Mathematical Treatment for the Pollutant Dispersion Considering the Ground as an Absorber-Reflector Surface for the Pollutant

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Abstract: A two – dimensional steady – state, mathematical modeling has been presented for the pollutant released from an elevated source in an inversion layer. The study presents a treatment for computing the pollutant concentration distribution under a physically realistic boundary condition which considers the ground as an absorber-reflector surface for the pollutant simultaneously. The wind speed is parameterized in terms of vertical height using the power law profile. The partial differential equation describing the advection-diffusion of pollutants has been solved using separation of variables method. An upper boundary condition which assumes the presence of capping inversion is taken into consideration. The mathematical formulation for the pollutant concentration distribution obtained in the present treatment is given in terms of Bessel and Gamma functions.
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Introduction

Mathematical modeling is a tool for establishing various aspects in air pollution like; emission control legislation, impact assessment, and emergency preparedness etc. [1]. The analytical solution of the advection-diffusion equation bears significant importance since all influencing parameters are expressed in mathematically closed form [2].From this modeling; it is possible to investigate dispersion from continuous point source given appropriate boundary and initial conditions. The model that is commonly used worldwide for regulatory purposes is the general Gaussian Plume Model (GPM).This model is based on various a assumptions:(1) the mean wind speed and eddy diffusivities do not have spatial variation (2)the ground surface is a perfect reflector for the pollutant (3)the diffusion in the vertical direction is unrestricted ,i.e., it is not capped by an inversion which tends to reflect back the pollutant hitting the inversion base[3]. In this respect, gradient transport theory is one of the analytical techniques that can overcome these short comings by inclusion of some of the above-mentioned physical processes, which will be more appropriate for treatment of atmospheric dispersion.

The analytical solution for the standard conditions of the advection-diffusion equation is obtained only by making some particular assumptions about the eddy diffusivities (homogeneous turbulence) and considering stationary conditions [4-6].

In the present work, we will present an analytical solution for the advection-diffusion equation which describes pollutant dispersion from a continuous elevated point source. In this formulation, the steady state condition is taken into consideration under the following postulates:

The down-wind speed profile is parameterized as a power-law depending on the vertical height (z) above ground level [2].

The pollutant dispersion remains confined to a layer capped by an inversion lid at the top, which serves as an impermeable upper boundary layer for the pollutant [7].

The inclusion of the ground surface as a reflector-absorber for the pollutants at the same time. This assumption is taken into consideration as an appropriate-realistic lower boundary condition.

2. Mathematical Description of the Problem

Considering a Cartesian coordinates system in which the x-axis coincides with the direction of the average wind and z is the vertical axis, then the steady-state of a contaminant released from a point source is described by the following partial differential equation[8];

$$u\frac{\partial \chi}{\partial x}+v\frac{\partial \chi}{\partial y}+w\frac{\partial \chi}{\partial z}=\frac{\partial}{\partial x}(k_x\frac{\partial \chi}{\partial x})+\frac{\partial}{\partial y}(k_y\frac{\partial \chi}{\partial y})+\frac{\partial}{\partial z}(k_z\frac{\partial \chi}{\partial z}) \quad (1)$$

Where χ denotes the average concentration, kx, ky, kz and u, v, w are the Cartesian components of the eddy diffusivities and wind, respectively. The crosswind integration of Eq.1,in stationary conditions and neglecting the longitudinal diffusion) leads to:

$$u\frac{\partial \chi}{\partial x}=\frac{\partial}{\partial z}(k_z\frac{\partial \chi}{\partial z}) \quad (2)$$

A power-law profile is used to describe the variation of wind speed u with height in the surface boundary layer, thus,u can be parameterized in terms of z as:

$$\frac{u(z)}{u(z_r)} = \left(\frac{z}{z_r}\right)^m \quad , 0 < m \le 1 \quad (3)$$

