ISSN NO. 2320-5407

Journal homepage:http://www.journalijar.com

INTERNATIONAL JOURNAL OF ADVANCED RESEARCH

RESEARCH ARTICLE

An analytical solution of two dimensional atmospheric diffusion equation in a finite boundary layer

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Manuscript Info

Manuscript History:

Received: 17 June 2013
Final Accepted: 27 June 2013
Published Online: July 2013

Key words:
Advection–diffusion equation,
Bessel Function,
Pollution,
Concentrations.

Abstract

An analytical model for the crosswind integrated concentrations released from a source in an inversion layer is formulated by considering the wind speed as a linear profile of vertical height and eddy diffusivity as a power law profile of vertical height, the separation of variables technique is used to solve the advection–diffusion equation.

The analytical model is compared with data collected from nine experiments conducted at Inshas, Cairo (Egypt). The model shows a good agreement between observed and calculated concentration.

1 – Introduction

Air pollutants released from various sources affect directly or indirectly man and his environment. Air pollutants emitted from different sources are transported dispersed or deposited my meteorological and topographical conditions. Dispersion of pollutants in the atmosphere is governed by the following dominant mechanisms (Wark and Warner, 1981), mean air flow that transports the pollutants downwind and turbulent velocity fluctuations that disperse the pollutants in all directions. Under moderate to strong winds, the continuously emitted pollutants from a cone- shaped plume in the downwind direction of the source. In this case, advection in the mean wind direction dominates over diffusion and dispersion in the crosswind and vertical directions is assumed to be non-Gaussian. Along-wind diffusion is particularly important near the leading edge of the plume, where uncontaminated fluid from upwind mixes with the mass initially released (Wilson, 1981).

For nearly thirty years it has known that vertical concentration profiles from field and laboratory experiments of near-surface point source releases exhibit non-Gaussian distribution (Elliot 1961; Malhorta and Cermak 1964; Nieuwstadt and Van Ulden 1978). Yokoyama et al.. (1979) have derived a puff formula for computing the concentration of smoke emitted from a point source in calm wind conditions by expressing the dispersion parameters as linear functions of time. The non-Gaussian shape has been attributed to the non-uniform turbulent mixing that occurs in boundary-layer flows. For elevated releases, Doran et al. (1978) and Khurshudyan et al. (1981) have shown that the agreement between a Gaussian reflected-plume formula and measured vertical profiles becomes progressively worse at larger downwind distances.

In an attempt to study the essential physics of shear-flow dispersion, several investigator have derived solutions to the diffusion equation that allow the mean velocity and vertical eddy diffusivity to vary with height (e.g. Reborts, personal communication in Sutton 1953; Smith 1957; Yeh and Huang 1975; Berlyand 1975; Huang 1979). These plume-dispersion models yield, in the general case, a non-Gaussian vertical distribution. The most general of these solutions, independently derived by Berlyand and Huang, is three dimensional, valid for both surface and elevated releases, and allows the velocity and vertical eddy-diffusivity profiles to vary independently as power-law functions.

Several researchers have highlighted the similarities between a non-Gaussian model and experimental data for surface releases (Tagliazucca et al . 1988, and Brown et al. 1992). For elevated releases, Ide et al. (1988) found favorable agreement between ground-level concentration measurements in a wind tunnel and a non-Gaussian model with a prescribed vertical diffusion coefficient σ_z. Hinrichson (1986) and Brown et al.(1989) have shown that a non-Gaussian model better simulates concentration profiles originating from surface sources that a Gaussian reflected-plume model.

In this study, we have formulated 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. An analytical solution has been obtained for the resulting advection-diffusion equation with the physically relevant boundary conditions. The moderate data collected during the convective conditions. From nine experimentsconducted at Inshas site, Cairo-Egypt (Essa et al. 2007) has been calculated by the solution obtained.

