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Mathematical model for dispersion of air pollutant considering settling of particles and dry deposition

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Abstract

A mathematical model for transport of air pollutant emitted from a point source considering settling of particles and dry deposition is developed. The solution of the mass transport equation together with these conditions is obtained by applying the Generalized integral Laplace transform technique (GILTT). The solution applies *within the earth's* boundary layer since variations in wind speed and vertical eddy diffusivity with height have been taken into account.

Key words: Mathematical Modeling, advection-diffusion equation, Generalized integral Laplace transform technique (GILTT), Planetary boundary layer, settling velocity, deposition velocity.

1. INTRODUCTION

Attention of researchers has been attracted by dispersion of air pollutant in many ways. There are various solution and approximation approaches that have been used in past to deal with air pollution dispersion (Turner 1970, Pasquil 1983; Horst 1983). In last few years a new approach, Laplace Transform Techniques have been used for solving advection-diffusion equation (Cotta R.M. 1993; Cotta and Mikhailov, 1997; Costa et al., 2006; Naveira et al. 2007; Almeida et al. 2008; Cassol et al. 2009). The Generalized Integral Laplace Transform Technique (GILTT) is a powerful hybrid numerical-analytical approach, which has been successfully applied to obtain solution for different classes of linear and non-linear diffusion/connection problems (Wortmann et al., 2006; Moreira et al, 2006; Daniela Buske et al., 2007 and Tirabassi et al., 2009). The removal of pollutants from the atmosphere can occurs in three main ways- general sedimentation of particles, dry deposition and wet deposition. Dry deposition occurs as trace gases and particle are absorbed or impact on objects (building, plants etc.) at the earth's surface. Dry deposition is modeled through a single parameter- the deposition velocity, which either is specified empirically or it estimated from appropriate theoretical relations. When the particles are dense enough and large enough, they fall to the surface by gravity effect also, which is represented in terms of settling velocity, so in dry deposition mechanism gravitational settling velocity and absorption at ground surface are of great importance. F.B. Smith (1962) gave solution for diffusion-deposition equation by Heaviside operational method but considered wind velocity constant with height. Recent solution of the advection-diffusion equation with dry deposition (Ermak, D.L.,1977; Koch 1989;Lin,et al.1997; Moreira et al., 2010) are restricted to the specific case in which the source is located at the ground level or with restriction to the wind and eddy diffusivity vertical profiles or ignoring the settling effect.

In this paper, we develop a mathematical model for transport of air pollutant considering settling of particles and dry deposition. The model's equations are solved by GILTT. Wind velocity and vertical eddy diffusivity vary with height, so obtaining the solution for the diffusion-deposition equation. The wind profile and vertical eddy diffusivity are specified by the power laws.

2. MATHEMATICAL MODEL

The two dimensional steady-state mass transport equation together with gravitational settling velocity and dry deposition on ground can be written as ,

$$u(z)\frac{\partial c}{\partial x} - w_s\frac{\partial c}{\partial z} = \frac{\partial}{\partial z}\left(k_z\frac{\partial c}{\partial z}\right) \qquad \ldots.(1)$$

The boundary conditions are-

$$k_z\frac{\partial c}{\partial z} + w_s c = v_d c \text{ at } z = 0 \qquad \ldots.(2)$$

$$k_z\frac{\partial c}{\partial z} = 0 \text{ at } z = h \qquad \ldots.(3)$$

And a continuous source condition

$$uc(0, z) = Q\delta(z - H_s) \qquad \text{at } x=0 \qquad \ldots.(4)$$

where c is the concentration of the pollutant and w_s is its settling velocity; u is the mean wind speed in x direction and k_z is the vertical eddy diffusivity, v_d is the deposition velocity, Q is the emission rate , H_s is the height of source, h is the planetary boundary layer height and δ is the Dirac delta function. It is assumed that the component of wind velocity in the x direction is very large in comparison of its component in z direction and $k_z >> k_x$, so the effect of diffusion in x-direction may be neglected as compared to advection in x-direction, while in the z-direction advection may be neglected as compared to diffusion.

3. METHOD OF SOLUTION

We solved the problem by GILTT. The main steps of the method include the construction of the auxiliary Strum-Liouville problem associated to the original problem, expansion of the pollutant concentration in a truncated series, having as base functions the eigenfunctions of the Strum- Liouville problem. The transformed equation is obtained from the eigenfunctions orthogonality properties by computing the moments that is, multiplying by the eigenfunctions and integrating over range of z. This procedure leads to a set of ordinary differential equations, which are solved by the application of Laplace transform techniques.