Where m is the power-law exponent which depends on thermal atmosphere stability (z_r) is the speed at a reference height z_r(usually z_r=10m).Eq. 3, can be written as:

$$u(z) = bz^m \quad (4)$$

Where $b = \frac{u_r}{z_r^m}$

The eddy diffusion coefficient k_z is assumed constant k in our derivation. Then Eq. 2, reduces to:

$$b\, z^m \frac{\partial \chi_y(x,z)}{\partial \chi} = k \frac{\partial^2 \chi_y(x,z)}{\partial z^2} \quad (5)$$

3. Method of Solution

The second order partial differential eq. 5 will be solved using the method of separation of variables. The concentration distribution function $\chi(x,z)$ is separated as:

$$\chi_y(x,z) = X(x) \bullet Z(z) \quad (6)$$

Differencing partially with respect to both x and z, and substituting in Eq. 6, we get:

$$b\, z^m\, Z(z) \frac{dX(x)}{dx} = k\, X(x) \frac{d^2 Z(z)}{dz^2} \quad (7)$$

Dividing both sides on z^m k X(x) Z (z) we get two ordinary differential equation in the two variables x and z as:

$$\frac{1}{X(x)} \frac{dX(x)}{dx} = -\frac{\beta^2}{b} k \quad (8)$$

And

$$\frac{z^{-m}}{Z(z)} \frac{d^2 Z(z)}{dz^2} = -\beta^2 \quad (9)$$

Where β^2 is a constant.

3.1. Boundary conditions

(i) The modified approach adopted in this study is to assume that the ground is assumed to be partially reflector and partially absorber surface to the pollutant.

Accordingly, diffusive flux at the ground surface does not vanish ,i.e.,

$$k \frac{dZ(z)}{dz} = v_d\, \chi_\circ \quad \text{at} \quad z = z_\circ \quad (10)$$

Where $\chi_\circ$ is the pollutant concentration at a reference height z_0, the roughness height, which is very close to the ground surface (z_0=0.3 m – 1.0 m)[9].

(ii) The pollutant is not able to penetrate through the top of the inversion / mixed layer located at height a ,i.e., the concentration vanishes at the height a;

$$\chi_y(x,z) = 0$$

At $z = a$ (11)

3.2. Solution of the differential equations

3.2.1. The horizontal equation in the variable x

Eq. 8, can be integrated to get the solution:

$$X(x) = \exp(-\frac{\beta^2 k}{b} x) \quad (12)$$

3.2.2. The vertical equation in the variable z

Eq. 9, can be transformed to Bessel differential equation [10] as;

$$Z(z) = z^{1/2}[c_1 J_n(2\beta n z^{1/2n}) + c_2 Y_n(2\beta n z^{1/2n})] + A \quad (13)$$

Where $J_n(2\beta n z^{1/2n})$ is the Bessel function of order n and first kind, while $Y_n(2\beta n z^{1/2n})$is the Bessel function of second kind. The order n is; $n = \frac{1}{m+2}$

A is a parameter which is determined from the boundary conditions such that it tends to zero for large values of z. c_1 and c_2 are constants.

From the characteristics of Bessel differential equations solution, if n is a fraction, the solution can be expressed in terms of two Bessel functions of first kind and of orders n and –n. Thus, the solution of the differential equation given by Eq. 13, is reduced to:

$$Z(z) = z^{1/2}[c_1 J_n(2\beta n z^{1/2n}) + c_2 J_{-n}(2\beta n z^{1/2n})] + A \quad (14)$$

3.3. Determination of the constants

From the boundary condition Eq. 10,which is valid very close to the ground surface, i.e. small values for the variable z, the Bessel function $J_n(x)$for small values of x is approximated as [11].

