Application of the Differential Transform Method to the Advection-Diffusion Equation in Three-Dimensions

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Advection diffusion equation with constant and variable coefficient has a wide range of practical, industrial and environmental applications. Due to the importance of atmospheric dispersion equation, we present this study which deals analytically with the atmospheric dispersion equation. The present model is proposed to estimate the concentration of an air pollutant in an urban area. The model is based on using Differential Transform Method (DTM) to solve the atmospheric dispersion equation. The model assumes 1) the pollutant is released from an elevated continuous point source; 2) there exist an elevated inversion layer; 3) the dispersion coefficients are parameterized as a function of downwind distance in a power law dependence. To test the model accuracy, the model predictions have been applied and compared with the experimental data for the Inshas research reactor (Egypt). The model predictions are shown to be in good agreement with the measurement of field data.

1 Introduction

The advection-diffusion equation of air pollution in the atmosphere is essentially a statement of conservation of the suspended material. The concentration of turbulent fluxes are assumed to be proportional to the mean concentration gradient which is known as Fick-theory.

This assumption, combined with the continuity equation, leads to the steady-state advection-diffusion equation, Blackadar [1]

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(k_x\frac{\partial C}{\partial x}\right) + \\ + \frac{\partial}{\partial y}\left(k_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z\frac{\partial C}{\partial z}\right) \tag{1}$$

where $C(x, y, z)$ denotes the concentration, k_x, k_y, k_z are the cartesian components of eddy diffusivity and u, v, w are the cartesian components of wind speed, where x, y are cartesian horizontal distance and z is the height above ground surface.

In order to solve (1) we included the following assumptions: the pollutants are inert and have no additional sinks or sources downwind from the point source, the vertical w and lateral v components of the mean flow are assumed to be zero, k_x is neglected, k_y and k_z are functions of downwind distance. The mean horizontal flow is incompressible and horizontally homogeneous (steady state). Then, (1) is simplified to be:

$$u\frac{\partial C}{\partial x} = k_y\left(\frac{\partial^2 C}{\partial y^2}\right) + k_z\left(\frac{\partial^2 C}{\partial z^2}\right). \tag{2}$$

Both z and y are confined in the range $0 < z < h$ and $0 < y < L_y$ where h is the height of the planetary boundary layer (PBL) and L_y is a cross-wind distance faraway from the source, while the downwind distance $x > 0$. The mathematical description of the dispersion problem (2) is completed by the following boundary conditions:

$$u\,C(x, y, z) = Q\,\delta(z)\,\delta(y), \quad \text{at } x = 0 \tag{3}$$

$$C(x, y, z) = 0, \quad \text{at } x, y, z \to \infty \tag{4}$$

$$\frac{\partial C}{\partial y} = 0, \quad \text{at } y = 0, L_y \tag{5}$$

$$C(x, y, z) = R, \quad \text{at } y = 0 \tag{6}$$

$$\frac{\partial C}{\partial z} = 0, \quad \text{at } z = h \tag{7}$$

$$k_z\frac{\partial C}{\partial z} = -v_d\,C, \quad \text{at } z = 0 \tag{8}$$

where v_d is the deposition velocity, Q is the emission rate and $R(x, z)$ is a variable.

The modeling of air pollution dispersion, including dry deposition, was first attempted by modifying the Gaussian plume equation (Chamberlain [2] and Overcamp [3]) and including operative algorithm, as in the surface depletion models (Horst [4, 5]). Ermak [6] found also an analytical solution but with diffusivity and wind as functions of down distance only and Berkowicz and Prahm [7] gave a numerical solution for the dependent time two dimensional equation including dry deposition. The solutions proposed by Smith [8] and Rao [9] also retained the framework of invariant wind speed and eddies with height (as the Gaussian approach). Tsuang [10] proposed a Gaussian model where the dispersion coefficients (the so-said "sigma") are functions of time and height.

Recent analytical solutions of the advection diffusion equation with dry deposition at the ground have utilized height-dependent wind speed and eddy diffusivities (Horst and Slinn [4], Koch [11], Chrysikopoulos et al. [12] and Tirbassi [13]). However, these solutions are restricted to the specific case in which the source is located at the ground level and/or with restrictions to the wind speed and eddy diffusivity vertical profiles. It is to be noted that the previous works, Moreira et al. [14, 15] assumed boundary conditions only of the second type (zero flux to the ground) and also Tirabassi et al. [16], but Tirabassi et al. [17] assumed boundary conditions of the the third kind (with deposition to the ground), which encompass the contaminant deposition speed and eddy, where eddy diffusivity profiles are functions in the z direction only.

