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New Technique for Solving the Advection-diffusion Equation in Three Dimensions using Laplace and Fourier Transforms

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Abstract

A steady-state three-dimensional mathematical model for the dispersion of pollutants from a continuously emitting ground point source in moderated winds is formulated by considering the eddy diffusivity as a power law profile of vertical height. The advection along the mean wind and the diffusion in crosswind and vertical directions was accounted. The closed form analytical solution of the proposed problem has obtained using the methods of Laplace and Fourier transforms. The analytical model is compared with data collected from nine experiments conducted at Inshas, Cairo (Egypt). The model shows a best agreement between observed and calculated concentration.

Keywords: Advection-diffusion equation; Laplace transform; Fourier transform; Bessel function

Introduction

Environmental problems caused by the huge development and the big progress in industrial, which cause's a lot of pollutions. The transport of these pollutants can be adequately described by the advection–diffusion equation. In the last few years, there has been increased research interest in searching for analytical solutions for the advection–diffusion equation (ADE). Therefore, it is possible to construct a theoretical model for the dispersion from a continuous point source from an Eulerian perspective, given adequate boundary and initial conditions and the knowledge of the mean wind velocity field and of the concentration turbulent fluxes. The exact solution of the linear advection–dispersion (or diffusion) transport equation for both transient and steady-state regimes has been obtained [1].

The two- and three-dimensional advection–diffusion equation with spatially variable velocity and diffusion coefficients has been provided analytically [2]. A mathematical treatment has been proposed for the ground level concentration of pollutant from the continuously emitted point source [3]. Essa and El-Otaify studied a mathematical model for hermitized atmospheric dispersion (self adjoined by itself) in low winds with eddy diffusivities as linear functions of the downwind distance [4]. More recently the generalized analytical model describing the crosswind-integrated concentrations is presented [5]. Also, an analytical scheme is described to solve the resulting two dimensional steady-state advection–diffusion equation for horizontal wind speed as a generalized function of vertical height above the ground and eddy diffusivity as a function of both downwind distance from the source and vertical height.

On the other hand, the literature presents several methods to analytically solve the partial differential equations governing transport phenomena [6-10]. For example, the method of separation-of-variables is one of the oldest and most widely used techniques. Similarly, the classical Green's function method can be applied to problems with source terms and inhomogeneous boundary conditions on finite, Semi-infinite, and infinite regions [10,11]. Integral transform techniques, such as the Laplace and Fourier transform methods, employ a mathematical operator that produces a new function by integrating the product of an existing function and a kernel function between suitable limits.

In this study, we obtained a mathematical model for dispersion of air pollutants in moderated winds by taking into account the diffusion in vertical height direction and advection along the mean wind. The eddy diffusivity is assumed to be power law in the vertical length. We provided analytical solutions to the advection–diffusion equation for three-dimensional with the physically relevant boundary conditions. The moderate data collected during the convective conditions. From nine experiments conducted at Inshas site, Cairo-Egypt [4], which used to investigate the analytical solution.

Mathematical Treatment

The dispersion of pollutants in the atmosphere is governed by the basic atmospheric diffusion equation. Under the assumption of incompressible flow, atmospheric diffusion equation based on the Gradient transport theory can be written in the rectangular coordinate system as:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)+S+R \qquad (1)$$

where C(x, y, z) is the mean concentration of a pollutant (Bq/m^3), (μg/m^3) and (ppm); in which t is the time, S and R are the source and removal terms, respectively; (u, v, w) and (k_x, k_y, k_z) are the components of wind and diffusivity vectors in x, y and z directions, respectively, in an Eulerian frame of reference.

