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Simulation of Pollutants with Dry Deposition in the Stable Atmospheric Boundary Layer

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Abstract

An unsteady atmospheric model represented in the atmospheric boundary layer over variable surface terrains. Here the pollutants are chemically reactive primary pollutants and are emitted from an elevated line source into a stable atmospheric boundary layer. The source of pollutants is considered as *Floor function* type. The time dependent model obtained through an analytical solution from a multiple Inverse Laplace transform of the atmospheric diffusion equation with the parabolic diffusion

coefficient (exchange coefficient) and the wind velocity taken to be of three different types viz. constant, constant shear and parabolic functions of vertical height. The pollutants considered to be of chemically reactive primary pollutants emitted from a time-dependent (floor function type) line source. In order to facilitate the application of the model the results for the general situation that includes chemical reaction rate, dry deposition rate & time dependent (floor function) line source incorporated in the model.

Keywords: Floor Function, Exchange Coefficient, Chemically Reactive, Stable Boundary Layer and Parabolic Wind

1. Introduction

The study of the atmospheric dispersion and diffusion of air pollutants in the atmospheric boundary layer emitted from various types of sources are received a great deal of attention during the last few decades. The effects of various sources emitting chemically reactive primary pollutants have investigated. In addition, the depletion of pollutants plumes will affect the pollutants concentration especially when the deposition occurs over a long distance. This paper addresses the problem of air pollution removal and deposition of analytical model for floor function type line sources. The deposition velocity depends upon such factors as the type and size of pollutant particles, the roughness of terrain and the type of ground cover and the meteorological conditions. The floor function type line sources assumed to be the series of industries, highways on during certain period of time and not continuous. The effect of continuous source studied in the previous work by C. Sulochana *et al* (2009). The purpose of this work is to develop an analytical model for the atmospheric dispersion of pollutants, emitted from a line source of floor function type, which treats pollutants deposition in a more physically realistic manner.

2. Mathematical Formulation of the Model

The situation analyzed is that, the dispersion of chemically reactive pollutants emitted from an elevated line source of floor function type and dry deposition. It is assumed that the emission of contaminant are in the gaseous state emitted from a time dependent elevated line source of infinite length into a stable ABL, the wind velocity is of variable type depending on the nature of the surface terrains viz. flat, buildup areas and elevated areas like mountain regions. The diffusion coefficient assumed to be of quadratic in nature, the atmospheric boundary layer is of stable boundary layer, where the mixing of pollutants is limited. To study the variation in the effect of pollutants the type of the source known i.e. continuous, impulse or step function type. This work focused on the source of floor function type, where the industries work during the certain fixed time. The pollutant transport governed by the atmospheric advection-diffusion equation with delayed removal. The height of the atmospheric boundary layer is assumed to be $z=H$, from the surface, the pollutants are chemically reactive.

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left(K_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial C}{\partial z} \right) - K''C + S \quad (1)$$

Where $C(x, y, z, t)$ is the concentration of pollutants in the atmosphere at any location (x, y, z) at any time t ; u, v, w are the components of velocity; K_x, K_y, K_z are the coefficients of eddy diffusivity (exchange coefficient) in the x, y, z directions respectively, K'' first order removal rate, S the source of the effluents.

The basic equation (1) simplified by assuming the following assumptions:

a. Model is of time dependent & advection dominates over horizontal diffusion

$$u \frac{\partial C}{\partial x} \gg \frac{\partial}{\partial x} \left(K_x \frac{\partial C}{\partial x} \right)$$

b. It is also assumed that the line source is in the direction of y -axis, which leads the concentration gradient and flux gradient to zero along y -direction.

$$v \frac{\partial C}{\partial y} = 0 \quad \& \quad \frac{\partial}{\partial y} \left(K_y \frac{\partial C}{\partial y} \right) = 0$$

c. The vertical diffusion dominates over advection

$$\frac{\partial}{\partial z} \left(K_z \frac{\partial C}{\partial z} \right) \gg w \frac{\partial C}{\partial z}$$

d. The source (S) is time dependent line source and is assumed to be

$$S = QW(t)\delta(x - x_0)\delta(z - z_0)$$

Based on the above assumptions the transport and diffusion equation (1) becomes:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left(K_z \frac{\partial C}{\partial z} \right) - K''C + QW(t)\delta(x - x_0)\delta(z - z_0) \quad (2)$$

Initial and boundary conditions are:

$$C(x, y, z) = 0 \quad \text{at } t = 0, \quad \forall x, z \in R^+ \quad 3(a)$$

$$C(x, y, z) = 0 \quad \text{at } x = 0, \quad t = 0, \quad x \geq 0 \quad 3(b)$$

$$K_z \frac{\partial C(x, y, z)}{\partial z} = 0, \quad z = 1 \quad \forall x, t \geq 0 \quad 3(c)$$

$$K_z \frac{\partial C(x, y, z)}{\partial z} = v_d C, \quad z = 0 \quad \forall x, t \geq 0 \quad 3(d)$$

Where, $C(x, y, z)$ = Pollutant concentration (ppm)

H = height of the inversion layer

z_0 = height of the source

(x_0, z_0) = the location of the source in xz -plane

K_z = Exchange coefficient along vertical direction

Q = Source strength at (x_0, z_0)

$\delta(\cdot)$ = Dirac's Delta function

v_d = the deposition velocity.

K'' = First order delayed removal

t = time in seconds

$W(t)$ = time dependent source of floor function type and is of the form:

$$W(t) = w_0 U(t - t_0) = \begin{cases} w_0, & 0 < t \leq t_0 \\ 0, & t > t_0 \end{cases} \quad (4)$$