The differential transform method is used in many fields and many mathematical physical problems such as a system of differential equations [18], a class of time dependent partial differential equations (PDEs) [19], wave, Laplace and heat equations [20], the fractional diffusion equations [21], two-dimensional transient heat flow [22], nonlinear partial differential equations [23], diffusion-convection equation [24], convection-dispersion problem [25], linear transport equation [26], two-dimension transient atmospheric pollutant dispersion [27], Helmholtz equation [28].

The aim of this work is to find the analytical solution developed for concentration of the pollutant released from an elevated source in an inversion layer by using the differential transform method (DTM) [29, 30] with different formulas of dispersion parameters (σ).

The paper is organized as follows. In section 2, we introduce the analytical solution using the differential transform method. In section 3, we apply both the standard method, power law, Briggs formula and other sigma to specific problems in analytical solution.

The validity of the present model is examined by comparing its results with the data for Cs^{137} which were performed around the Atomic Energy Authority (AEA) First Research Reactor in Egypt. The results are tabulated with the observed data and clarified in the conclusion.

2 Analytical solution

Applying DTM for (2) with respect to x, we get:

$$\frac{\partial U_i(x,y)}{\partial x} = k_y \frac{\partial^2 U_i(x,y)}{\partial y^2} + (i+1)(i+2)\, k_z U_{i+2}(x,y) \tag{9}$$

where the inverse of the differential transform is defined as:

$$C(x,y,y,z) = \sum_{i=0} z^i U_i(x,y)\,; \tag{10}$$

from boundary condition (8), we obtain:

$$U_1 = \left(\frac{-v_g}{k_z}\right) U_0\,; \tag{11}$$

from equations (9) and (11), we find that:

$$U_2 = \frac{1}{2k_z}\left(u\,\frac{\partial U_0(x,y)}{\partial x} - k_y \frac{\partial^2 U_0(x,y)}{\partial y^2}\right), \tag{12}$$

$$U_3 = \frac{-v_g}{6k_z}\left[u\,\frac{\partial}{\partial x}\left(\frac{U_0(x,y)}{k_z}\right) - \left(\frac{k_y}{k_z}\right)\frac{\partial^2 U_0(x,y)}{\partial y^2}\right]; \tag{13}$$

from boundary condition (7), we obtain:

$$\begin{aligned}&\left(\frac{-2k_z v_g}{hk_y(2k_z - hv_g)}\right) U_0(x,y) + \left(\frac{u}{k_y}\right)\frac{\partial U_0(x,y)}{\partial x} - \\ &-\left(\frac{2hk_z u v_g}{k_y(2k_z - hv_g)}\right) U_0(x,y)\,\frac{\partial}{\partial x}\left(\frac{1}{k_z}\right) = \frac{\partial^2 U_0(x,y)}{\partial y^2}\,.\end{aligned} \tag{14}$$

By using separation of variables method for (14), we get:

$$\frac{d^2 Y}{dy^2} + \lambda^2 Y = 0 \tag{15}$$

and

$$\frac{dX}{dx} - (A - B)X = 0 \tag{16}$$

where

$$A = \left(\frac{hk_z v_g \frac{\partial}{\partial x}\left(\frac{1}{k_z}\right)}{2k_z - hv_g}\right)$$

and

$$B = \frac{hk_z\lambda^2(2k_z - hv_g) - 2v_g k_z}{hu(2k_z - hv_g)}\,.$$

The solution of (14) becomes:

$$U_0(x,y) = c_1\, e^{\int (A-B)dx} \cos\lambda y \tag{17}$$

where $\lambda = n\pi/l_y$.

For practical application of solutions, we need to find the dispersion parameters σ_y, σ_z and the wind speed u. The dispersion parameters are an important function of downwind distance and stability. The empirical σ_y, σ_z curves suggested by Pasquill [31], Gifford [32] and Turner [33] have often been used and are based on the stability. There are different methods to find these parameters.

The meteorological conditions defining Pasquill turbulence types are

- A- Extremely unstable conditions
- B- Moderately unstable conditions
- C- Slightly unstable conditions
- D- Neutral conditions
- E- Slightly stable conditions
- F- Moderately stable conditions.

Here, we used four methods for estimating dispersion parameters:

1. Standard method: This method is based on a single atmospheric stability. Analytical expressions based on Pasquill-Gifford (P-G) curves used for the dispersion estimates have the forms [34]: .

$$\sigma_y = \frac{rx}{(1+x/a)^p}, \tag{18}$$

$$\sigma_z = \frac{sx}{(1+x/a)^q}, \tag{19}$$

where r, s, a, p and q are constants depending on the atmospheric stability. Table 1 shows the values of these constants for different stability classes [35].