To find the eigenfunctions of the associated Strum- Liouville problem, we divided the problem in to two cases-

Case 1-

When $w_s = v_d$

Then the associated Strum- Liouville problem and respective boundary conditions are-

$$\phi_i''(z) + \lambda_i^2\,\phi_i(z) = 0 \text{ at } 0 < z < h \quad \ldots.(5)$$

$$\phi_i'(z) = 0 \text{ at } z = 0, h \quad \ldots.(6)$$

The solution is $\phi_i(z) = \cos(\lambda_i z)$, where $\lambda_i = i\pi/h$, $\lambda_0 = 0$.

Case 2 –

When $w_s \neq v_d$

Then the associated Strum- Liouville problem and respective boundary conditions are-

$$\phi_i''(z) + \lambda_i^2\,\phi_i(z) = 0 \text{ at } 0 < z < h \quad \ldots.(7)$$

$$k_z\,\phi_i'(z) + w_s\,\phi_i(z) = v_d\,\phi_i(z) \text{ at } z = 0 \quad \ldots.(8)$$

$$\phi_i'(z) = 0 \text{ at } z = h \quad \ldots.(9)$$

The solution is $\phi_i(z) = \cos[\lambda_i(h-z)]$, where λ_i is given by the equation

$\lambda_i \tan(\lambda_i h) = (v_d - w_s)/\,k_z(z_0)$, which is solved by numerical methods. The k_z is not evaluated at z=0 but at z_0 (the roughness length) where v_d is also defined.(Arya 1999).

The functions ϕ_i (z) and λ_I known respectively, as the eigenfunctions and eigenvalues associated with the Strum- Liouville problem.

Equation (1) can be written as

$$u(z)\frac{\partial c}{\partial x} = k_z\frac{\partial^2 c}{\partial z^2} + \left(w_s + \frac{\partial k_z}{\partial z}\right)\frac{\partial c}{\partial z} \quad \ldots.\,(10)$$

Let $\psi_i(z)$ be orthonormal eigenfunctions associated with the Strum- Liouville problem, then we assume solution of eq. (1) as

$$c(x, z) = \sum_{i=0}^{\infty}\bar{c}_i(x)\psi_i(z) \quad \ldots.\,(11)$$

Substituting equation (11) in (10) and multiplying by $\psi_j(z)$, then integrating with respect to z from 0 to h, we get

$$\sum_{i=0}^{\infty}\bar{c}_i{}'(x)\int_0^h u(z)\psi_i\psi_j\,dz + \sum_{i=0}^{\infty}\bar{c}_i x\left[\lambda_i^2\int_0^h k_z\psi_i\psi_j\,dz - \int_0^h\left(w_s + \frac{\partial k_z}{\partial z}\right)\psi_i{}'\psi_j\,dz\right] = 0 \quad \ldots.\,(12)$$

Now, taking $Y(x) = \{\bar{c}_i(x)\}$, $H = E^{-1}F$, $E = \{e_{ij}\}$,

where $e_{ij} = \int_0^h u\,\psi_i\psi_j\,dz$

$F = \{f_{ij}\}$ where $fij = \lambda_i^2\int_0^h k_z\psi_i\psi_j\,dz - \int_0^h\left(w_s + \frac{\partial k_z}{\partial z}\right)\psi_i{}'\psi_j\,dz$

Equation (7) can be written in matrix form as

$$Y'(x) + HY(x) = 0 \quad \ldots.\,(13)$$

Then using (4),

$$c_0(0) = \frac{Q\psi_0(H_s)\sqrt{h}}{\int_0^h u(z)\psi_0^2(z)dz}, \qquad \text{for } i = 0 \quad \ldots.(14)$$

$$c_i(0) = \frac{Q\psi_i(H_s)\sqrt{h}/2}{\int_0^h u(z)\psi_i^2(z)dz}, \qquad \text{for } i \neq 0 \quad \ldots.(15)$$

Taking Laplace transform of (13), we get

$$(p+H)\,\bar{Y}(p) - Y(0) = 0 \quad \ldots.\,(16)$$

where the $\bar{Y}(p)$ represents the Laplace transform of Y(x). The matrix H can be decomposed into eigenvectors and eignevalues as

$$H = XDX^{-1} \quad \ldots.\,(17)$$

where X is the matrix of the eignevectors and D is the diagonal matrix of the eigenvalues of H. Then equation (16) becomes

$$\bar{Y}(p) = X(pI + D)^{-1} X^{-1} Y(0) \quad \text{, where I is the identity matrix.} \qquad \ldots. (18)$$

