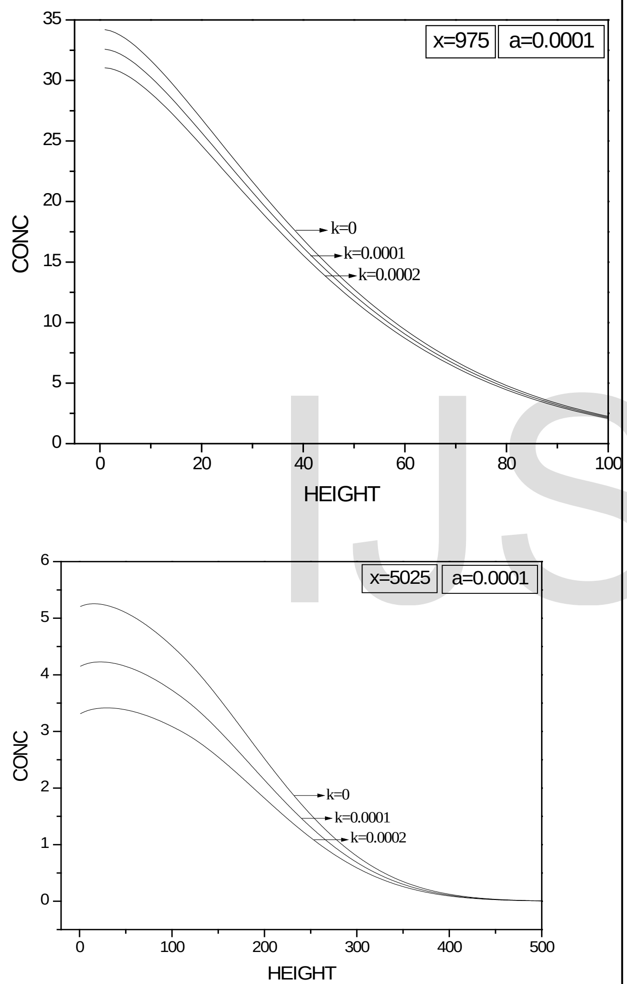

Fig. 5. Concentration versus Height for different chemical reaction rate coefficient for Neutrale case

In figure 6 the effect of chemical reaction on pollutant concentration with respect to distance is analysed for both stable and neutral case. The chemical reaction reduces the pollutant concentration throughout the region of interest. The concentration of pollutants is maximum in the case of stable atmospheric conditions compared to that of neutral atmospheric conditions.

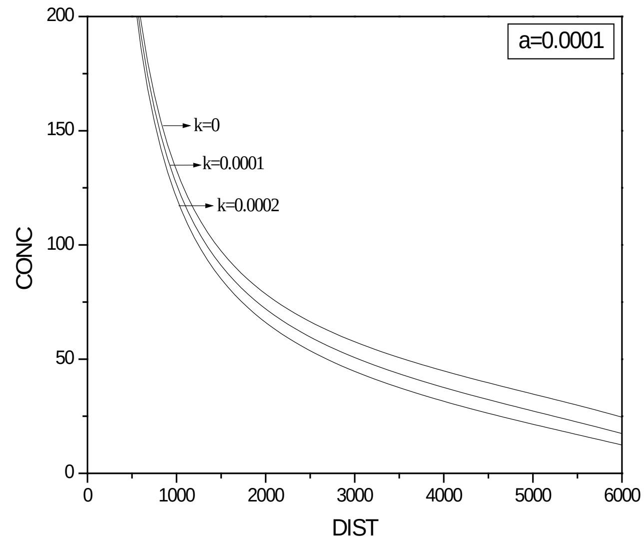

Fig. 6a. Concentration versus Distance for different chemical reaction rate coefficient for Stable case

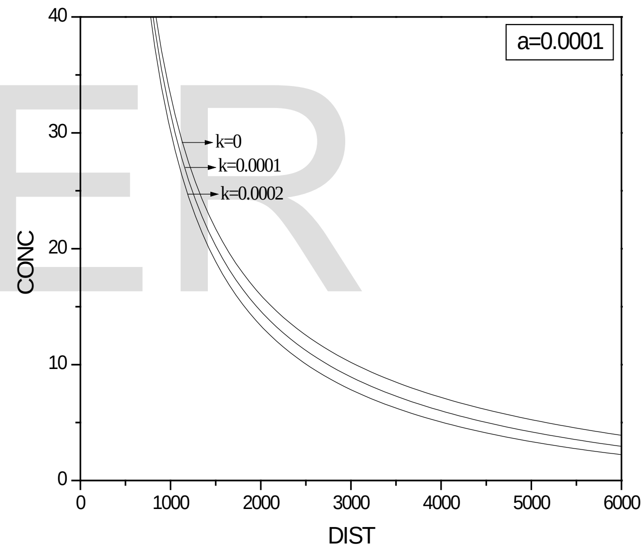

Fig. 6b. Concentration versus Distance for different chemical reaction rate coefficient for Neutral case

5 Conclusions

A mathematical model has been developed to compute the ambient concentration of air pollutants emitted from a line source along with the effect of mesoscale type wind and chemical reaction. The results have been analyzed for the dispersion of air pollutants in the downwind and the vertical direction for stable and neutral atmospheric conditions. From the figures we conclude that the mesoscale wind aggravates the air pollutants concentration for stable and neutral conditions of atmosphere. Also, the results obtained in this model show that as the chemical reaction rate coefficient increases, the concentration of pollutants decreases everywhere. We found that the magnitude of concentration is more in stable case and less in neutral case and the concentration level reaches maximum height in neutral case compared to stable case, indicating that the neutral condition enhances the vertical diffusion of pollutants in the atmosphere.

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