Romanian Reports in Physics, Vo ume. 55, Number 1, P. 94 -101, 2003

ANALYTICAL FORM OF POLLUTANTS DISPERSION FOR DIFFERENT ATMOSPHERIC CONDITIONS

A. B. MAYHOUB, KHALED S.M. ESSA and SHERIF ALY

Mathematics and Theoretical Physics Dept., Atomic Energy Authority,
Nuclear Research Center, Cairo-Egypt
(Received March 25, 2001)

Abstract. The dispersion of pollutants from a point source is analytically investigated for varying wind velocity, and vertical diffusivity coefficient. At the surface, the diffusing particles are deposited and then interact with it. The concentration of pollutants was calculated for downwind and crosswind distances, taking into account the vertical dispersion, which is limited by elevated inversion, and the atmospheric stability conditions. The corresponding decay distances and the source depletion strength are evaluated.

Key words: radioactive waste.

1. INTRODUCTION

The most common model computing the dispersion of air pollution from a single point source is the Gaussian plume model, which was initially proposed by Sutton (1932). Although that model has its limitations, it is used widely to solve dispersion problems. Its assumptions are:

- No spatial variation of wind velocity.
- The ground reflects pollutants.
- The terrain is flat.
- No temperature inversion suppresses vertical diffusion of airborne material.

The Gaussian formula has been extended to include complex multiple source situations (Turner 1964, Runca et al 1976). The effect of ground level absorption on the dispersion of pollutants has been studied analytically by Heines (1974).

Benntt (1988) introduced a physical model for dry deposition of pollutants to a rough surface. Mayhoub et al (1992) used simple integral method for modeling atmospheric dispersion of pollutants. In this paper we apply an analytical method to solve the diffusion equation with specific boundary conditions. We also study the variation of wind velocity and diffusivity coefficients with height under neutral and stable conditions of the atmosphere. Decay distances and the corresponding concentrations in addition to the depletion of the source at decay distances are calculated.

2. THE MATHEMATICAL MODEL

Assume a rectangular coordinate system with x-axis oriented along the wind direction U(z), the y-axis along the crosswind direction, and the z-axis oriented vertically upward, then the conservation of mass for a steady turbulent flow may be described by the second order partial differential equation (Gifford 1975):

$$\mathrm{U}(z)\frac{\partial C(x,z)}{\partial x}=\frac{\partial}{\partial z}\left[K(z)\frac{\partial C(x,z)}{\partial z}\right], \tag{1}$$

where C(x,z) is the pollutant's air concentration, K(z) is the diffusion coefficient, and U(z) is the wind velocity.

(2-a) Neutral condition

In neutral condition, the wind velocity U(z) and K(z) are taken of the form:

$$U(z) = \frac{u_*}{k}\ln(\frac{z}{z_0}), \tag{2}$$

$$K(z) = k_0 + k u_* z, \tag{3}$$

where u_* is the friction velocity, k is the Von-Karman constant (≈ 0.4), k_0 is constant, and z_0 is the roughness length which may be computed as:

$$z_0 = \varepsilon/30, \tag{4}$$

where ε is the average height of the obstacles in the study area.

The dispersion equation (1) may be solved under the boundary conditions, which are:

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

$$\partial C(x,z)/\partial z = 0 \quad \text{at } z = a, \tag{6}$$

$$K(z)\partial C(x,z)/\partial z = -V_g C \quad \text{at } z = a, \tag{7}$$

$$\partial^2 C(x,z)/\partial z^2 = 0 \quad \text{at } z = a. \tag{8}$$

Assuming the solution of equation (1) by a polynomial and using the boundary conditions (5-8) one gets:

$$C(x,z) = F(x)(1-z/a)^{n}, \tag{9}$$

where a is the inversion height, which is considered to be constant, and V_g is the deposition velocity.

Integrating equation (1) over the whole mixing layer $0 \le z \le a$ yields:

$$\frac{d}{dx}\int_0^a U(x)C(x,z)dz = -V_g F(x) \tag{10}$$

Substituting U(z) and C(x,z) from equation (2) and equation (9) respectively, into equation (10) to get:

$$\frac{dF(x)}{dx}\frac{u_*}{k}\int_0^a ln(\frac{z}{z_0})(1-\frac{z}{a})^n dz = -V_g F(x), \tag{11}$$

the solution of that equation is:

$$F(x) = F_0(x)\exp\left\{-\frac{V_g k}{u_* A(a,n)}x\right\}, \tag{12}$$

where $A(a,n) = a[-\text{EulerGamma}+ln(a)+ln(1/z_0) - \text{PolyGamma}(0,2+n)]/(n+1)$,

where EulerGamma is mathematical constant equal to $\cong$ 0.577 and PolyGamma (0,2+n) has numerical values depending on n's values.