The following assumptions are made in order to simplify equation (1):

1) Steady -state conditions are considered, i.e., $\partial C/\partial t = 0$

2) We are going to study Eq. (1) in case, when the components of

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wind (v, w) tends to zero

3) Source and removal (physical/chemical) pollutants are ignored so that S=0 and R=0

4) Under the moderate to strong winds, the transport due advection dominates over that due to longitudinal diffusion: $\left|u\frac{\partial C}{\partial x}\right| >> \left|\frac{\partial}{\partial x}\left(k_x\frac{\partial C}{\partial x}\right)\right|$

With the above assumptions, equation (1) reduces to:

$$u\frac{\partial \tilde{C}(x,y,z)}{\partial x} = \frac{\partial}{\partial y}\left(K_y\frac{\partial \tilde{C}(x,y,z)}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial \tilde{C}(x,y,z)}{\partial z}\right) \tag{2}$$

Under the following boundary conditions:

$$\tilde{C}(x,y,z) = 0 \qquad \forall \qquad x,y,z \Rightarrow \infty \tag{3}$$

$$\tilde{C}(x,y,z) = \frac{Q}{u}\delta_x\delta_y \quad at \quad z = h \tag{4}$$

$$\tilde{C}(x,y,z) = \frac{Q}{u}\delta_y\delta_z \quad at \quad x = 0 \tag{5}$$

$$\frac{\partial \tilde{C}(x,y,z)}{\partial y} = 0 \quad at \quad y = \pm\infty \tag{6}$$

where δ (…) is Dirac's delta function, and h is the mixing height.

The wind speed u and eddy diffusivity k_y, k_z is expressed as a functions of power law of z as:

$$\begin{aligned} &u = z^m;\ z \neq 0; \quad u = u_0;\ z = 0; \\ &k_y = \alpha z^m; \quad \alpha \neq 0; \\ &k_z = \beta z^n; \quad n < 1; \qquad \beta \neq 0; \end{aligned} \tag{7}$$

Where α, β, m, n are turbulence parameters and depend on atmospheric stability.

The Analytical Solution

Eq. (2) can solve analytically as follows:

Transform the variable x to s by applying the Laplace transform on Eq. (2) to become

$$-Q\delta(y)\delta(z-z_0) + sz^m\tilde{C}(s,y,z) = \alpha z^m\frac{\partial^2\tilde{C}(s,y,z)}{\partial y^2} + \beta z^n\frac{\partial^2\tilde{C}(s,y,z)}{\partial z^2} + \beta n z^{n-1}\frac{\partial \tilde{C}(s,y,z)}{\partial z} \tag{8}$$

Again transform the variable y to λ by applying the Fourier transform on Eq. (8) to become

$$-Q\delta(z-z_0) + sz^m\tilde{C}_*(s,\lambda,z) = -\alpha\lambda^2 z^m\tilde{C}_*(s,\lambda,z) + \beta z^n\frac{\partial\ \tilde{C}_*(s,\lambda,z)}{\partial z} + \beta n z^{n\ \ 1}\frac{\partial \tilde{C}_*(s,\lambda,z)}{\partial z} \tag{9}$$

Eq. (9) simplified to the form

$$\beta z^n\frac{\partial^2\tilde{C}_*(s,\lambda,z)}{\partial z^2} + \beta n z^{n-1}\frac{\partial \tilde{C}_*(s,\lambda,z)}{\partial z} - (\alpha\lambda^2 + s)z^m\tilde{C}_*(s,\lambda,z) = -Q\delta(z-z_0) \tag{10}$$

Now we will solve the homogeneous equation of Eq. (10) which takes the form

$$z^2\frac{\partial^2\tilde{C}_*(s,\lambda,z)}{\partial z^2} + nz\frac{\partial \tilde{C}_*(s,y,z)}{\partial z} - \frac{(\alpha\lambda^2 + s)}{\beta}z^{m-n+2}\tilde{C}_*(s,\lambda,z) = 0 \tag{11}$$