2 - Model Formulation

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:

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

where C is the mean concentration of a pollutant (Bq/m^3), (µg/m^3) and (ppm); 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 w 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) As the vertical velocity is much smaller than the horizontal one in x-direction, the term $w\,(\partial C / \partial z)$ is neglected.
3) x-axis is oriented in the direction of mean wind u=U and U much greater than the wind speed v in y-direction the term $v\,(\partial C / \partial y)$ is neglected).
4) Source and removal (physical / chemical) pollutants are ignored so that S=0 and R=0.

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

$$\mathrm{U}\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) \quad (2)$$

The Advection term in x direction is larger than the diffusion in x direction then we will neglect the diffusion term in x direction,

$$\mathrm{U}\frac{\partial C}{\partial x} = \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) \quad (3)$$

Eq. (3) is solved together with the following boundary conditions

- The is assumed to be a perfectly total absorption i.e.,

$$C(x, y, z) = 0 \quad at\ z = 0 \quad (4)$$

- The pollutant is totally penetrate through the top of the inversion/mixed layer located at height h, i.e.

$$C(x,y,z)=0 \quad at\ z=h \tag{5}$$

- A continuous point source with strength Q is assumed to be located at the point $(0,y_s,z_s)$, i.e.

$$UC=Q\delta(y-y_s)\delta(z-z_s) \qquad \text{as} \qquad z=0 \tag{6}$$

where δ (…) is Dirac's delta function.

- Far away from the source, the concentration decreases to zero, i.e.

$$C\rightarrow 0 \ \text{as} \quad x.y,z\rightarrow\infty \tag{7}$$

Here U is taken as linear of z:

$$\mathrm{U}=\mathrm{k}_o u_* z \quad z\neq 0 \ \text{ and } \ \mathrm{U}=\mathrm{U}_0 \ \text{ at } z=0 \tag{8}$$

where k_o is Von-Karmen constant and u_* is the friction velocity.
The eddy diffusivity k_z is expressed as functions of power law of *z* as:

$$k_z=u_1 z^n \tag{9}$$

Where u_1 is turbulence intensity.
Also after integrating Eq. (3) with respect to y from (-∞ to ∞), Eq. (2) becomes:

$$\mathrm{k}_o u_* z\,\frac{\partial C_y}{\partial x}=\frac{\partial}{\partial z}\left(u_1 z^n\frac{\partial C_y}{\partial z}\right) \tag{10}$$

which is simply reads:

$$\frac{\partial C_y}{\partial x}=\frac{u_1}{\mathrm{k}_o u_*}z\,n-1\,\frac{\partial^2 C_y}{\partial z^2}+\frac{u_1 n}{\mathrm{k}_o u_*}z^{n-2}\frac{\partial C_y}{\partial z} \tag{11}$$

One can solve the two-dimensional partial differential equation (11) analytically by using the separation of variables technique. We take the solution of Eq. (11) of the form:

$$\mathrm{C}_y\,(\mathrm{x,z})=\mathrm{X(x).Z(z)} \tag{12}$$

Differentiating (12) partially with respect to x and z and substituting in Eq. (11), we get two ordinary differential equations in the variables X and Z as follows:

$$\frac{1}{X}\frac{dX}{dx}=-\lambda^2 \tag{13}$$

and.

$$\frac{\alpha z^{n-1}}{Z}\frac{d^2Z}{dz^2}+\frac{\beta z^{n-2}}{Z}\frac{dZ}{dz}=-\lambda^2 \quad (14)$$

where λ^2 is a constant, $\alpha = u_1 / k_o u_*$ and $\beta = u_1 n / \mathrm{k}_o u_*$.

The general solution of Eq. (13) is given by

$$X(x)=\gamma e^{-\lambda^2 x} \quad (15)$$

where γ is a constant.

