Proceedings of the Third International Symposium on Air Quality Management at Urban, Regional and Global Scales. pp. 690-698, 26-30 September 2005, Istanbul – Turkey

QUANTITATIVE ASSESSMENT OF AIR QUALITY THROUGH MODELING OF POLLUTION CONCENTRATION IN ATMOSPHERE WITH KNOWN SURFACE VALUE IN CIRCULAR REGIONS

V.P. Saxena and H.S. Jat*

School of Mathematics and Allied Sciences, Jiwaji University, Gwalior – 474011, India saxena_vp@rediffmail.com
*Department of Mathematics, M.P. College of Technology, Gwalior– 474006, India
drhsjat@yahoo.co.in

ABSTRACT

This paper deals with the mathematical model of atmospheric pollution problem when the a near circular ground source emits specific pollutant species vertically upward in still air. The eddy diffusivity is assumed to vary continuously in upward direction and attains very small value at some given height. The values of the concentration distribution are monitored at the ground and at the boundary points of the region under consideration. The Mathematical model, which is expressed in terms of partial differential equation, is solved in exact form yielding Bessel functions and Legendre polynomials. The numerical values of the concentration are computed for certain specific cases.

Key Words : Air Pollution, Mathematical Modeling, Numerical Computation, Initial and Boundary Conditions, Concentration Distribution.

1. INTRODUCTION

Many of the urban air pollution are related with near circular area source and vertical and radial distribution above the surface. The vertical distribution is influenced by the variation of eddy diffusivity which varies in vertical direction (Seinfeld, 1986) almost parabolically. This paper considers pollution distribution in an atmosphere with circular symmetry incorporating the above situations. Solution of the mathematical model is presented using Laplace transform in terms of modified Bessel functions and Legendre polynomials (Rainville, 1960).

Earlior, attempts have been made to solve mathematical models of pollution by simplified approach (Khan (1992), Kakamari (2001)) and also by advanced method for difficult problems (Saxena, Juneja, Aslan and Durukanoglu (2001)), (Tokgozlu, Saxena, Ocak and Erturk(2001)). Closed form solutions have also been obtained in certain cases (Saxena, Jat, Miri and Juneja (2003A)), (Saxena, Jat, Miri and Juneja (2003 B)), (Saxena and Juneja (2003)).

The mathematical solution of air pollution model obtained in this paper provides a closed from expression which can give air quality and pollution status at any desired interval and at any location in vertical as well as in horizontal direction. As indicated above the eddy diffusivity of the substances present is assumed to vary in vertical direction in a particular fashion so that it reduces to minimum value at a particular height. The numerical computation is carried out for a particular situation of initial air quality to obtain pollution density in the whole region for different values of time. However, more result can be obtained for other situations also. At the same time model can be utilized for manipulating the air quality for a given pollutant.

2. MATHEMATICAL FORMULATION

We consider a near circular ground with known concentration of pollutant all over and a cylindrical region above it which is equally polluted initially but the pollution level falls down gradually. The concentration beyond this resign is supposed to be estimated vertically.

The governing partial differential equation and the allied conditions can be stated as:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rK_r\frac{\partial C}{\partial r}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)=\frac{\partial C}{\partial t} \qquad (1)$$

where t is time, C is the concentration of pollutants and K_r and K_z are the turbulent diffusion coefficients along radial direction r and z – directions respectively.

We take

C (r, z, o) = L, C (r, o, t) = L and C (a, z, t) = g(z,t) (given)
Here a = ground radius and L is a fixe value of C.