3. Dimensional Analysis:

Introducing the non-dimensional parameters

$$Z = \frac{z}{H}, \quad \frac{K_z}{K_o} = (1-Z)^2, \quad X = \frac{K_o}{H^2 u_o} x, \quad \frac{u(z)}{u_o} = \left[\frac{z}{H} \right]^n = Z^n, \quad V_D = \frac{K_o}{H^2} v_d$$

$$T = \frac{K_o}{H^2} t, \quad C = \frac{H \langle u \rangle}{W_o Q} c, \quad \text{where } \langle u \rangle = \frac{u_o}{n+1}, \quad W(T) = \frac{W(t)}{w_o},$$

$$\text{and } u_b = \frac{4.7 u_* H}{kL}, K_o = \frac{k}{4.7} u_* L \quad (\text{Robson R.E(1987)})$$

where, u_* = is friction velocity

L = the Monin – Obukov length

k = Vankarman Constant

H = the boundary layer height

n = the constant decided on the stability of boundary layer

In addition, non-dimensional source term is as follows:

$$W(T) = \frac{W(t)}{W_o} = U(T - T_o) \quad (5)$$

Incorporating all the above non-dimensional parameters in the equation (2) and dropping out the capitals, we get

$$\frac{\partial c}{\partial t} + z^n \frac{\partial c}{\partial x} = \frac{\partial}{\partial z} \left((1-z)^2 \frac{\partial c}{\partial z} \right) - \alpha c + \frac{W(t)}{n+1} \delta(x - x_0) \delta(z - z_0) \quad (6)$$

Where,

$$\alpha = \frac{k H^2}{K_o} \quad (7)$$

Initial and boundary conditions are:

$$c(x, z, t) = 0 \quad \text{at } t = 0, x \geq 0, z \geq 0 \quad (8(a))$$

$$c(x, z, t) = 0 \quad \text{at } x = 0, t \geq 0, z \geq 0 \quad (8(b))$$

$$(1-z)^2 \frac{\partial c}{\partial z} = 0, \quad \text{at } z = 1 \quad (8(c))$$

$$(1-z)^2 \frac{\partial c}{\partial z} = v_d c(x, z, t), \quad \text{at } z = 0 \quad (8(d))$$

4. Method of Solution

The partial differential equation reduced to the ordinary differential equation by applying multiple Laplace transform along t and x , followed by the corresponding boundary conditions. Applying the transform along we get:

$$s \bar{c}(x, z, s) - c(x, z, 0) + z^n \frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial z} \left((1-z)^2 \frac{\partial \bar{c}}{\partial z} \right) - \alpha \bar{c} + \frac{W(s)}{n+1} \delta(x - x_0) \delta(z - z_0) \quad (9)$$

Boundary conditions:

$$c(x, z, t) = 0 \quad \text{at } x = 0, t \geq 0, z \geq 0 \quad (10(a))$$

$$(1-z)^2 \frac{\partial \bar{c}(x, z, s)}{\partial z} = 0, \quad \text{at } z = 1 \quad (10(b))$$

$$(1-z)^2 \frac{\partial \bar{c}(x, z, s)}{\partial z} = v_d \bar{c}(x, z, s), \quad \text{at } z = 0 \quad (10(c))$$

Where,

$$\bar{c}(x, z, s) = \int_0^\infty e^{-st} c(x, z, t) dt \quad (11)$$

Again, taking Laplace transform along x -axis which is assumed to of semi-infinite region, then (9) becomes

$$s\hat{c}(p, z, s) + z^n \left(p\hat{c}(p, z, s) - \bar{c}(0, z, s) \right) = \frac{d}{dz} \left((1-z)^2 \frac{d\hat{c}}{dz} \right) - \alpha\hat{c} + \frac{\overline{W(s)}}{n+1} e^{-sx_0} \delta(z - z_0) \quad (12)$$

Where,

$$\hat{c}(p, z, s) = \int_0^\infty e^{-st} \bar{c}(x, z, s) dt \quad (13)$$

Differential equation (12) becomes

$$\frac{d}{dz} \left((1-z)^2 \frac{d\hat{c}}{dz} \right) - (\alpha + s + p z^n) \hat{c} = -\frac{\overline{W(s)}}{n+1} e^{-sx_0} \delta(z - z_0) \quad (14)$$

and boundary conditions:

$$(1-z)^2 \frac{d\hat{c}(p, z, s)}{dz} = 0, \quad \text{at } z = 1 \quad (15(a))$$

$$(1-z)^2 \frac{d\hat{c}(p, z, s)}{dz} = v_d \hat{c}(p, z, s), \quad \text{at } z = 0 \quad (15(b))$$

Case I:

When the wind profile is of constant (n = 0)

The movements of air near the earth's surface retarded by frictional effect proportional to the surface roughness. Thus, the nature of the terrain the location and density of trees, the location and size of lakes, rivers, hills and buildings produces different wind velocity gradients in the vertical direction (Warn & Walker). The wind of constant type is experienced in case of flat open country, lakes and seas. This case dealt with constant wind profile. Then the equation (14) becomes

$$\frac{d}{dz} \left((1-z)^2 \frac{d\hat{c}}{dz} \right) - (\alpha + s + p) \hat{c} = -\overline{W(s)} e^{-px_0} \delta(z - z_0) \quad (16)$$

Under the boundary conditions:

$$(1-z)^2 \frac{d\hat{c}(p, z, s)}{dz} = 0, \quad \text{at } z = 1 \quad (17)$$

$$(1-z)^2 \frac{d\hat{c}(p, z, s)}{dz} = v_d \hat{c}(p, z, s), \quad \text{at } z = 0 \quad (18)$$

The complete solution of the above equation through Green's function technique assumed to be of the following form:

$$\hat{C}(p, z, s) = \begin{cases} G_1(z/z_0), & z < z_0 \\ G_2(z/z_0), & z > z_0 \end{cases} \quad (19)$$

$$\hat{C}(p, z, s) = -\overline{W(s)} e^{-px_0} \begin{cases} \frac{\phi_a(z) \phi_b(z_0)}{A_1}, & z < z_0 \\ \frac{\phi_a(z_0) \phi_b(z)}{A_1}, & z > z_0 \end{cases} \quad (20)$$

Where, ϕ_a, ϕ_b are the two independent solutions of homogeneous differential equation,

$$\frac{d}{dz} \left((1-z)^2 \frac{d\phi}{dz} \right) - (\alpha + s + p) \phi = 0 \quad (21)$$

Under the boundary conditions:

$$(1-z)^2 \frac{d\phi}{dz} = 0, \quad \text{at } z = 1 \quad (22(a))$$

$$(1-z)^2 \frac{d\phi}{dz} = v_d \phi, \quad \text{at } z = 0 \quad (22(b))$$

Moreover, and are found to be

$$\varphi_a = (1-z)^{\frac{-(\lambda+1)}{2}} + R_1 (1-z)^{\frac{(\lambda-1)}{2}} \quad (23)$$

$$\varphi_b = (1-z)^{\frac{(\lambda-1)}{2}} \quad (24)$$

In addition, A_1 is determined through Wronskian of

$$W[\varphi_a, \varphi_b]_{z=z_0} = \varphi_a(z) \varphi_b'(z) - \varphi_a'(z) \varphi_b(z) = \frac{A_1}{(1-z_0)^2} \quad (25)$$