The elements of the diagonal matrix (pI + D) have the form $\{p+d_i\}$, where d_i is the eigenvalue of the matrix H. Inverse of a diagonal matrix is the inverse of their elements. So the diagonal elements of $(pI + D)^{-1}$ are $1/(p + d_i)$, whose transformed inverse of Laplace is $e^{-d_i x}$, A(x) being the diagonal matrix with elements $e^{-d_i x}$, then the solution of equation (18) is given by

$$Y(x) = \{\bar{c}_i(x)\} = XA(x)\, X^{-1}\, Y(0) \qquad \ldots. (19)$$

Thus the final solution is,

$$c(x,z) = \sum_{i=0}^{\infty} XA(x)\; X^{-1} Y(0)\, \psi_i(z) \qquad \ldots. (20)$$

4. RESULTS AND DISCUSSION

To obtain the numerical value of c(x,z), the wind and vertical eddy diffusivity profiles have to be specified. The wind speed and the vertical eddy diffusivity can be expressed as a function of height and represented by the following power laws with the power indexes p and n respectively, as follows

$$u(z) = u_1 z^p$$

and $$k_z(z) = k_1 z^n.$$

where u_1 and k_1 are constants. To obtain solution of diffusion-equation, power law assumption for wind and eddy diffusivity has been used by a number of researchers (Calder, 1949; Rounds, 1955; Haung and Drake, 1977; Van Uden, 1978 and Haung, 1979).

The meteorological conditions and diffusion parameters used for the calculations of concentration are as follows; wind speed $u = 5\ ms^{-1}$ at a height of 10m; the power law indexes are p = 0.15 and n = 1

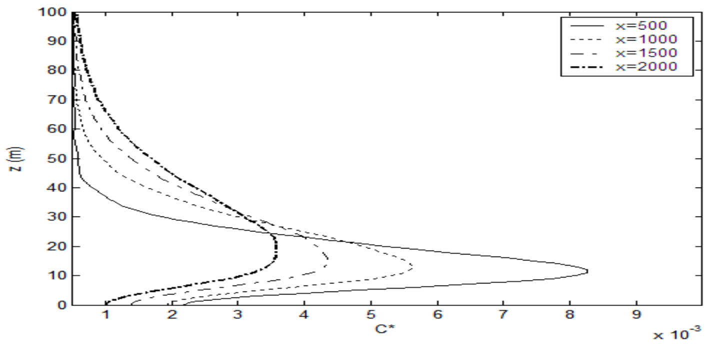

Fig. 1. Vertical profiles of C* for various downward distances.

The change in concentration (c* = c/Q) profiles with respect to vertical distance z and downward distance x is shown in Fig.1. Its verified the traditional behavior of pollution dispersion, larger value of concentration for short distance, which become smaller with increase in the downward distance. For stable flow, the value of c* first increases with increasing value of z and becomes maximum at some height and then decreases with increasing value of z and finally tends to zero for large value of z, which fairly matches with natural behavior of pollutant dispersion. Relation between ground surface concentration and source height is shown in Fig 2. The peak in an area near to the source decreases with the increase in source height, verified that near the source the ground surface concentration increases rapidly in a short distance and then decreases. This shows that concentration with nearby areas of source is more and then gradually decreases with distance. It's also verified that the ground level concentration is quite sensitive to source height. For low source height very high ground surface concentration near the source, so in order to dispose pollutants over a large area, large value of source height should be considered.

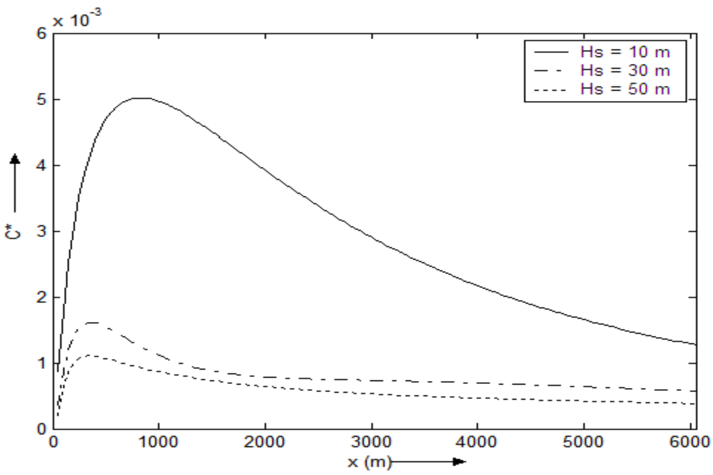

Fig. 2. Ground surface concentration curves with downward distance for various source heights.