Then the concentration will be

$$C(x,z) = F_0(x)\exp\left\{-\frac{V_g k}{u_* A(a,n)}x\right\}(1-\frac{z}{a})^{n}. \tag{13}$$

If C(x,z) decreases exponentially with x like $\exp(-x/\overline{x_1})$, where $\overline{x_1}$ is the decay distance at which the source strength will be reduced to one-tenth or more from its original value, equation (13) can be rewritten as:

$$C(x,z) = F_0(x)\exp(\frac{-x}{\overline{x_1}})(1-\frac{z}{a})^n, \tag{14}$$

where

$$\bar{x}_1 = u_* A(a,n)/V_g k, \tag{15}$$

and $F_0(x)$ can be calculated using the boundary conditions:

$$Q = \int_0^a \int_0^{\bar{x}_1} U(z) C(x,z)\, dx dz. \tag{16}$$

Substituting by U(z) from equation (2) and performing the integration yields:

$$F_0(x) = \frac{Q}{0.63 \bar{x}_1^2 V_g}. \tag{17}$$

Therefore, the equation (14) will be:

$$C(x,z) = \frac{Q}{0.63 \bar{x}_1^2 V_g} \exp(\frac{-x}{\bar{x}_1})(1-\frac{z}{a})^n, \tag{18}$$

This represents the complete solution of the dispersion problem to considering case.

2-b. Stable condition

The wind velocity U(z) and K(z) in x-direction are taken as:

$$U(z) = \frac{u_*}{k}\left\{\ln(\frac{z}{z_0}) - \frac{5z}{L}\right\}, \tag{19}$$

$$K(z) = \frac{k u_* z}{(1+\frac{5z}{L})} + k_0, \tag{20}$$

where u_*, k, k_0, and z_0 are previously defined, where L is the Monin-Obukove length. L is a parameter, which characterizes the stability of the surface layer and is calculated from ground-level measurements.

Using the same boundary conditions equations (5-8) to solve the diffusion equation (1) to get:

$$C(x,z) = E(x)(1-z/a)^n, \tag{21}$$

integrating equation (1) over the whole mixing layer $0 \le z \le a$ yields:

$$\frac{d}{dx}\int_0^a U(x) C(x,z) dz = -V_g E(x). \tag{22}$$

Substituting U(z) and C(x,z) from equation (19) and equation (21) respectively into equation (22) gives:

$$\frac{dE(x)}{dx} \frac{u_*}{k} \int_0^a ln(\frac{z}{z_0})(1-\frac{z}{a})^n dz = -V_g E(x), \tag{23}$$

The solution of that equation is:

$$E(x) = E_0(x) \exp\left\{-\frac{V_g k}{u_* B(a,n)} x\right\}, \tag{24}$$

where

$$B(a,\mathrm{n}) = \frac{a}{(\mathrm{n}^2+3\mathrm{n}+2)\mathrm{L}}\{5a-(2-\mathrm{n})\mathrm{L}\ \mathrm{EulerGamma} + (\mathrm{n}+2)\mathrm{L}\times$$
$$\ln(\frac{a}{z_0}) - (\mathrm{n}+2)\mathrm{L}\ \mathrm{polyGamma}(0,n+2)\}. \quad (25)$$

Then the concentration becomes:

$$C(x,z) = E_0(x)\exp\left\{-\frac{V_g k}{u_* B(a,n)}x\right\}(1-\frac{z}{a})", \quad (26)$$

$$C(x,z) = E_0(x)\exp(\frac{-x}{\bar{x}_2})(1-\frac{z}{a})^n, \quad (27)$$

where

$$\bar{x}_2 = u_* B(a,n)/V_g k \quad (28)$$

is the decay distance and $E_0(x)$ can be calculated using the boundary conditions:

$$Q = \int_0^a \int_0^{\bar{x}_2} U(z)C(x,z)dxdz. \quad (29)$$

Substituting U(z) from equation (19) and performing the integration yields:

$$E_0(x) = \frac{Q}{.63\bar{x}_2^2 V_g}, \quad (30)$$

$$C(x,z) = \frac{Q}{0.63\bar{x}_2^2 V_g}\exp(\frac{-x}{\bar{x}_2})(1-\frac{z}{a})^n, \quad (31)$$

which represents the solution to the atmospheric equation.