By Wronskian A_1 found to be

$$A_1 = -\lambda \quad (26)$$

Where,

$$\lambda = \sqrt{1 + 4(\alpha + s + p)} \quad (27)$$

and

$$R_1 = \frac{\lambda + 1 - 2v_d}{\lambda - 1 + 2v_d} \quad (28)$$

The arbitrary constant R_1 , in the general solution 22(a), determined by using the boundary conditions. There of the solution $\varphi_a(z)$ and $\varphi_b(z)$ satisfies the b.c's., at $z = 0$ and $z = 1$ respectively. Taking the multiple inverse Laplace transform using standard tables (Erdelyi *et al* 1954) the solution (6) becomes.

$$C_1(x, z, t) = \frac{U(t-t_0+x)e^{-(\alpha+\frac{1}{4})x}}{4\sqrt{(1-z)(1-z_0)}} \left\{ \frac{e^{-\frac{h_1^2}{4x}} + e^{-\frac{h_2^2}{4x}}}{\sqrt{\pi x}} + 2V e^{-V h_2 + V^2 x} \text{Erfc}\left(\frac{h_2}{2\sqrt{x}} - V\sqrt{x}\right) \right\} \quad z < z_0 \quad (29)$$

Where,

$$h_1 = \log\left(\frac{1-z}{1-z_0}\right) \quad (30)$$

$$h_2 = \log\left(\frac{1}{(1-z)(1-z_0)}\right) \quad (31)$$

$$V = \frac{1}{2} - v_d \quad (32)$$

$$L^{-1}\left\{\frac{e^{-sx}(1-e^{-st_0})}{s}\right\} = U(t-x) \quad (33)$$

The complete solution for $z > z_0$ obtained by interchanging z and z_0 in the above solution (29).

Case II:

When the wind profile is of constant shear ($n=1$)

The wind profile of constant shear $u(z) = z$ is experienced in the region of highly buildup areas. The velocity varies linearly with vertical height then differential equation (9) reduced to the form for quadratic diffusion coefficient.

$$\frac{d}{dz}\left((1-z)^2 \frac{d\hat{c}}{dz}\right) - (\alpha + s + pz)\hat{c} = -\frac{\overline{W(s)}}{2} e^{-px_0} \delta(z-z_0) \quad (34)$$

Following boundary conditions,

$$(1-z)^2 \frac{d\hat{c}}{dz} = 0, \quad \text{at } z = 1 \quad (35(a))$$

$$(1-z)^2 \frac{d\hat{c}}{dz} = v_d \hat{c}, \quad \text{at } z = 0 \quad (35(b))$$

The solution of the above equation through Green's function technique assumed to be of the following form:

$$\hat{C}(p, z, s) = \begin{cases} \frac{-\overline{w(s)} e^{-px_0} \psi_a(z) \psi_b(z_0)}{2A_2}, & z < z_0 \\ \frac{-\overline{w(s)} e^{-px_0} \psi_a(z_0) \psi_b(z)}{2A_2}, & z > z_0 \end{cases} \quad (36)$$

$$\hat{C}(p, z, s) = \frac{-\overline{w(s)} e^{-px_0}}{2} \begin{cases} \frac{\psi_a(z) \psi_b(z_0)}{A_2}, & z < z_0 \\ \frac{\psi_a(z_0) \psi_b(z)}{A_2}, & z > z_0 \end{cases} \quad (37)$$

Where, A_2 determined by Wronskian of $\psi_a(z)$ and $\psi_b(z)$:

$$W[\psi_a, \psi_b]_{z_0} = \psi_a \psi_b' - \psi_a' \psi_b = \frac{A_2}{(1-z_0)^2} \quad (38)$$

$\psi_a(z)$ and $\psi_b(z)$ are the two linearly independent solutions of the homogeneous differential equation:

$$\frac{d}{dz} \left((1-z)^2 \frac{d\psi}{dz} \right) - (\alpha + s + pz) \psi = 0 \quad (39)$$

Under the boundary conditions:

$$(1-z)^2 \frac{d\psi}{dz} = 0, \quad \text{at } z = 1 \quad (40)$$

$$(1-z)^2 \frac{d\psi}{dz} = v_d \psi, \quad \text{at } z = 0 \quad (41)$$

$$\text{Let } (1-z) = \eta \quad (42)$$

$$\psi'' + \frac{2}{\eta} \psi' + \left(\frac{p}{\eta} - \frac{\alpha + p + s}{\eta^2} \right) \psi = 0 \quad (43)$$

This is a **Bessel's** differential equation when compared with the generalized **Bessel's equation**

$$R'' + \left(\frac{1-2m}{x} - 2\alpha \right) R' + \left[p^2 \alpha^2 x^{2p-2} + \alpha^2 + \frac{\alpha(2m-1)}{x} + \frac{m^2 - p^2 v^2}{x^2} \right] R = 0 \quad (44)$$

(Sherwood and Reed, 1939, p -65) [8], and the solutions are found to be

$$\psi_a(z) = \frac{1}{\sqrt{\eta}} [J_{-v}(2\sqrt{p\eta}) + R_2 J_v(2\sqrt{p\eta})] \quad (45)$$

$$\psi_b(z) = \frac{J_v(2\sqrt{p\eta})}{\sqrt{\eta}} \quad (46)$$

Where,

$$v = \sqrt{1 + 4(\alpha + s + p)} \quad (47)$$

$$R_2 = \frac{1}{p^v} \frac{\Gamma(1+v)}{\Gamma(1-v)} \left(\frac{v+2V}{v-2V} \right) \quad (48)$$