Eq. (14) becomes:

$$z^2\frac{d^2Z}{dz^2}+nz\frac{dZ}{dz}+\frac{\lambda^2}{\alpha}z^{3-n}Z=0 \quad (16)$$

which is simply reads

$$z_*^2\frac{d^2Z_*}{dz_*^2}+z_*\frac{dZ_*}{dz_*}+\left[\eta^2 z_*^2-\mu^2\right]Z_*=0 \quad (17)$$

where $\eta^2 = 4\lambda^2 / \alpha(3-n)^2$, $\mu=(1-n)/(3-n)$

The solution of Eq. (14) is obtained in different boundary conditions as follows:
Eq. (10) along with the following boundary condition corresponding to Eq. (4) and Eq. (5):

$$Z=0 \quad at\ z=0,h \quad (18)$$

On changing the dependent (Z) and independent (z) variables in Eq. (16) by means of the substitutes:

$$\left.\begin{aligned} Z &= z_*^{\frac{1-n}{3-n}} Z_* \\ &\text{and} \\ z_* &= z^{\frac{3-n}{2}} \end{aligned}\right\} \quad (19)$$

Equation (17) is a Bessel equation and has a solution:

$$Z=z^{\frac{1-n}{2}}\left[AJ_{\mu}(\eta z^{\frac{3-n}{2}})+BJ_{-\mu}(\eta z^{\frac{3-n}{2}})\right] \quad (20)$$

Where J_{μ} and $J_{-\mu}$ the Bessel functions of first kind of order are μ and $-\mu$, respectively, A and B are constants, application of the boundary condition Eq. (18) at $z=0$ in Eq. (20) yields $B=0$ and condition $z=h$ Eq. (18) gives rise:

$$h^{\frac{1-n}{2}}J_{\mu}(\eta h^{\frac{3-n}{2}})=0 \quad (21)$$

this represents Storm-Liouville Eigen value problem which have the corresponding Eigen functions:

$$Z_{\alpha}(z) = z^{\frac{1-n}{2}} J_{\mu}(\eta_{\alpha} z^{\frac{3-n}{2}}), \quad \alpha = 1, 2, 3, ...\infty \tag{22}$$

The general of Eq. (10) is obtained by using Eq. (15), Eq. (21) and Eq. (22) as:

$$C_y(x,z) = z^{\frac{1-n}{2}} \left[\sum_{\alpha=1}^{\infty} A_{\alpha} J_{\mu}(\eta_{\alpha} z^{\frac{3-n}{2}}) \exp(-\lambda^2 x) \right] \tag{23}$$

Where $A_{\alpha}, \quad \alpha = 1, 2, 3, ...\infty$ arethe unknown coefficients. Eq. (23) represent the concentration distribution C_y through the Fourier-Bessel series (Gradshteyn&Ryzhik, 1965, pp 672)) corresponding to a set of Eigen function Z_{α}.

Estimation of the coefficients A_{α}'s for crosswind integrated concentrations:

The source at $x = 0$, Eq. (6) gives:

$$k_o u_* z^{\frac{3-n}{2}} \left[\sum_{\alpha=1}^{\infty} A_{\alpha} J_{\mu}(\eta_{\alpha} z^{\frac{3-n}{2}}) \right] = Q_p \delta(z - z_s) \tag{24}$$

To determine the values of A_{α}we use the orthogonally of Eigen functions series (Gradshteyn&Ryzhik, 1965, pp 672)).

Multiplying Eq. (24) by $z^{\frac{1-n}{2}} J_{\mu}(\eta_{\beta} z^{\frac{3-n}{2}})$, $\beta \geq 0$ and integrating according to z from 0 to h, we get:

$$A_{\beta} = \frac{2 Q_p z_s^{\frac{1-n}{2}}}{k_o u_* h^2} * \frac{J_{\mu}(\eta_{\beta} z_s^{\frac{3-n}{2}})}{J_{\mu+1}^2(\eta_{\beta} h^{\frac{3-n}{2}})} \qquad \beta \geq 1 \tag{25}$$

SubstitutingA_{β}in Eq. (23), the final solution is given as follows:

$$C_y(x,z) = Q_p \frac{2 (z z_s)^{\frac{1-n}{2}}}{k_o u_* h^2} \sum_{\alpha=1}^{\infty} \frac{J_{\mu}(\eta_{\alpha} z^{\frac{3-n}{2}}) J_{\mu}(\eta_{\alpha} z_s^{\frac{3-n}{2}})}{J_{\mu+1}^2(\eta_{\beta} h^{\frac{3-n}{2}})} \exp(-\lambda^2 x) \tag{26}$$