3. CALCULATION OF DECAY DISTANCE AND CORREPONDENCE CONCENTRATION IN CROSSWIND DISTANCE

Equation (1) in the crosswind distance takes the form:

$$U(z)\frac{\partial C(y,z)}{\partial y} = \frac{\partial}{\partial z}[K(z)]\frac{\partial C(y,z)}{\partial y}, \quad (32)$$

where U(z) is the geostrophic wind velocity of the form:

$$U(z) = u_g e^{-\psi z}\sin(\psi z), \quad (33)$$

$\psi = (F/2k)^{0.5}$, where $F = 2\Omega\sin\Phi$ is the Cariolis parameter, $K = k_0 + kz^n$ and Φ is the latitude.

Applying the following boundary conditions:

$$C(y,z) = 0 \quad \text{at } z = a, \quad (34)$$
$$\partial C(y,z)/\partial z = 0 \quad \text{at } z = a, \quad (35)$$
$$K(z)\,\partial C(y,z)/\partial z = -V_g C \quad \text{at } z = 0, \quad (36)$$
$$\partial^2 C(y,z)/\partial z^2 = 0 \quad \text{at } z = a \quad (37)$$

we assume the solution of equation (32) as a polynomial and using the boundary conditions (34-37) one gets:

$$C(x,z) = F_3(y)(1-z/a)^n, \quad (38)$$

where a is the inversion height, which is considered to be constant.

Integrating equation (32) over the whole mixing layer $0 \le z \le a$ yields:

$$\frac{d}{dx}\int_0^a U(z)C(x,z)dz = -V_g F_3(y). \tag{39}$$

Substituting U(z) and C(x,z) from equations (32), (38) respectively into equation (39) yields:

$$\frac{dF_3(y)}{dy} u_g \int_0^a e^{-\Psi z}\sin(\psi z)(1-\frac{z}{a})^n dz = -V_g F_3(y). \tag{40}$$

The solution of the above equation is calculated for every value of n.

<u>For n = 2</u>

$$\int_0^a e^{-\Psi z}\sin(\psi z)(1-\frac{z}{a})^n = a\sin(\sqrt{F/k_0})/3\exp(\sqrt{F/k_0}). \tag{41}$$

<u>For n = 3</u>

$$\int_0^a e^{-\Psi z}\sin(\psi z)(1-\frac{z}{a})^n =$$

I/2(a/4+(7I)/6s-1.154sI + (11s^2)/(6a) – (0.577s^2)/ a – ((9I)/50s^3)/a^2 + (I/9.7s^3)/a^2 – (3053s^4)/(1058400a^3) + (0.577s^4)/(1260a^3)-(32/35 + (32I)/35)$\sqrt{as}$ PFQ[{-7/2}, {1/2, 3/2}, {(I/2s)/a}] + (I/453600s^{5}PFQ[{1, 1}, {5,11/2,6},{(I/2s)/a}])/a^4 + Isln[a] + (s^{2}ln[a])/(2a) – (I/30s^3ln[a])/a^2 – (s^{4}ln[a]/(2520a^3) + 2Isln[.5-.5I)/$\sqrt{S}$] + (s^2ln[(1/2 – I/2)/$\sqrt{S}$])/a – (I/15s^3ln[(1/2 – I/2)/$\sqrt{S}$])/a^2 – (s^4ln[(1/2 – I/2)/$\sqrt{S}$])/(1260a^3) – a/4 – (7I)/6s + 1.154Is + (11s^2)/(6a) – (0.577s^2)/a + ((9I)/50s^3)/a^2 – (I/8.7s^3)/a^2 – (3053s^4)/(1058400a^3) + (0.577s^4)/(1260a^3) – (32/35 – (32I)/35))$\sqrt{as}$ PFQ[{-7/2}, {1/2, 3/2}, {(-I/2s)/a}]/(2a) - (I/453600s^{5}PFQ[{1, 1}, {5,11/2,6},{(-I/2s)/a}])/a^4 + Isln[a] +(s^{2}ln [a])/(2a) + (I/30s^3ln[a])/a^2 – (s^4ln[a]/(2520a^3) - 2Isln[1/2 + I/2)/$\sqrt{S}$] + (S^2ln[(1/2 + I/2)/$\sqrt{S}$])/a + (I/15s^3ln[(1/2 + I/2)/$\sqrt{S}$])/a^2 - (s^4ln[(1/2 + I/2)/$\sqrt{S}$])/(1260a^3),

where PFQ is the generalized hypergeometric function.