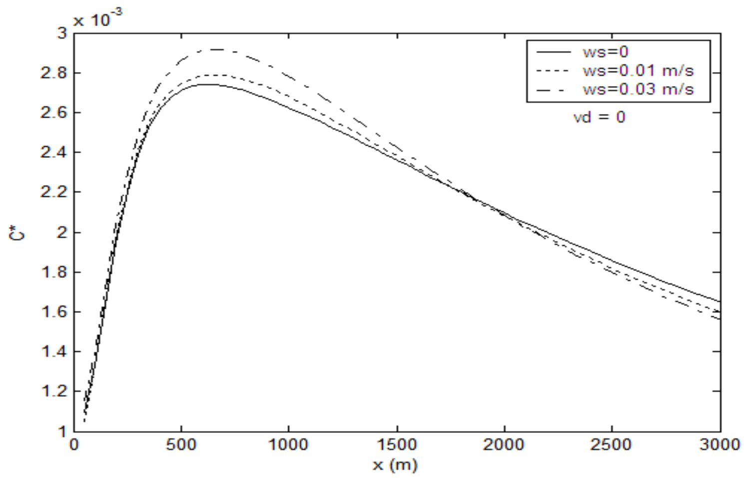

Fig. 3. Variation of ground level downward concentration for different settling velocities**.**

The effect of gravitational settling on the ground-level concentration is shown in Fig. 3. With increase in settling velocity the ground-level concentration increases upto some distance and after that it change its pattern, this is because of the fact that as the settling velocity increases, then after some downwind distance only light particles left in the smoke and gravity force becomes almost ineffective on these particles.

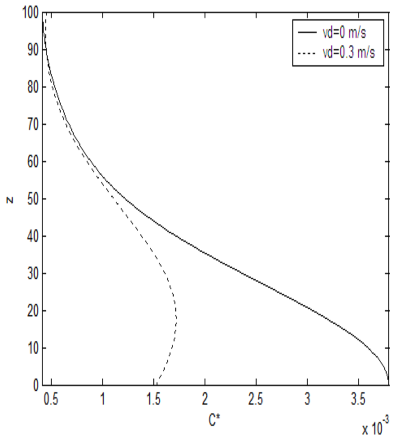

Fig. 4. Vertical profile of concentration with deposition and non deposition at x=1000 m

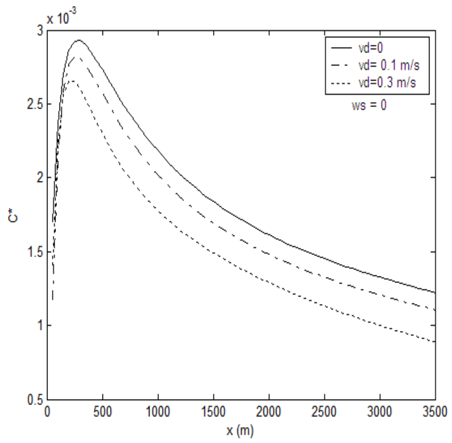

Fig. 5.Variation in ground level concentration with downwind distance for different diposition velocities.

There is a decrease in concentration near the ground surface when deposition is considered as shown in Fig.4, since dry deposition by trees,leaves,plants and buildings etc. clearly decreases the ground level concentration. Fig. 5 shows the variation of downward ground-level concentration for various dry deposition velocities.Ground level concentration decreases with increasing value of deposition velocities at the same downward distance.

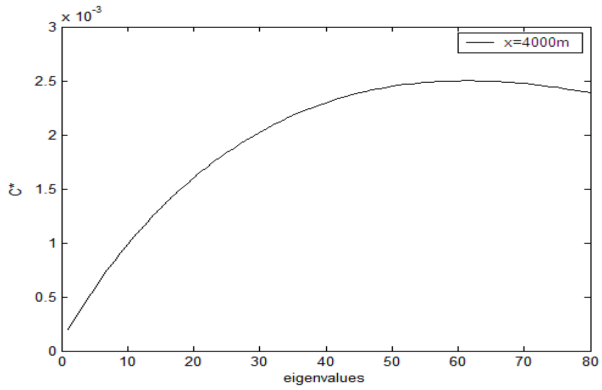

Fig. 6. Convergence of the model for ground level concentration

In Fig. 6 we have shown the numerical convergence of the proposed solution for the the concentration by GILTT at x=4000 m and Hs = 10 m,with the increasing number of eigenvalues.From this figure , we notice that we can reach a prescribed accuracy varying the number of eigenvalues.

5. Conclusion

In this work, the Generalised Integral Laplace Transform Technique (GILTT) was successfully employed for the modelling of air polutant dispersion by considering gravitational settling and dry deposition . The result were presented graphically for showing the effect of gravitational setting and dry deposition on the ground level concentration . Results obtained in this work show good agreement with literature avilable.

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