Table 1: Meteorological data of the eight convective test runs [35]

Pasquil classes	A	B	C	D	E	F
σ_θ	25°	20°	15°	10°	5°	2.5°
$a(km)$	0.927	0.370	0.283	0.707	1.07	1.17
$s(m/km)$	102.0	96.2	72.2	47.5	33.5	22.0
q	-1.918	-0.101	0.102	0.465	0.624	0.70
$r(m/km)$	250	202	134	78.7	56.6	37.0
p	0.189	0.162	0.134	0.135	0.137	0.134

2. Power law of sigma: In this method σ_z and σ_y can be calculated from:

$$\sigma_y = cx^m \tag{20}$$

$$\sigma_z = dx^n\,. \tag{21}$$

The parameters c, d, m, n in Smith's (1968) [8] are estimated in table 2.

Table 2: Meteorological data of the eight convective test runs [36]

Pasquil classes	c	m	d	n
A-B	1.46	0.71	0.01	1.54
C	1.52	0.69	0.04	1.17
D	1.36	0.67	0.09	0.95
E-F	0.79	0.70	0.40	0.67

3. Briggs formulas: Formulas had been recommended by Briggs 1973 [37]; they should be used in place of the formulas in Table 3 to estimate σ_z and σ_y.

Table 3: Meteorological data of the eight convective test runs [35,37]

stability class	σ_y	σ_z
A-B	$0.32x\,(1+0.0004x)^{-\frac{1}{2}}$	$0.24x\,(1+0.001x)^{\frac{1}{2}}$
C	$0.22x\,(1+0.0004x)^{-\frac{1}{2}}$	$20x$
D	$0.16x\,(1+0.0004x)^{-\frac{1}{2}}$	$0.14x\,(1+0.0003x)^{-\frac{1}{2}}$
E-F	$0.11x\,(1+0.0004x)^{-\frac{1}{2}}$	$0.08x\,(1+0.00015x)^{-\frac{1}{2}}$

4. Hosker expression: Hosker 1973 [38] well-known analytical "best-fit" expression as:

$$\sigma_z = \left(\frac{\alpha x^\beta}{1+\gamma x^\delta}\right) F(z_0, x) \tag{22}$$

where z_0 is the roughness length, α, β, γ and δ are constants depending on the stability classes in Table 4 and $F(z_0, x)$ is defined as:

$$F(z_0, x) = \ln\left(mx^g\left[1+\left(lx^j\right)^{-1}\right]\right), \quad z_0 \geqslant 0.1m \tag{23}$$

where m, g, l, j are constants depend on the value of the roughness length, where our application z_0 (roughness length) = 0.5, so $l = 18.6$, $m = 5.16$, $j = 0.225$ and $g = 0.098$.

Table 4: The constant values of the roughness length, α, β, γ and δ [38]

Pasquil classes	α	β	γ	δ
A	0.112	1.06	5.0×10^{-4}	0.815
B	0.130	0.950	6.52×10^{-4}	0.750
C	0.112	0.920	9.05×10^{-4}	0.718
D	0.098	0.889	1.35×10^{-3}	0.688
E	0.0609	0.895	1.96×10^{-3}	0.684
F	0.0638	0.783	1.36×10^{-3}	0.672

On the other hand, Briggs 1973 [37] proposed a series of algebraic interpolation formulae based on a wide variety of data sources containing surface and elevated sources with a range of initial buoyancies:

$$\sigma_y = b_1(1+b_2x)^{b_3}\,. \tag{24}$$

The coefficient values b_1, b_2 and b_3 were derived for both rural and urban terrain and are given in Table 5 [37].

Table 5: The coefficient values b_1, b_2 and b_3 for equation (24) [37]

PG stability	b_1	b_2	b_3
A	0.20	0	–
B	0.12	0	–
C	0.08	0.0002	-0.5
D	0.06	0.0015	-0.5
E	0.03	0.0003	-1
F	0.016	0.0003	-1

3 Results and discussion

Meteorological data provided by Inshas meteorological tower for four months at a smooth flat site (Inshas area, Egypt) for the year (2006) are given in Table 6, [39]. Air samples were collected from 98 m to 186 m around the first and second research reactor in AEA, Egypt. The study area is flat, dominated by sand soil with poor vegetation cover. The study area was divided into 16 sectors (with 22.5° width for each sector), beginning from the north direction. Aerosols were collected at a height of 0.7 m above the ground of 10.3 cm diameter filter paper with a desired collection efficiency (3.4%)

Table 6: Meteorological Data of the nine Convective test runs at Inshas Site

No.	Stability	Down distance x (m)	Mixing height (m)	Emission rate Q (Bq)	Wind speed (m/s)	Initial wind velocity u_0(m/s)
1	A	98	600.85	0.555429	4	3.95
2	A	100	801.13	0.567	4	3.7
3	B	106	973.0	0.023143	6	5.1
4	C	106	888.0	0.254577	4	3.95
5	A	135	921.0	0.266143	4	3.1
6	D	136	443.0	0.277714	4	3.95
7	E	154	1271.0	0.543857	4	3.95
8	C	165	1842.0	0.563529	4	3.1
9	A	186	1642	0.558321	4	3.95