Wronskian determines A_2 with help of the above solutions we get:

$$A_2 = -\frac{\sin v\pi}{\pi} \quad (49)$$

The solutions of equation (34) followed by the boundary conditions defined in two regions viz. below the source level $z < z_0$ and above the source level $z > z_0$ are follows:

$$\hat{c}(p, z, s) = \frac{\pi W(s)}{2 \sin v\pi} \begin{cases} \frac{1}{\sqrt{\eta}} [J_{-v}(2\sqrt{p\eta}) + R_2 J_v(2\sqrt{p\eta})] \frac{J_v(2\sqrt{p\eta}o)}{\sqrt{\eta_o}}, & z < z_0 \\ \frac{1}{\sqrt{\eta_o}} [J_{-v}(2\sqrt{p\eta}o) + R_2 J_v(2\sqrt{p\eta}o)] \frac{J_v(2\sqrt{p\eta})}{\sqrt{\eta}}, & z > z_0 \end{cases} \quad (50)$$

For, the limiting case where p is infinitesimally small i.e. $x \gg 1$, for large values of x , $J_v(2\sqrt{p\eta})$ and $J_{-v}(2\sqrt{p\eta})$ are approximated (Beck *et al* 1992) [4] as follows:

$$J_v(2\sqrt{p\eta}) \cong \frac{(\sqrt{p\eta})^v}{\Gamma(1+v)} \quad (51)$$

$$J_{-v}(2\sqrt{p\eta}) \cong \frac{(\sqrt{p\eta})^{-v}}{\Gamma(1-v)}, \quad v \notin \text{Integers} \quad (52)$$

Equation (50) reduced after approximation of the Bessel's functions as

$$\hat{c}_1(p, z, s) \cong \frac{W(s)}{2 \sin v\pi \sqrt{\eta\eta_o}} \left[\frac{(p\eta)^{-v}}{\Gamma(1-v)} + R_2 \frac{(p\eta)^v}{\Gamma(1+v)} \right] \frac{(p\eta)^v}{\Gamma(1+v)}, \quad z < z_0 \quad (53)$$

Then the solution for $z < z_0$ is

$$\psi_1(x, z, t) \cong \frac{U(t-t_0-x)e^{-(\alpha+\frac{1}{4})x}}{4\sqrt{(1-z)(1-z_0)}} \left[F(x) + 2V e^{\frac{-h_2 V + V^2 x}{2}} \text{Erfc} \left(\frac{h_2}{2\sqrt{x}} - V\sqrt{x} \right) \right] \quad (54)$$

Where,

$$F(x) = \frac{e^{-\frac{h_1^2}{4x} + \frac{h_2^2}{4x}}}{\sqrt{\pi x}} \quad (55)$$

$$h_1 = \log \left(\frac{1-z}{1-z_0} \right) \quad (56)$$

$$h_2 = \log \left(\frac{1}{(1-z)(1-z_0)} \right) \quad (57)$$

$$V = \frac{1}{2} - vd \quad (58)$$

This is the complete solution of the equation (34) followed by the boundary conditions 35(a) & 35(b) for $z < z_0$. Similarly, the solution for $z > z_0$ can be obtained by interchanging z and z_0 in the above solution. We dealt only with the case below the source height $z < z_0$ i.e. at the ground level $z = 0$.

Case III:

When the wind profile is of parabolic type ($n=2$)

The wind profile of parabolic type $u(z) = z^2$ $n = 2$ experienced when the study area is located near the deep valley and near oceans, then the differential equation (14) reduced to the form with diffusion coefficient of quadratic in nature.

$$\frac{d}{dz} \left((1-z)^2 \frac{d\hat{c}}{dz} \right) - (\alpha + s + pz^2) \hat{c} = -\frac{\overline{W(s)}}{3} e^{-px_0} \delta(z - z_0) \quad (59)$$

Boundary conditions:

$$(1-z)^2 \frac{d\hat{c}}{dz} = 0, \quad \text{at } z = 1 \quad (60)$$

$$(1-z)^2 \frac{d\hat{c}}{dz} = v d\hat{c}, \quad \text{at } z = 0 \quad (61)$$

Solutions of equation (59) through Green's Function technique assumed to be of the form

$$\hat{C}(p, z, s) = -\frac{\overline{W(s)}e^{-px_0}}{3s} \begin{cases} \frac{\xi_a(z)\xi_b(z_0)}{A_3}, & z < z_0 \\ \frac{\xi_a(z_0)\xi_b(z)}{A_3}, & z > z_0 \end{cases} \quad (62)$$

Where A_3 is determined by the Wronskian

$$W[\xi_a, \xi_b]_{z=z_0} = \xi_a \xi_b' - \xi_a' \xi_b = \frac{A_3}{(1-z_0)^2} \quad (63)$$

Moreover, $\xi_a(z)$ and $\xi_b(z)$ are the linearly independent solutions of the homogeneous part of the differential equation (59).

$$\frac{d}{dz} \left((1-z)^2 \frac{d\xi}{dz} \right) - (\alpha + s + pz)\xi = 0 \quad (64)$$

With boundary conditions

$$(1-z)^2 \frac{d\xi}{dz} = 0, \quad \text{at } z = 1 \quad (65)$$

$$(1-z)^2 \frac{d\xi}{dz} = v_d \xi, \quad \text{at } z = 0 \quad (66)$$

Taking, $\mu = 2\sqrt{p}(1-z)$ in the above differential equation then it reduces to the form

$$\mu^2 \frac{d^2 \xi}{d\mu^2} + 2\mu \frac{d\xi}{d\mu} + \left\{ \frac{-\mu^2}{4} + \lambda_2 \mu - \lambda_1 \right\} \xi = 0 \quad (67)$$

Taking the transformation

$$\xi(\mu) = \frac{1}{\mu} W(\mu) \quad (68)$$

Then the equation (62) becomes

$$\frac{d^2 W}{d\mu^2} + \left\{ \frac{-1}{4} + \frac{\lambda_2}{\mu} - \frac{\lambda_1}{\mu^2} \right\} W = 0 \quad (69)$$

This is a **Whittaker's** differential equation, where $\lambda_1 = \alpha + s + p$ and $\lambda_2 = \sqrt{p}$ the two independent solutions of equation (64) are the **Whittaker's Confluent Hyper-geometric function** as follows:

$$W_a(\mu) = W_{k,m}(\mu) + R_3 W_{k,-m}(\mu) \quad (70)$$

$$W_b(\mu) = W_{k,-m}(\mu) \quad (71)$$

Where,

$$W_{k,m}(\mu) = \mu^{\frac{1}{2}+m} e^{-\frac{\mu}{2}} F\left(\frac{1}{2} - k + m, 1 + 2m, \mu\right) \quad (72)$$

and also

$$W_{k,-m}(\mu) = \mu^{\frac{1}{2}-m} e^{-\frac{\eta}{2}} F\left(\frac{1}{2} - k - m, 1 - 2m, \mu\right) \quad (73)$$