Transform $z\ to\ z_* : z_* = z^{\frac{m-n+2}{2}}$ then Eq. (11) becomes

$$z_*^2\frac{\partial^2\tilde{C}_*}{\partial z_*^2} + \frac{m+n}{m-n+2}z_*\frac{\partial \tilde{C}_*}{\partial z_*} - \frac{4(\alpha\lambda^2 + s)}{\beta(m-n+2)^2}z_*^2\tilde{C}_* = 0 \tag{12}$$

Again transform $\tilde{C}_*\ to\ \tilde{C}_{**} : \tilde{C}_* = z_*^{\frac{1-n}{m-n=2}}\tilde{C}_{**}$ then Eq. (12) become

$$z_*^2\frac{\partial^2\tilde{C}_{**}}{\partial z_*^2} + z_*\frac{\partial \tilde{C}_{**}}{\partial z_*} - ((\eta z_*)^2 + \nu^2)z_*^2\tilde{C}_{**} = 0 \tag{13}$$

where $\nu = \frac{1-n}{m-n=2}$; $and\ \eta = \sqrt{\frac{4(s+\alpha\lambda^2)}{\beta(m-n+2)^2}}$

But Eq. (13) is modified Bessel equation which has solution [12].

$$\tilde{C}_{**} = AI_\nu(\eta z_*) + BK_\nu(\eta z_*) \tag{14}$$

$$\tilde{C}_* = z_*^\nu\tilde{C}_{**} = z_*^\nu[AI_\nu(\eta z_*) + BK_\nu(\eta z_*)] \tag{15}$$

where A and B are constant

Now the general solution of the non-homogeneous Eq. (10) takes the form

$$\tilde{C}_* = z_*^\nu[A_*I_\nu(\eta z_*) + B_*K_\nu(\eta z_*)] \tag{16}$$

where A_* and B_* are constants

Apply the boundary condition Eq. (3) on Eq. (16) which become

$$\tilde{C}_*(\mathrm{s},\lambda,\mathrm{z}) = B_*z_*^\nu K_\nu(\eta z_*) \tag{17}$$

Apply the boundary condition Eq. (5) on Eq. (16) which gives

$$B_* = \frac{Q}{u}\frac{\Gamma(1-\nu)\sin(\nu\pi)}{\frac{\pi}{2}(\frac{\eta}{2})^{-\nu}} \tag{18}$$

Substitute B_* Eq. (16) in Eq. (17) which gives:

$$\tilde{C}_*(\mathrm{s},\lambda,\mathrm{z}) = \frac{2Q}{\pi u_0}(\frac{\eta}{2})^\nu\Gamma(1-\nu)\sin(\nu\pi)z_*^\nu K_\nu(\eta z_*) \tag{19}$$

Apply inverse Fourier and inverse Laplace respectively on Eq. (19) we get:

$$C(x,y,z) = \frac{2\sqrt{2}Q\Gamma(1-\nu)\sin(\nu\pi)}{u_0\sqrt{\alpha\pi}}(2\mathrm{x})^{\nu-\frac{1}{2}}\left(\frac{z^{\frac{m-n+2}{2}}}{(m-n+2)\sqrt{\beta}}\right)^\nu\left(\frac{4z^{m-n+2}}{(\mathrm{m-n+2})^2\beta} + \frac{y^2}{\alpha}\right)^{-\nu-\frac{1}{2}}e^{\left[-\left(\frac{z^{m-n+2}}{(\mathrm{m-n+2})^2\mathrm{x}\beta} + \frac{y^2}{4\alpha x}\right)\right]} \tag{20}$$

Source Data

The diffusion data for the estimating were gathered during ^{135}I isotope tracer nine experiments in moderate wind with unstable conditions at Inshas, Cairo. During each run, the tracer was released from source has height 43 m for twenty four hours working, where the air samples were collected during half hour at a height 0.7 m. We collected air samples from 92 m to 184 m around the source in AEA, Egypt. The study area is flat, dominated by sandy soil with poor vegetation cover. The air samples collected were analyzed in Radiation Protection Department, NRC, AEA, Cairo, Egypt using a high volume air sampler with 220 V/50 Hz bias [13]. Meteorological data have been provided by the measurements done at 10 m and 60 m.