Table 7: Observed and calculated concentrations (Bq/m^3) for nine experiments

Run no.	Observed Con. [39]	Calculated concentrations			
		Standard Model	Power law of sigma	Briggs formulas	Hosker expression
1	0.002	0.0140799	0.0189143	0.013563	0.01379
2	0.004	0.0153392	0.011873	0.01475	0.014014
3	0.005	0.00448	0.00507518	0.004391	0.04422
4	0.007	0.0062904	0.013799	0.00624019	0.00625
5	0.009	0.00859466	0.00870	0.0081565	0.0081117
6	0.007	0.0070497	0.01596	0.0068969	0.00674
7	0.007	0.0137824	0.015015	0.019399	0.013155
8	0.019	0.0177893	0.019194	0.0171672	0.017135
9	0.006	0.0141444	0.01312	0.0132115	0.01311

using a high volume air sampler with 220 V / 50 Hz bias. The air sampler had an air flow rate of approximately 0.7 m^3/min (25 ft^3/min). Sample collective time was 30 min with an air volume of 21.2 m^3 (750 ft^3). This air volume was corrected to standard conditions (25 C^o and 1013 mb) [39].

Table 7 indicates comparison between experimental data of the nine convective test runs at Inshas site and our calculation of concentration by Briggs formula, power law variation, standard method and Hosker's expression, which shows that the power law formula for the dispersion coefficients achieves the best agreement with the experimental results.

3.1 Statistical evaluation

Statistical analysis of the predictions and observations is central to the model performance evaluation. The predicted and the corresponding observed concentrations are treated as pairs in this evaluation.

The statistical index FB indicates weather the predicted quantities underestimate or overestimate the observed ones. The statistical index NMSE represents the quadratic error of the predicted quantities in relation to the observed ones. Best results are indicated by values nearest zero in NMSE, FB, nearest 1 in MG, VG and FAC2 and are factor of two if are greater than 1 and less than 2. The statistical measures chosen to compare performances of the models described here [40]:
(i) Fractional bias FB is defined as:

$$\mathrm{FB} = \frac{\bar{C_o} - \bar{C_p}}{0.5(\bar{C_o} + \bar{C_p})}$$

where the subscripts o and p refer to the observed and predicted values, respectively, and the overbars indicate mean values. A good model should have FB value close to zero.
(ii) Normalized mean square error (NMSE) is defined as:

$$\mathrm{NMSE} = \frac{\overline{(C_o - C_p)^2}}{\bar{C_o}\bar{C_p}} .$$

This provides information on the overall deviations between predicted and observed concentrations. It is a dimensionless statistic and its value should be as small as possible for a good model.
(iii) The geometric mean bias is defined as:

$$MG = \exp\left(\overline{\ln C_o} - \overline{\ln C_p}\right) .$$

(iv) The geometric variance is defined as:

$$VG = \exp\left(\overline{(\ln C_o - \ln C_p)^2}\right) .$$

Table 8: Comparison between the Standard method, Power law of sigma, Briggs formulas and Hosker expression in terms of FB, FAC2, NMSE, MG and VG

	Standard method	Power law of sigma	Briggs formulas	Hosker expression
FB	-0.42543	-0.65368	-0.445	-0.69646
FAC2	1.540371	1.971068	1.572352	2.068563
NMSE	0.189565	0.478407	0.208342	0.551991
MG	0.605381	0.46362	0.601944	0.490099
VG	1.286468	1.805587	1.293883	1.662927

(v) Fraction within a factor of two (FAC2) is given by:

$$0.5 \leqslant (C_p/C_o) \leqslant 2\,.$$

Statistical evaluation of the models results are given in Table 8, which compares the Standard method, Power law of sigma, Briggs formulas and Hosker expression in terms of FB, FAC2, NMSE, MG and VG.

4 Conclusion

In the present study, an analytical treatment for the dispersion of air pollutant released from point source is formulated. A mathematical solution has been obtained for the steady-state form of the three-dimensional advection-diffusion equation using the Differential Transform Method. Different realistic formulae for the dispersion coefficients as a function of downwind distance have been adopted (namely: Briggs formula, power law variation, standard method and Hosker's expression). In order to validate and verify our model, and for the sake of comparison, we apply our obtained mathematical formulae on the experimental data performed for the release from the first Research Reactor in Egypt. The comparison shows that the power law formula for the dispersion coefficients achieves the best agreement with the experimental results. Finally, the good agreement between the power law variation of the dispersion parameter and the experiential data gives us confidence to extend this work for the case of different sources types, namely, line, area and volume sources. In addition, it is also our intention to perform the mathematical analysis of this method for the case of high penetrated inversion layer (i.e. different stability conditions that permits the pollutant penetration and diffusion through the mixing height).

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