Now we use the transformation

y (r, z, t) = L – C (r, z, t)

Then equation (1) becomes

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rK_r\frac{\partial y}{\partial r}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial y}{\partial z}\right)=\frac{\partial y}{\partial t} \qquad (2)$$

and condition becomes

y (r, z, o) = 0, y (r, o, t) = 0 and y (a, z, t) = L – g (z, t)

Further, assuming variable diffusivity in vertical direction reaching lowest value at the top (z=H), we take

$K_z = \lambda\ (1 - z^2/H^2)$

Also, we assume

$K_r = K$, and $z/H = u$

Accordingly

$$K\left(\frac{\partial^2 y}{\partial r^2} + \frac{1}{r}\frac{\partial y}{\partial r}\right) + \frac{\lambda}{H^2}\frac{\partial}{\partial u}\left[(1-u^2)\frac{\partial y}{\partial u}\right] = \frac{\partial y}{\partial t}$$

(3)

The initial and boundary conditions are

y (r, u, o) = 0, y (r, o, t) = 0
y (a, u, t) = G (u,t)

(4)

3. **SOLUTION**

The Laplace transform is defined as

$$\mathscr{L}\ \{y(r,u,t)\} = \bar{y}(r,u) = \int_0^\infty \exp(-pt)\, y(r,u,t)\, dt \quad \mathrm{Re}(p) > 0 \tag{5}$$

with the inversion formula

$$\text{y(r,u,t)} = \frac{1}{2\pi i}\int_{\sigma - i\infty}^{\sigma + i\infty} \exp(pt)\,\bar{y}(r,u)\,dp \tag{6}$$

where $0 < \sigma < 1$. Also we know that

$$\mathscr{L}\ \left\{\frac{\partial}{\partial t} y(r,u,t)\right\} = p\,\mathscr{L}\ \{y(r,u,t)\} - y(r,u,0)$$

(7)

Hence with the help of initial condition (4), the equation (3) takes the form

$$\frac{\partial^2 \bar{y}}{\partial r^2} + \frac{1}{r}\frac{\partial \bar{y}}{\partial r} + \frac{\lambda}{KH^2}\frac{\partial}{\partial u}\left[(1-u^2)\frac{\partial \bar{y}}{\partial u}\right] = \frac{p}{k}\,\bar{y}(r,u) \tag{8}$$

with the conditions

$$\mathscr{L}\ \{y(r,o,t)\} = 0 \tag{9}$$
$$\mathscr{L}\ \{y\ (a, u,t)\} = G(u)$$

where

$$G(u) = \mathcal{L}\ \{G(u,t)\}$$

Using the properties of Legendre's polynomial (Rainville(1962)), we have that if

$$y_n(r) = \int_0^1 \bar{y}(r,u) P_{2n+1}(u)\,du \tag{10}$$

then

$$\bar{y}(r,u) = \sum_{n=0}^{\infty} (4n+3) y_n(r) P_{2n+1}(u) \tag{11}$$

We also know that the Legendre's polynomial $P_{2n+1}(u)$ is solution of the differential equation

$$\frac{d}{du}\left[(1-u^2)\frac{d}{du}P_{2n+1}(u)\right] + (2n+1)(2n+2)P_{2n+1}(u) = 0 \tag{12}$$

Hence using equation (10) and (11), we get equation (8) in the form

$$\frac{\partial^2 y_n}{\partial r^2} + \frac{1}{r}\frac{\partial y_n}{\partial r} - \xi_n^2 y_n = 0 \tag{13}$$

where

$$\xi_n^2 = \frac{\lambda}{KH^2}(2n+1)(2n+2) + \frac{p}{k}$$

Equation (13) is known as Bessels equation and its solution is given as

$$y_n = AI_0(\xi_n r) + B\,Ko(\xi_n r) \tag{14}$$

But as $r \longrightarrow 0$, $K_0(\xi_n r) \rightarrow \infty$

Therefore B = 0 and from (5)

A = Yn/ I_0 (ξ_na),

$$y_n = \int_0^1 P_{2n+1}(u)\overline{G}(u)du$$

(15)

Substituting in (14), (11) and (6), we get

$$y(r, u, t) = \sum_{n=0}^{\infty}(4n+3)P_{2n+1}(u)\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} Y_n \frac{I_0(\xi_n r)}{I_0(\xi_n a)}\exp(pt)dp$$