In which $\eta_{\beta} h^{\frac{3-n}{2}}$ is given as

$$J_{\mu}(\eta_{\beta} h^{\frac{3-n}{2}}) = 0 \tag{27}$$

3 - 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 43m for twenty four hours working, where the air samples were collected during half hour at a height 0.7m. We collected air samples from 92m to 184m around the source in AEA, Egypt. The study area is flat, dominated by sand 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 220V /50Hz bias (Essa et al 2005). Meteorological data have been provided by the measurements done at 10 and 60 m. Table 1. gives the data information about the diffusion tests and the wind vectors. In addition, it contains values of vertical velocity scale (w*) and mixing height (zi). The data from these nine unstable test runs have been utilized for the following analysis.

Table 1. Meteorological data of the nine convective test runs at Inshas site in March and May 2006.

Run no.	Working hours	Release rate (Bq)	Wind speed (m s^{-1})	Wind direction(deg)	W* (ms^{-1})	Zi (m)	P-G stability class
1	48	1028571	4	301.1	2.27	600.85	A
2	49	1050000	4	278.7	3.05	801.13	A
3	1.5	42857.14	6	190.2	1.61	973	B
4	22	471428.6	4	197.9	1.23	888	C
5	23	492857.1	4	181.5	0.958	921	A
6	24	514285.7	4	347.3	1.3	443	D
7	28	1007143	4	330.8	1.51	1271	C
8	48.7	1043571	4	187.6	1.64	1842	C
9	48.25	1033929	4	141.7	2.1	1642	A

4 - Model parameters

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 3m/s most of the time even at 10m 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) (Golder 1972) based on friction velocity, temperature, and surface heat flux.

5 - Results and Discussion

The concentration is computed using data collected at vertical distance of a 30m 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 (12) which contains eddy diffusivities as function with power law at y = 0.0 for half hourly averaging.

Table 2. Observed and predicted concentrations for Run 9 experiments

Test	Downwind distance (m)	Vertical distance (m)	Observed conc. (Bq/m^3)	Predicted conc. (Bq/m^3)
1	100	5	0.025	0.051
2	98	10	0.037	0.031
3	115	5	0.091	0.070
4	135	5	0.197	0.160
5	99	2	0.272	0.234
6	184	11	0.188	0.138
7	165	12	0.447	0.339
8	134	7.5	0.123	0.107
9	96	5.0	0.032	0.034

As an illustration, results computed from these approaches are shown in Table 2, for nine typical tests conducted at Inshas site, Cairo-Egypt (Essa et al. 2007). This Table shows that the observed and predicted concentrations for ^{135}**I** using Eq. (12) with power law of eddy diffusivities and the wind speed in linear form of "z" are very near to each other of ^{135}**I**.