Inter-relation between **Whittaker's** to **Bessel's** function derived as follows (Carslaw & Jaeger)

$$F\left(\alpha, \beta, \frac{\alpha^2}{4t}\right) = e^{\frac{\alpha^2}{4t}} (\alpha - \beta)! (\beta - 1)! \left(\frac{\alpha}{2}\right)^{1-\beta} \cdot t^{\beta-\alpha} \cdot p^{\frac{\beta}{2}-\alpha+\frac{1}{2}} J_{\beta-1}\left(\alpha p^{1/2}\right) \quad (74)$$

Where,

$$p^n = \frac{t^n}{(-n)!} \quad (75)$$

Where, $F(\alpha, \beta, x)$ the confluent Hyper geometric functions and is defined as

$$F(\alpha, \beta, x) = \sum_{k=0}^{\infty} \frac{(\alpha)_k}{k! (\beta)_k} x^k \quad (76)$$

By the above transformations (69) the solution (65) and (66) becomes

$$W_a(\mu) = \sqrt{\mu} e^{\frac{\mu}{2}} \left[J_{-2m}\left(2\sqrt{\frac{\mu}{\pi}}\right) + R_3 J_{2m}\left(2\sqrt{\frac{\mu}{\pi}}\right) \right] \quad (77)$$

$$W_b(\mu) = \sqrt{\mu} e^{\frac{\mu}{2}} \left[J_{2m}\left(2\sqrt{\frac{\mu}{\pi}}\right) \right] \quad (78)$$

Then the complete solution of the equation (53) becomes

$$\xi_a(z) = \frac{\mu}{\sqrt{\mu}} \left[J_{-2m}\left(2\sqrt{\frac{\mu}{\pi}}\right) + R_3 J_{2m}\left(2\sqrt{\frac{\mu}{\pi}}\right) \right] \quad (79)$$

$$\xi_a(\mu) = \frac{\mu}{\sqrt{\mu}} J_{2m}\left(2\sqrt{\frac{\mu}{\pi}}\right) \quad (80)$$

The solution (62) using standard tables, Erdyle *et al* (1954), Schaum Series (1950) Beck *et al* (1992)^[4], the multiple inverse lap lace transform can be carried out for the solutions, assuming $x_0 = 0$ we get,

$$\hat{C}(p, z, s) = -\frac{\overline{W(s)}}{3} \frac{e^{\left(\frac{\mu+\mu_0}{2}\right)}}{\sqrt{\mu\mu_0}} \left\{ \begin{array}{l} \frac{\left[J_{-2m}\left(2\sqrt{\frac{\mu}{\pi}}\right) + R_3 J_{2m}\left(2\sqrt{\frac{\mu}{\pi}}\right) \right] J_{2m}\left(2\sqrt{\frac{\mu_0}{\pi}}\right)}{A_3}, \quad z < z_0 \\ \frac{\left[J_{-2m}\left(2\sqrt{\frac{\mu_0}{\pi}}\right) + R_3 J_{2m}\left(2\sqrt{\frac{\mu_0}{\pi}}\right) \right] J_{2m}\left(2\sqrt{\frac{\mu}{\pi}}\right)}{A_3}, \quad z > z_0 \end{array} \right. \quad (81)$$

Where R_3 can be determined through on of the boundary conditions at $z = 0$, and is found to be

$$R_3 = -\left(\frac{\pi^2}{4p}\right)^m \left[\frac{v_d + \sqrt{p-m+1/2}}{v_d + \sqrt{p+m+1/2}} \right] \quad (82)$$

and A_3 is determined though Wronskian and is found to be

$$A_3 = -4m(1 - z_0)^2 \sqrt{a_2 p} e^{\sqrt{a_2 p}(1 - z_0)} \quad (83)$$

Then equation (76) becomes by assuming that the concentration is for from the source i.e. distance $x \gg 1$ or $p \rightarrow 0$. Then the Bessel's function approximated

$$\hat{C}(p, z, s) = -\frac{\overline{W(s)}}{3^{-m} \frac{e^{2\sqrt{p}(1-z_0)}}{\sqrt{p}}}\left\{\begin{array}{l} \frac{e^{\mu/2}}{\sqrt{\mu}} \left[\left(\frac{\mu}{\pi} \right)^{-m} + R_3 \left(\frac{\mu}{\pi} \right)^m \right] \frac{e^{\mu_0/2}}{\sqrt{\mu_0}} \left(\frac{\mu_0}{\pi} \right)^m, \quad z < z_0 \\ \frac{e^{\mu_0/2}}{\sqrt{\mu_0}} \left[\left(\frac{\mu_0}{\pi} \right)^{-m} + R_3 \left(\frac{\mu_0}{\pi} \right)^m \right] \frac{e^{\mu/2}}{\sqrt{\mu}} \left(\frac{\mu}{\pi} \right)^m, \quad z > z_0 \end{array}\right. \quad (84)$$

$$\hat{C}_1(p, z, s) = \overline{W(s)} \frac{e^{\sqrt{p}(z_0-z)}}{6\sqrt{(1-z)(1-z_0)}} \left[\frac{e^{-mh_1}}{m} - \left(\frac{v_d + \sqrt{p} - m + 1/2}{v_d + \sqrt{p} + m + 1/2} \right) \frac{e^{-mh_2}}{m} \right], \quad z < z_0 \quad (85)$$