<u>For n = 4</u>

$$\int_0^a e^{-\Psi z}\sin(\psi z)(1-\frac{z}{a})^n =$$

(((1 + I)a((6-6I)a^4 + 77$a^3$$\sqrt{S}$ + (51 + 51I)a^2s + 19Ias$^{(3/2)}$ – (1 – I)s^2))/Exp((1 + I)$\sqrt{S}$ /a) – (2+2I)(30$a^4$$\sqrt{S}$ + (60 + 60I)a^3s + 60Ia^2s$^{(3/2)}$ – (10- 10I)as^2 -s$^{(5/2)}$Γ[0, ((1+ I)$\sqrt{S}$ /a])/(60a^4) – (((1 – I)a((6 + 6I)a^4 + 77$a^3$$\sqrt{S}$ + (51 – 51I)a^2s – 19Ias$^{(3/2)}$ – (1 + I)s^2))/Exp((1 – I) $\sqrt{S}$ /a) + (2 + 2I)(30I$a^4$$\sqrt{S}$ + (60 + 60I)a^3s + 60a^2s$^{(3/2)}$+ (10-10I) as^2 - Is$^{(5/2)}$) Γ[0, (1– I)$\sqrt{S}$ /a])/(60a^4),

where

s = (F/2k_0) and I = $\sqrt{-1}$.

Since the solution of equation (40) depends on the value of n, then one can write:

$$F_3(y) = F_{03}(y)\exp\left\{-\frac{V_g}{u_g M(a,S,n)}y\right\}, \tag{42}$$

where M(a,S,n) is the solution of integration depending on n’s values. Then the concentration becomes:

$$C(y,z) = F_{03}(y)\exp\left\{-\frac{V_g}{u_g M(a,S,n)}y\right\}(1-\frac{z}{a})^{n}. \tag{43}$$

If C(y,z) decreases exponentially with y like exp($-y/\bar{y}$), where $\bar{y}$ is the decay distance at crosswind direction, equation (43) can be rewritten as:

$$C(y,z) = F_{03}(y)\exp(\frac{-y}{\bar{y}})(1-\frac{z}{a})'' , \quad (44)$$

where

$$\bar{y}_3 = u_g M(a,S,n)/V_g , \quad (45)$$

and $F_{03}(y)$ can be calculated using the boundary conditions:

$$Q = \int_0^a \int_0^{\bar{y}} U(z)C(y,z)dydz. \quad (46)$$

Substituting U(z) from equation (33) and performing the integration yields:

$$F_{03}(y) = -\frac{Q}{.63\bar{y}_3^2 V_g}. \quad (47)$$

Therefore, the equation (43) will be:

$$C(y,z) = \frac{Q}{.63\bar{y}_3^2 V_g}\exp(\frac{-y}{\bar{y}_3})(1-\frac{z}{a})'' , \quad (48)$$

which represents the concentration at crosswind direction.

4 – DEPLETING SOURCE STRENGTH CALCULATIONS

The plume can be progressively depleted along the downwind distance and crosswind distance as a result of removal of particles from the original source strength. The removal particles may be attributed to many reasons such:

- Impact on surfaces, such as walls, leaves and ground.
- Interaction of pollutants chemically with other paticles present in the atmosphere.
- The proper effect of deposition velocity.
- The wind velocity.
- Type of stability conditions.

The source strength Q is defined as:

$$Q = \int_0^a \int_0^{\bar{x}} \int_0^{\bar{y}} C(x,z)dydxdz. \quad (49)$$

(4-a) In downwind distance

- **For neutral condition**

$$Q = \int_0^a \int_0^{\bar{x}_1} C(x,z)dxdz,$$

$$Q_1 = \frac{Q_1^*}{0.63V_g\bar{x}_1^2}\int_0^a \int_0^{\bar{x}_1} \exp(\frac{-x}{\bar{x}_1})(1-\frac{z}{a})'' dxdz, \quad (50)$$

$$Q_1 = \frac{Q_1^* a}{V_g\bar{x}_1(n+1)}, \quad (51)$$

where Q_1^* is the depleted quantity from the original source strength Q_1 at downwind distance.