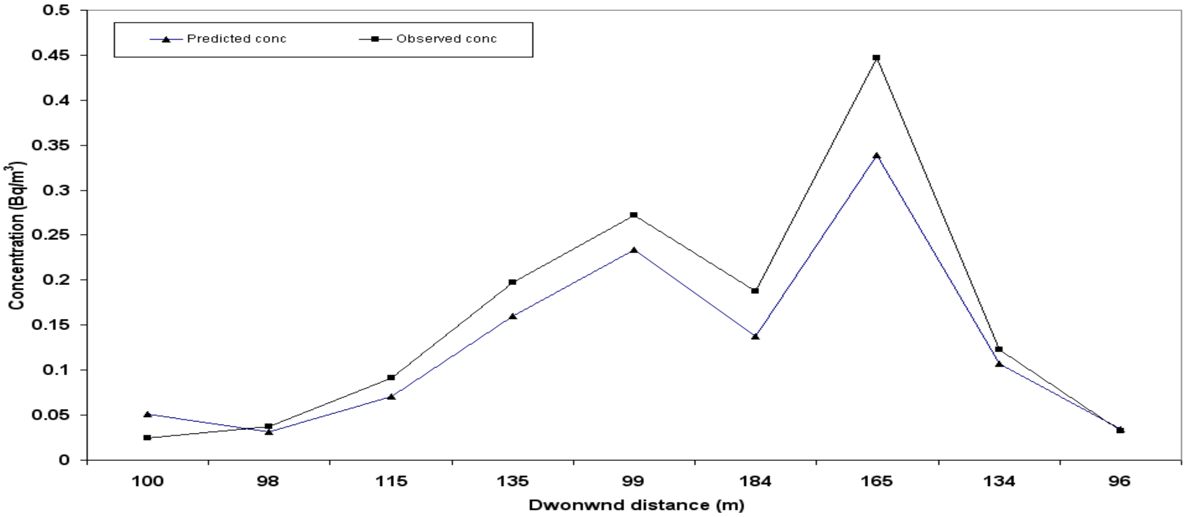

Fig. 1. Maximum computed concentrations compared with observed maximum value for each test run.

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

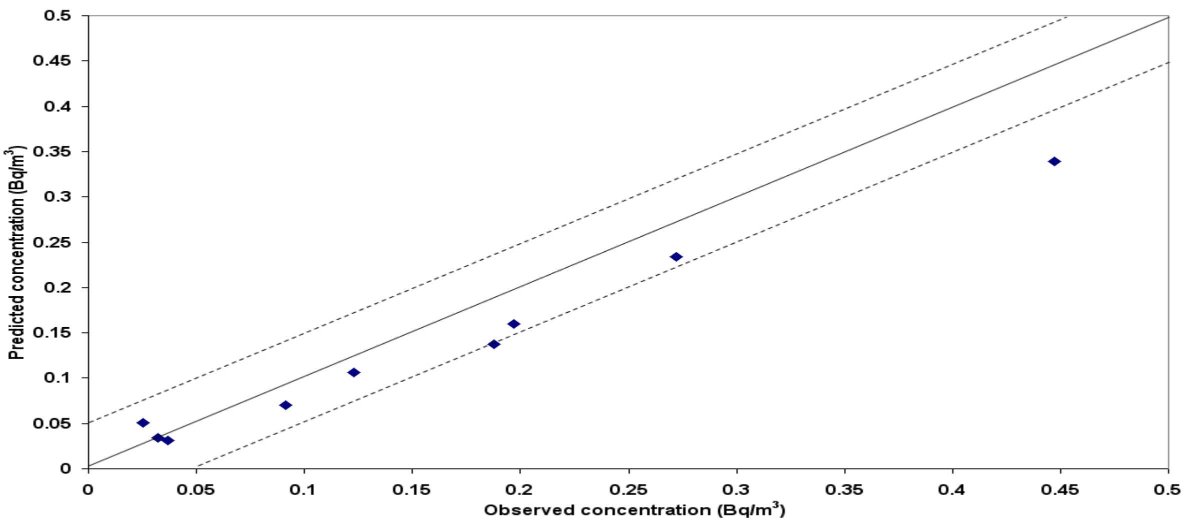

Fig. 2. Diagram of Predicted model for Eq. (12) with corresponding observation. Solid lines indicate one to one and dashed lines a factor of two.

Fig. 2 shows that the predicted concentrations which are estimated from Eq. (12) are a factor of two with the observed concentration.

6- Statistical method

Now, the statistical method is presented and comparison among analytical, statically and observed results will be offered (Essa et al 2005). The following standard statistical performance measures that characterize the agreement between prediction (Cp=Cpred) and observations (Co=Cobs):

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:

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

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 and it 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
$0.5 \le (Cp/Co) \le 2$

Where σ_p and σ_o are the standard deviations of Cp and Co 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

Table (3): Comparison between averages predicted isotopes for ^{135}Iand observed concentrations.

Statistical functions	^{135}I			
	NMSE	FB	COR	FAC2
Predicted Concentrations model	0.10	0.19	0.99	0.4

From the statistical method of Table (3), 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.

7 - Conclusions

In this paper, we have formulated a mathematical model for dispersion of air pollutants in moderated winds. The diffusion in vertical height direction and advection along the mean wind are taking into account. The eddy diffusivity is assumed to be power law in the vertical height “z” and the wind speed is function in linear form of “z”.