Where,

$$h_1 = \log \left(\frac{1-z}{1-z_0} \right) \quad (86)$$

$$h_2 = \log \left(\frac{1}{(1-z)(1-z_0)} \right) \quad (87)$$

$$m = \sqrt{\frac{1}{4} + p + s + \alpha} \quad (88)$$

Taking inverse lap lace transform along 's', we get

$$\bar{C}_1(p, z, t) = \frac{e^{\sqrt{p}(z_0-z)}}{6\sqrt{(1-z)(1-z_0)}} L_s^{-1} \left\{ \overline{W(s)} \left[\frac{e^{-mh_1}}{m} - \left(\frac{v_d + \sqrt{p} - m + 1/2}{v_d + \sqrt{p} + m + 1/2} \right) \frac{e^{-mh_2}}{m} \right] \right\}, \quad z < z_0 \quad (89)$$

$$\text{By assuming } z=0 \text{ we get } h_1 = h_2 = \log \left(\frac{1}{(1-z_0)} \right) = h \text{ say} \quad (90)$$

$$\bar{C}_1(p, 0, t) = \frac{e^{\sqrt{p}z_0}}{3\sqrt{(1-z_0)}^3} L_s^{-1} \left\{ \overline{W(s)} \frac{e^{-mh}}{V + \sqrt{p} + m} \right\}, \quad z < z_0 \quad (91)$$

$$\bar{C}_1(p, 0, t) = \frac{e^{\sqrt{p}z_0}}{3\sqrt{(1-z_0)}^3} \int_0^t W(u) F(t-u) du \quad (92)$$

$$F(t) = L_s^{-1} \left\{ \frac{e^{-mh}}{V + \sqrt{p} + m} \right\} \quad (93)$$

$$\begin{aligned} L_s^{-1} \left\{ \frac{e^{-mh}}{V + \sqrt{p} + m} \right\} &= e^{-(\frac{1}{4} + \alpha + p)t} L_s^{-1} \left\{ \left(\frac{e^{-h\sqrt{s}}}{V + \sqrt{p} + \sqrt{s}} \right) \right\} \\ &= e^{-(\frac{1}{4} + \alpha + p)t} \left\{ \frac{-\frac{h^2}{4t}}{\sqrt{\pi t}} - \beta_1 e^{h\beta_1 + \beta_1^2 t} \operatorname{Erfc} \left(\frac{h}{2\sqrt{t}} + \beta_1 \sqrt{t} \right) \right\} \end{aligned}$$

$$F(t) = L_s^{-1} \left\{ \frac{e^{-mh}}{V + \sqrt{p} + m} \right\} = e^{-(\frac{1}{4} + \alpha + p)t} \left\{ \frac{-\frac{h^2}{4t}}{\sqrt{\pi t}} - \beta_1 e^{h\beta_1 + \beta_1^2 t} \operatorname{Erfc} \left(\frac{h}{2\sqrt{t}} + \beta_1 \sqrt{t} \right) \right\} \quad (94)$$

Then equation (92) becomes

$$\bar{C}_1(p, 0, t) = \frac{e^{\sqrt{p}x_0}}{2\sqrt{(1-z_0)^3}} \left\{ \int_0^{t_0} W(u)F(t-u)du + \int_{t_0}^t W(u)F(t-u)du \right\} \quad (95)$$

$$\bar{C}_1(p, 0, t) = \frac{e^{\sqrt{p}x_0}}{2\sqrt{(1-z_0)^3}} \left\{ \int_{t-t_0}^t F(t)dt \right\} \quad (96)$$

$$\bar{C}_1(p, 0, t) = \frac{-\hbar e^{\sqrt{p}x_0}}{6\sqrt{(1-z_0)^3}} \{ \varphi(x, t) - \varphi(x, t - t_0) \} \quad (97)$$

$$\varphi(x, t) = \frac{e^{\beta_2^2 t - \frac{h^2}{4t}}}{(\beta_2^2 t - \frac{h^2}{4t})(\beta_1 \sqrt{t} + \frac{h}{2\sqrt{t}})} \quad (98)$$

$$\beta_1 = v_d + 1/2 + \sqrt{p} \quad (99)$$

$$\beta_2 = \sqrt{\frac{1}{4} + \alpha + p} \quad (100)$$

$$h = \log\left(\frac{1}{1-z_0}\right) \quad (101)$$

$$C_1(x, o, t) = \frac{-\hbar}{6\sqrt{(1-z_0)^3}} L_p^{-1} \{ e^{x_0 \sqrt{p}} [\varphi(x, t) - \varphi(x, t - t_0)] \} \quad (102)$$

Let

$$L_p^{-1} \{ e^{x_0 \sqrt{p}} \varphi(x, t) \} = \int_0^x G_1(u) G_2(x-u) du \quad (103)$$

$$G_1(x) = L_p^{-1} \left\{ \frac{e^{\beta_2^2 t - \frac{h^2}{4t}}}{(\beta_2^2 t - \frac{h^2}{4t})(\beta_1 \sqrt{t} + \frac{h}{2\sqrt{t}})} \right\} \quad (104)$$

$$G_1(x) = e^{\lambda_3^2 x} \begin{cases} e^{\lambda_3^2 x}, & 0 < x < -t \\ 0, & x > -t \end{cases} \quad (105)$$

$$G_2(x) = \frac{1}{\sqrt{t}} \left[\frac{e^{-\frac{\lambda_1^2}{4x}}}{\sqrt{\pi x}} - \lambda_2 e^{\lambda_1 \lambda_2 + \lambda_2^2 x} \operatorname{erfc} \left(\frac{\lambda_1}{2\sqrt{x}} + \lambda_2 \sqrt{x} \right) \right] \quad (106)$$

$$L_p^{-1} \{ e^{x_0 \sqrt{p}} \varphi(x, t) \} = \frac{e^{\lambda_3^2 x}}{2\sqrt{t}} [F_1(x, t) - F_2(x, t) - F_3(x, t)] \quad (107)$$

Therefore, equation (102) becomes

$$C_1(x, o, t) = \frac{\hbar e^{\lambda_3^2 x}}{6\sqrt{\pi(1-z_0)^3}} \{ \psi_1(x, t) - \psi_1(x, t - t_0) \} \quad (108)$$