$$\Gamma(p) = \int_0^\infty x^{p-1} e^{-x} dx \quad (15)$$

Where Gamma function Γ(n+1) has the formula :

$$J_n(x) = \frac{x^n}{2^n \Gamma(n+1)} \quad (16)$$

When substituting Eq. 15, on Eq. 14, we find that the constant c_2 should vanish, since the function $J_{-n}(z)$ has imaginary argument . By applying the boundary condition Eq. 10, we get

$$k c_1 \frac{(\beta n)^n}{\Gamma(n+1)} = \nu_d \chi_\circ$$

Then the constant c_1 can found as:

$$c_1 = \frac{\nu_d \chi_\circ \Gamma(n+1)}{k(\beta n)^n} \qquad (17)$$

Thus, Eq. 14 can be written in the form:

$$Z(z) = z^{1/2} \frac{\nu_d \chi_\circ \Gamma(n+1)}{k(\beta n)^n} J_n(2\beta n z^{1/2n}) + A \qquad (18)$$

On substituting both Eq. 12, and Eq.18 in Eq. 6, we get the concentration distribution function as:

$$\chi_y(x,z) = \exp(-\frac{\beta^2}{b} k\, x)\left[A + z^{1/2}\frac{\nu_d \chi_\circ \Gamma(n+1)}{k\,(\beta\, n)^n} J_n(2\beta\, n z^{1/2n})\right]$$

(19)

4. Application of the Upper Boundary Condition

Is the boundary condition given by Eq.11, for large values of z. In this case A will be zero, and the boundary condition then reads:

$$\exp(-\frac{\beta^2}{b} kx)\left[z^{1/2}\frac{\nu_d \chi_\circ \Gamma(n+1)}{k\,(\beta\ n)^n} J_n(2\beta\ n z^{1/2n})\right] = 0$$

at z=a (20)

Then, we get

$$\beta = \frac{(3n+2)\pi}{8n\, a^{1/2n}} \qquad (21)$$

5. The Boundary Condition at the Point of Emission

It is well known that the pollutant concentration $\chi_y(x,z)$ both in air and on ground level is directly proportional to the source strength Q and inversely with both the source height h_s and the wind velocity at the emission point u (h_s).These concepts can be expressed as:

$$\chi_y(x,z) = \frac{Q}{h_s\, u(h_s)} \quad \text{at} \quad x=0, z=h_s \qquad (22)$$

Applying this condition, Then the constant A may have the formula:

$$A = \frac{Q}{b h_s^{m+1}} - h_s^{1/2} \frac{\nu_d \chi_\circ \Gamma(n+1)}{k(\beta\, n)^n} J_n(2\beta\, n h_s^{1/2n})$$

(23)

The resulting expression for the concentration $\chi_y(x,z)$ can be obtained from Eq. 19,. When substituting the values of the constants A (Eq.23) and B (Eq.21).If we assume a Gaussian distribution for the contaminated plume in y-direction, the final formula of the total pollutant concentration $\chi\ (x, y, z)$ can be written as:

$$\chi\ (x, y, z) = \chi_y (x, z) \exp[\ -\frac{y^2}{2\sigma_y{}^2}\ ] * \frac{1}{\sqrt{2\pi}\sigma_y}$$

(24)

6. Summary and Conclusions

In this work we present an analytical treatment to solve the advection – diffusion equation describing the atmospheric dispersion of pollutants released from an elevated point source. In the model, we take into account more realistic physical boundary conditions.

The ground is considered as reflector and absorber surface for the pollutants reaching it. Also, we take into consideration the existence of capping inversion layer at which the pollutants are not able to penetrate, and we assume that this layer is located at height a above the ground surface. The wind velocity profile is taken as power law variation with the height z in the vertical direction.

The solution of the differential equation is obtained in terms of Bessel function of the first kind. Due to the very limited data concerning atmospheric dispersion under the same group of boundary conditions adopted in our study, specially, the reflectivity and absorptive of the ground surface for the pollutants, the present model could not be validated by comparison its result with either experimental data or another models. We think when suitable data becomes available, namely, absorption and reflection of ground surface for the pollutants, deposition velocities of the pollutants under consideration, inversion layer heights and the source characteristics, we are confident to point out that the results of the present model can be validated easily.

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