The analytical 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.

References

Berlyand M. E. (1975) Contemporary problems of atmospheric diffusion and air pollution. Hydromet press, 448 pp.

Brown M. J., Arya S. P. S., and Snyder W. H. (1989) Vertical dispersion from surface and elevated releases. Sixth Joint Conf. on Appl. Of Air Poll. Meteor. Anaheim, Amer. Meteor. Soc., 163-166.

Brown M. J., Arya P. S., and Snyder W. H. (1993) Vertical dispersion from surface and elevated releases: An investigation of a non-Gaussian plume model. 32, 490-505.

Doran J. C., Horst T. W. and Nickola P. W. (1978) Experimental observations of thedependence of lateral and vertical dispersion characteristics on source height. Atmos. Environ. 12, 2259-2263.

Elliot W. P. (1961) The vertical diffusion of gas from a continuous source. Int. J. Air Water Pollut., 4,33-46.

Golder Donald: "Relation among Stability Parameters in the Surface Layer", Boundary Layer Meteorology, 3, pp. 47:58 (1972).

Gradshteyn I.S. and Ryzhik I. M. (1965) “Table of Integrals, Series, and Products”, New York

Gradshteyn, I.S., Ryzhik, I.M., 1965. Table of Integrals, Series and Products. Academic Press, New York, 1160pp.

Hinrichson K. (1986) Comparison of four analytical dispersion models for near-surfacereleases above a grass surface. Atmos. Environ. 20, 29-40.

Huang C. H. (1979) A theory of dispersion in turbulent shear flow. Atmos. Environ., 13,453-463.

Ide Y., Okamato H., and Okabayashi K. (1988) On the parameterization of diffusion in the turbulent boundary layer. Atmos. Environ., 22, 1863-1870.

IrvingJ. and Mullineux (1959)“Mathematics in Physics and Engineering, New York.

Khaled S. M. Essa; Fawzia Mubarak and Sanaa Abu Khadra (2005) Comparison of Some Sigma Schemes for Estimation of Air Pollutant Dispersion in Moderate and Low Winds,Atmospheric Science Letter Vol. 6, issue 2, 90-96.

Khaled S. M. Essa, and Maha S. El-Otaify (2007) Mathematical model for hermitized atmospheric dispersion in low winds with eddy diffusivities linear functions downwind distance, Meteorology and Atmospheric Physics, 96, 265-275 (2007).

Khurshudyan L. H., Snyder W. H., and Nekrasov I. V. (1981) Flow and dispersion of pollutants over two-dimensional hills: Summary report on Joint Soviet-American study.Rep. No. EPA-600/4-81-067, Env. Prot. Agency, 130pp.

Malhorta R. C., and Cermak J. E. (1964) Mass diffusion in neutral and unstably stratified boundary-layer flows. Int. J. Heat Mass Trans., 7, 169-186.

Nieuwstadt F. T. M., and van Ulden A. P. (1978) A numerical study on the verticaldispersion of passive contaminants from a continuous source in the atmospheric surface layer. Atmos. Environ. 12, 2119-2124.

Smith F. B. (1957) The diffusion of smoke from a continuous elevated point-source into a turbulent atmosphere. J. Fluid Mech. 2, 49-76.

Sutton O. G. (1953) Atmospheric Turbulence. Methuen, 111pp.

Tagliazucca M. T. Nanni, and Tirabassi T. (1985) An analytical dispersion model for sources in the surface layer. II NuovoCimento, 8C, 771-781.

Wark K., and Waner C. F. (1981) Air pollution. Its Origin and Control. Harper and Row, New York.

Wilson D. J. (1981) Along-wind diffusion of source transients. Atmospheric Environment 15, 489-495.

Yeh G. T. and Huang C. H. (1975) Three-dimensional air pollutant modeling in the lower atmosphere. Bound-layer Meteor., 9, 381-390.

Yokoyama O. et al. (1979) Study on atmospheric dispersion of pollutants. Rep. National Res. Inst. for Pollution and Resources, MITI, 15, 408.