Where,

$$\psi_1(x, t) = F_1(x, t) - F_2(x, t) - F_3(x, t) \quad (109)$$

$$F_1(x, t) = \frac{\lambda_2 e^{\lambda_1 \lambda_2 + (\lambda_2^2 - \lambda_3^2)x}}{(\lambda_2^2 - \lambda_3^2)} \operatorname{erfc} \left(\frac{\lambda_1}{2\sqrt{x}} + \lambda_2 \sqrt{x} \right) \quad (110)$$

$$F_2(x, t) = e^{\lambda_1 \lambda_3} \operatorname{erfc} \left(\frac{\lambda_1}{2\sqrt{x}} + \lambda_3 \sqrt{x} \right) \quad (111)$$

$$F_3(x, t) = e^{-\lambda_1 \lambda_3} \operatorname{erfc} \left(\frac{\lambda_1}{2\sqrt{\zeta}} - \lambda_3 \sqrt{\zeta} \right) \quad (112)$$

$$\lambda_1 = -z_0 \quad (113)$$

$$\lambda_2 = v_d + \frac{1}{2} + \frac{h}{2t} \quad (114)$$

$$\lambda_3 = \sqrt{\frac{h^2}{4t} - \left(\frac{1}{4} + \alpha \right)} \quad (115)$$

$$\zeta = x + t \quad (116)$$

$$h = \log \left(\frac{1}{1-z_0} \right) \quad (117)$$

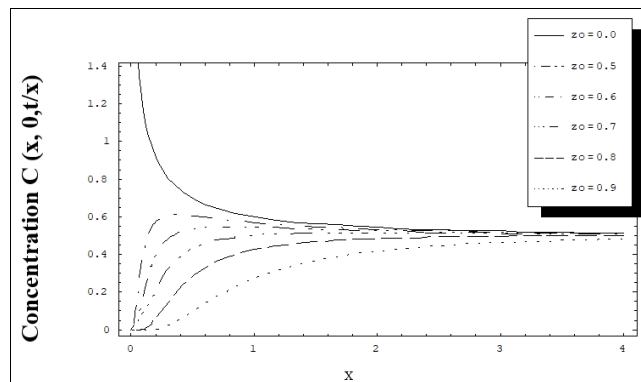


Fig 1: Ground level concentration for various source heights $z_0 = 0, z_0 = 0.5, z_0 = 0.6, z_0 = 0.7, z_0 = 0.8, z_0 = 0.9$ corresponding to the quadratic diffusion and Wind coefficient of constant shear. Compared the results the results with R.E. Robson (1987) [3] as limiting case where chemical reaction rate $\alpha=0$

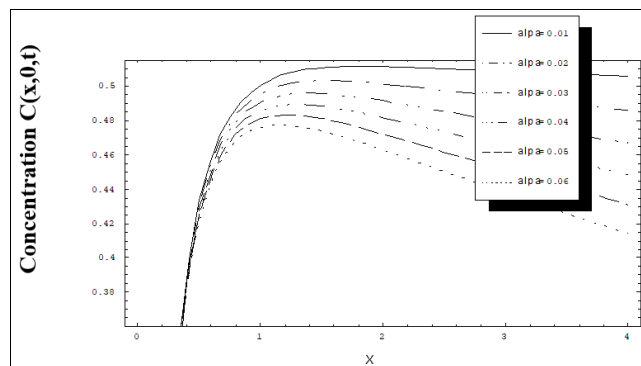


Fig 2: Ground level concentration for variable chemical reaction rate corresponding to the quadratic diffusion and wind coefficient of constant shear, settling velocity $v_d = 0, z_0 = 0.0$

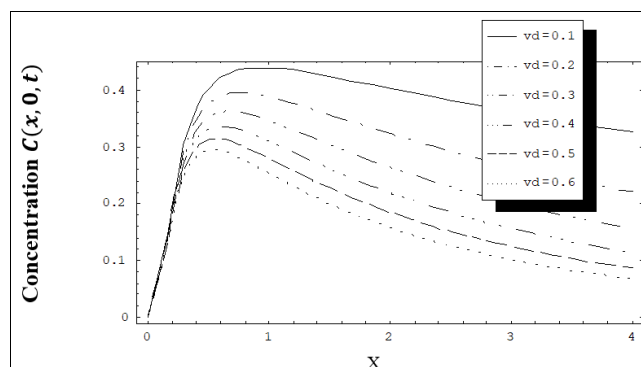


Fig 3: Ground level concentration for various settling velocities corresponding to $v_d = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$, Chemical reaction rate $\alpha = 0$ and source height at $z_0 = 0.7$ settling velocity is zero for the quadratic diffusion coefficient and wind velocity of constant shear with height

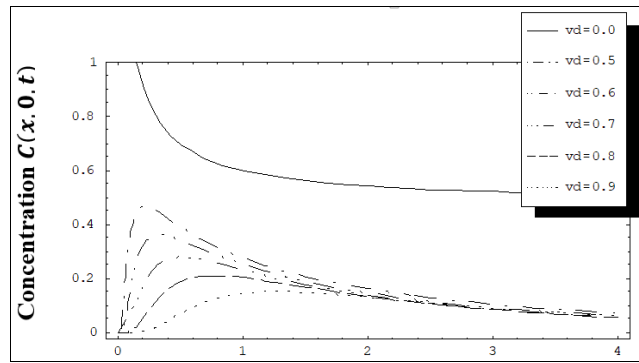


Fig 4: Ground level concentration for various settling velocities corresponding to $v_d = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$, Chemical reaction rate $\alpha = 0$ and source height at $z_o = 0.0$ settling velocity is zero for the quadratic diffusion coefficient and wind velocity of constant shear with height

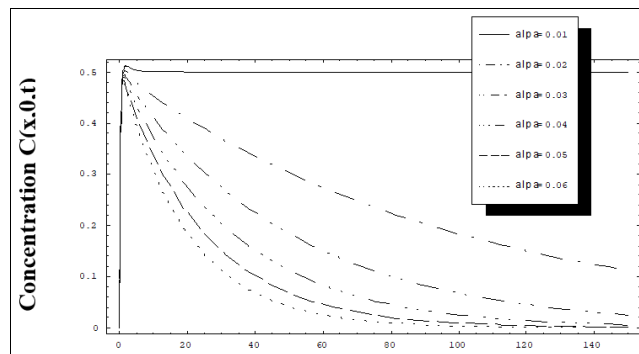


Fig 5: Ground level concentration for variable chemical reaction rate corresponding to the quadratic diffusion and wind coefficient of constant shear, settling velocity $v_d = 0$ $z_o = 0.7$