For the concentration computations, we require the knowledge of wind speed, wind direction, source strength, the dispersion parameters, mixing height and the vertical scale velocity. Wind speeds are greater than 3 m/s most of the time even at 10 m level. Further the variation wind direction with time is also visible. Thus in the present study, we have adopted dispersion parameters for urban terrain which are based on power law functions. The analytical expressions depend upon downwind distance, vertical distance and atmospheric stability. The atmospheric stability has been calculated from Monin-Obukhov length scale (1/L) [14] based on friction velocity, temperature, and surface heat flux.

Results and Discussion

The concentration is computed using data collected at vertical distance of a 30 m multi-level micrometeorological tower. In all a test runs were conducted for the purpose of computation. The concentration at a receptor can be computed in the following way:

Applying formula Eq. (21) which contains eddy diffusivities as function with power law at y = 0.0 for half hourly averaging.

As an illustration, results computed from these approaches are shown in Table 1, for nine typical tests conducted at Ins has site, Cairo-Egypt [4]. This table shows that the observed and predicted concentrations for ^{135}I using Eq. (20) with power law of eddy diffusivities and the wind speed are very near to each other of ^{135}I.

Test	Downwind distance (m)	Observed conc. (Bq/m^3)	Predicted conc. (Bq/m^3)
1	100	0.025	0.047
2	98	0.037	0.076
3	115	0.091	0.127
4	135	0.197	0.225
5	99	0.272	0.282
6	184	0.188	0.196
7	165	0.447	0.503
8	134	0.123	0.162
9	96	0.032	0.039

Table 1: Observed and predicted concentrations for run 9 experiments.

Figure 1 shows the variation of predicted and observed concentration of ^{135}I with the downwind distance. One gets very good agreement between observed and predicted concentration.

Figure 2 shows that the predicted concentrations which are estimated from Eq. (20) are a factor of two with the observed concentration.

Statistical Methods

Now, the statistical method is presented and comparison among analytical, statically and observed results will be offered [13]. The following standard statistical performance measures that characterize the agreement between prediction ($C_p = C_{pred}$) and observations ($C_o = C_{obs}$):

1. Normalized mean square error (NMSE), It is an estimator of the overall deviations between predicted and observed concentrations. Smaller values of NMSE indicate a better model performance. It is defined as:

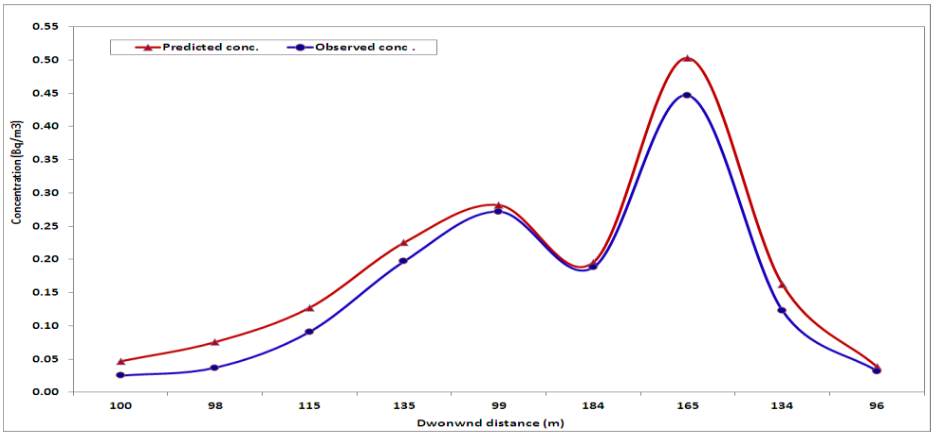

Figure 1: Maximum computed concentrations compared with observed maximum value for each test run.