- **For stable condition**

One can find out a similar formula to Q_2 at downwind distance as:

$$Q_2 = \frac{Q_2^* a}{V_g \bar{x}_2 (n+1)}. \tag{52}$$

(4b-b) crosswind direction

The source strength is given by:

$$Q_3 = \int_0^a \int_0^{\bar{y}} C(y,z)dydz, \tag{53}$$

$$Q_3 = \frac{Q_3^*}{0.63\bar{y}^2} \int_0^a \int_0^{\bar{y}} \exp(\frac{-y}{\bar{y}})(1-\frac{z}{a})^n dydz,$$

$$Q_3 = \frac{Q_3^* a}{V_g \bar{y}(n+1)}. \tag{54}$$

Then the total depleted source strength for either neutral or stable conditions can be estimated as:

$$Q = Q_1 Q_3, \quad \text{(neutral conditions)},$$

$$Q = \frac{Q_1^* a}{V_g \bar{x}_1 (n+1)} \frac{Q_3^* u_g a}{V_g \bar{y}(n+1)},$$

$$Q = \frac{Q_1^* Q_3^* a^2}{V_g^2 \bar{x}_1 y (n+1)^2}. \tag{55}$$

Let Q_{13}^* is the total depleted source strength at neutral condition, then

$$Q_{13}^* = Q_1^* Q_3^*,$$

$$Q_{13}^* = \frac{QV_g^2 \bar{x}_1 \bar{y}(n+1)^2}{a^2}. \tag{56}$$

For stable condition we can also calculate the total depleted source strength as

$$Q_{23}^* = \frac{Q' V_g^2 \bar{x}_2 \bar{y}(n+1)^2}{a^2}, \tag{57}$$

where $Q' = Q_2 Q_3$ and $Q_{23}^* = Q_2^* Q_3^*$

5. SAMPLE APPLICATIONS

To apply the concentration formulae indicated by equations (18,48) practically, calculations must be made for the decay distances $\bar{x}, \bar{y}$ supposing all other parameters are known.

Assuming that the environmental lapse rate is adiabatic and that the terrain is flat, typical values of V_g over growing wheat when the wind speed is measured at 10 m/s in neutral stability conditions are given from Smith (1990).

The relation between the decay distances (downwind and crosswind) corresponding to the order of n and the inversion height which are indicated from equations (15 and 45) is plotted as shown in figures (1,2) for downwind decay distance and in figures (3,4) for crosswind direction.

The normalized concentrations derived from equation (18) and equation (48) are plotted against both the downwind distance for a dry day, as shown in figures (5,6) and the crosswind distance, as shown in figures (7,8).

6. CONCLUSION

The present study deals with modeling of air polllution in atmosphere. In this treatment we assume that the vertical distribution of pollutants is given by a simple polynomial. The variation of both wind velocity and diffusivity coefficient with height rather than with different atmospheric stability classes (neutral and stable) are considered.
The diffusivity coefficient K(z) is taken, as should be, non-zero at ground surface for vertical diffusion to be possible.
The prediction of concentrations of pollutants released from elevated source in downwind and crosswind directions are estimated, while both the deposition to the ground surface and elevated inversion are considered.
Decay distances along downwind and crosswind distances are obtained also their relations with the elevated inversion heights are discussed.
The depleted source strength in both downwind and crosswind distances are estimated and then the total source strength depletion is predicted.

REFERENCES

A. B. Mayoub and A. O. ElShal, A simple analytical model of pollutant dispersion with ground absorption. Arab Journal of nuclear sciences and application 25,2, (1992)
M. Benntt, A simple physical model of dry deposition to a rough surface. Atmos. Environ. Vol. 22, No. 12, 2701, (1988).
F. A. Gifford, Atmospheric dispersion models for environmental pollution applications. In Haugen (1975), 35-58, (1975)
T. S. Heines and L. K. Peters, The effect of the ground level absorption on the dispersion of the pollutant in the atmosphere. Atmos. Environ. 8, 1143-1153, (1974).
E. Melli P. Runca and P. Zannetti, Computation of long term average SO_2 concentration in the Venetian area. Appl. Math. Mod. 1, 9-15, (1976).
F. B. Smith, Dry deposition processes. College on atmospheric boundary layer physics SMR/463-3. Trieste, (1990).
O. G. Sutton, A theory of eddy diffusion in the atmosphere. Proc. R. Soc. Lond. 135 A, 143-165, (1932).
D. B. Turner, A diffusion model for an urban area. J. Appl. Meteor., 3:83, (1964).