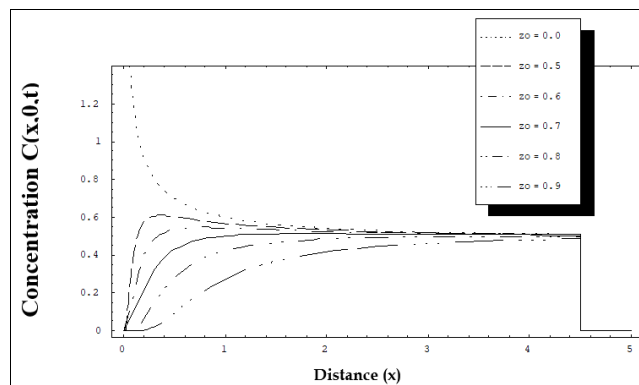


Fig 6: Ground level concentration vs. source heights corresponding to the Quadratic diffusion and constant shear wind coefficient, settling velocity $v_d = 0.0$ Chemical reaction rate $\alpha = 0.0$ at time $t = 5.0$, $t_o = 0.5$

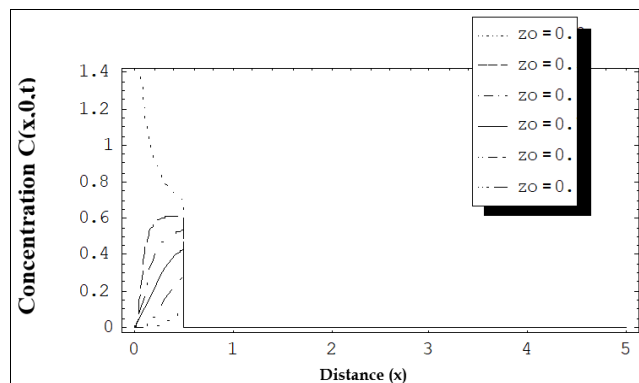


Fig 7: Ground level concentration vs. source heights corresponding to the Quadratic diffusion and constant shear wind coefficient, settling velocity $v_d = 0.0$ Chemical reaction rate $\alpha = 0.0$ at time $t = 1$, $t_o = 0$

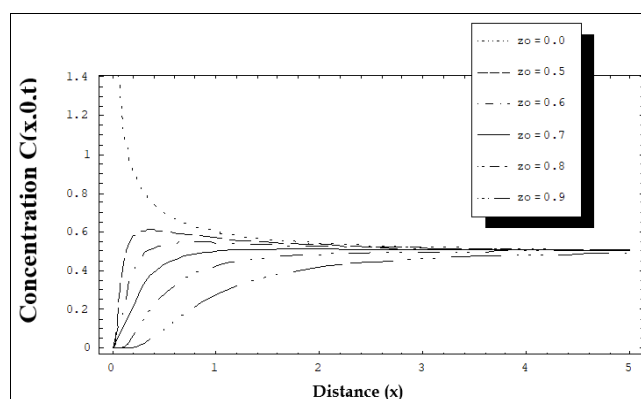


Fig 8: Ground level concentration vs. source heights corresponding to the quadratic diffusion and constant shear wind coefficient, settling velocity $v_d = 0.0$ Chemical reaction rate $\alpha = 0.0$ at time $t = 15, t_o = 0.5$

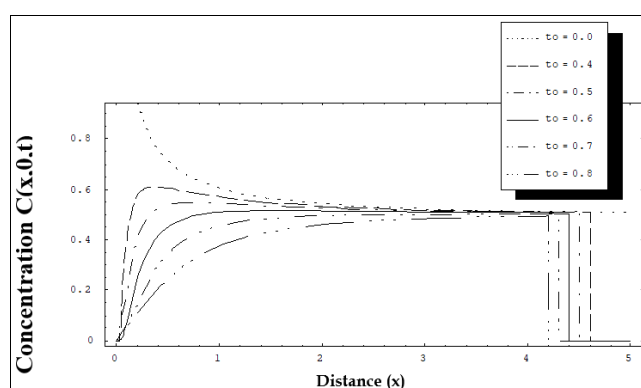


Fig 9: Ground level concentration vs. downwind distance corresponding to the quadratic diffusion and constant shear wind coefficient, settling velocity for various time $t_o, v_d = 0.0$ Chemical reaction rate $\alpha = 0.0$ at time $t = 5, t_o = 0.5$

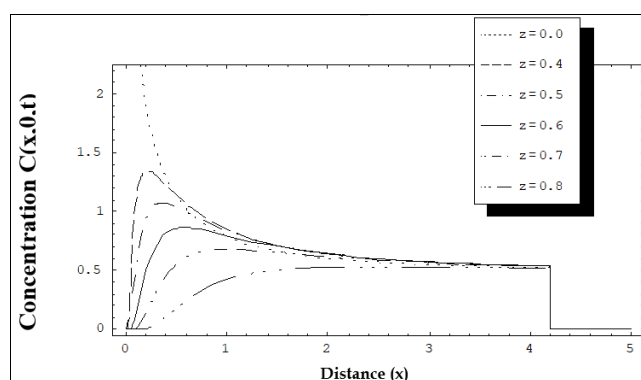


Fig 10: Ground level concentration vs. Distance for various heights on the surface to the quadratic diffusion and constant shear wind coefficient, settling velocity $v_d = 0.0$ chemical reaction rate $\alpha = 0.0$ at time $t = 5, t_o = 0.5$

5. Results and Discussions

In this paper, the dispersion of chemically reactive pollutants emitted from a time dependent line source into a stable atmospheric boundary layer is analyzed by quadratic diffusion coefficient and wind profile $u \propto z^n$ with $n=0, 1$ and 2 . An analytical solution for the constant wind and ($n=0$), but for $n=1$ (constant shear wind profile) the numerical inversion of Laplace transform analyzed earlier (Robson 1987) [3]. However, an analytical solution found for all the cases like the constant wind, constant shear and parabolic type of wind profiles, in the time dependent model, which is more interesting and much realistic with the hypothetical cases in the meteorological parameter. The effect of floor function containing model is simulated. The results are validated for the limiting case for $t \rightarrow \infty$ is verified for steady state model by R.E. Robson. The parabolic wind profile case is validating for the limiting case with no settling C. Sulochana (2009).

6. Conclusions

In the present paper, an unsteady state mathematical model of chemically reactive primary pollutants is studied. The source assumed to be of time dependent (floor function type, specifically defined in the formulation) elevated line source. In addition to this, the settling velocity of pollutants incorporated in the model. Simulated the model for various meteorological parameters and studied the effect of chemical reaction rate, settling velocity and time dependent source. The solution is obtain is

analytically, no numerical technique is performed during solution. The results validated for the case where no settling, chemically reaction rate and no time dependent case were validated with that of R.E. Robson (1987) ^[3].

7. References

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