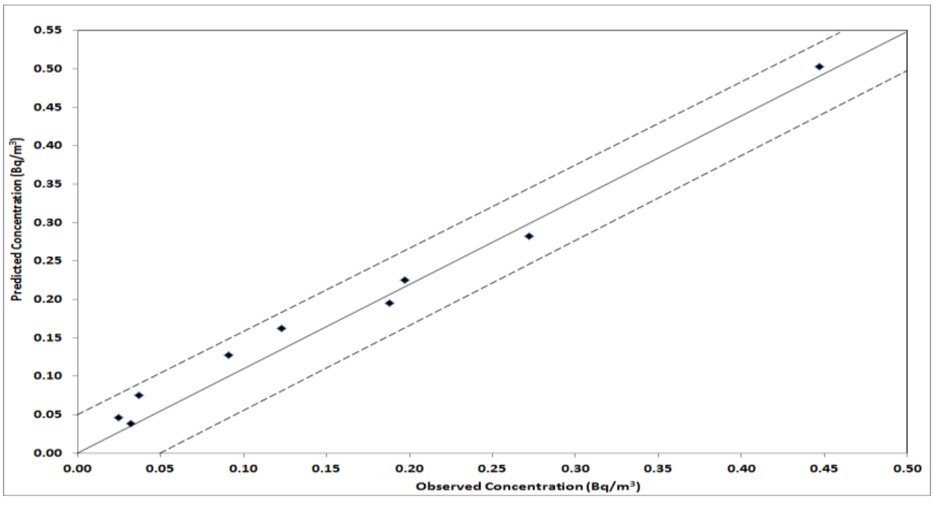

Figure 2: Diagram of predicted model for Eq. (20) with corresponding observation. Solid lines indicate one to one and dashed lines a factor of two.

Statistical functions	^{135}I			
	NMSE	FB	COR	FAC2
Predicated Concentrations model	0.03	-0.16	0.99	1.36

Table 2: Comparison between averages predicted isotopes for ^{135}I and observed concentrations.

$$NMSE = \frac{\overline{(C_o - C_p)^2}}{\overline{C}_o \overline{C}_p}$$

2. Fractional bias (FB): It provides information on the tendency of the model to overestimate or underestimate the observed concentrations. The values of FB lie between -2 and +2 andit has a value of zero for an ideal model. It is expressed as:

$$FB = \frac{(\overline{C}_o - \overline{C}_p)}{0.5(\overline{C}_o + \overline{C}_p)}$$

3. Correlation coefficient (R): It describes the degree of association between predicted and observed concentrations and is given by:

$$R = \frac{\overline{(C_o - \overline{C}_o)(C_p - \overline{C}_p)}}{\sigma_o \sigma_p}$$

4. Fraction within a factor of two (FAC2) is defined as:

FAC2 = fraction of the data for which

$0.5 \leq (C_p/C_o) \leq 2$

Where σ_p and σ_o are the standard deviations of C_p and C_o respectively. Here the over bars indicate the average over all measurements (Nm). A perfect model would have the following idealized performance: NMSE = FB = 0 and COR = FAC2 = 1.0

From the statistical method of Table 2, we find that the predicted concentrations for ^{135}I lie inside factor of 2 with observed data. Regarding to NMSE, FB and COR the predicted concentrations for ^{135}I are better with observed data.

Conclusion

In this paper, a steady-state three-dimensional mathematical model for the dispersion of pollutants from a continuously emitting ground point source in moderated winds is formulated. Besides advection along the mean wind, the model takes into account the diffusion in crosswind and vertical directions. The eddy diffusivity and the wind speed are assumed to be power law in the vertical height z.

The closed form analytical solution of the proposed problem has obtained using the methods of Laplace and Fourier transforms.

In general, the present model is compared with data collected from nine experiments conducted at Inshas, Cairo (Egypt). One gets the predicted concentrations are in a best agreement with the corresponding observation. Moreover, the Statistical results here are in agreement with the analytical results.

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