(16)

or

$$y(r, z/H, t) = \sum_{n=0}^{\infty}(4n+3)P_{2n+1}(z/H)\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} \frac{Y_n I_0(\xi_n r)}{I_0(\xi_n a)}\exp(pt)dp$$

(17)

But

y (r, z, t) = L – C (r, z, t)

Therefore

C (r, z, t) = L – y (r, z, t)

and

$$C(r, z/H, t) = L - \sum_{n=0}^{\infty}(4n+3)P_{2n+1}(z/H)\frac{1}{2\pi i}\int_{\sigma-i\infty}^{a+i\infty} \frac{Y_n I_0(\xi_n r)}{I_0(\xi_n a)}\exp(pt)dp$$

(18)

4. SPECIAL CASE

Now as a particular case, we take

$$C\ (a, z,t) = \left(\frac{L}{H}\right)z$$

So that from equation (9) and (16) and the integrals

$$\int_0^1 x^y P_{2n+1}(x)dx = \frac{1}{4n+3}, y = 2n+1$$
$$= 0, y \neq 2n+1$$

(19)

we get

$$Y_n = \frac{L}{3Hp}$$

Therefore

$$C\ (r, z/H, t) = \frac{Lz}{H}\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{I_0(\xi_0 r)}{pI_0(\xi_0 a)}\exp(pt)dp$$

(20)

Here

$$\xi_0 = \left[\frac{2}{H^2} + p/k\right]^{1/2} \qquad \text{at } \lambda = k$$

The zeros of I_0 (ξ_0a) are

$$\frac{2}{H^2} + p/k = -\alpha_n^2$$

(21)

$$\Rightarrow \left(2/H + \alpha_n^2\right) = -p/k$$

or

$$p = -k\left(\frac{2}{H^2} + \alpha_n^2\right)$$

(22)

where α_n are roots of the equation $J_0(a\alpha) = 0$.

Hence evaluating the integral on the right hand side of (20) with the help of residue method, we obtain

$$C(r,z,t) = L - \frac{L\,z}{H}\left[1-\frac{2}{a}\sum_{n=1}^{\infty}\frac{\alpha_n \exp\left\{-k\left(\frac{2}{H^2}+\alpha^2\right)t\right\}J_0(r\alpha_n)}{\left(2/H^2+\alpha_n^2\right)J_1(a\alpha_n)}\right]$$

(23)

5. NUMERICAL COMPUTATION

On taking H = 1 km, we get

$$\begin{aligned} C(r, z, t) = L\,[&1-z + z\,(1.3915)\exp(-25.127\,kt) \times J_0(4.809\,r) \\ &- z\,(1.0440)\exp(-123.881\,kt)\ J_0(11.040\,r) \\ &+ z\,(0.8512)\exp(-301.5322\,kt)\ J_0(17.307\,r) \\ &- z\,(0.7275)\exp(-558.1579\,kt)\ J_0(23.583\,r)\ t \end{aligned} \quad (24)$$

Here

A = .5 km

The numerical values of C_1 (r,z,t), where

C_1(r,z,t) = C(r,z,t)/L

for different r and at the different time values are shown in the Table-1 and Table-2.

Table 1. The concentration distribution at different radius values and different height where t = 60 sec. and k = $3.5\text{x}10^{-3}$ km/gm/sec.

z ↓ \r →	0.0	0.1	0.2	0.3	0.4	0.5
0.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.1	.9629	.9596	.9650	.9340	.9193	.9001
0.2	.9258	.9192	.9300	.8687	.8386	.8003
0.3	.8888	.8788	.8950	.8031	.7579	.7005
0.4	.8517	.8384	.8600	.7375	.6772	.6007
0.5	.8147	.7980	.8251	.6719	.5966	.5009
0.6	.7776	.7576	.7934	.6062	.5159	.4010
0.7	.7405	.7173	.7551	.5406	.4352	.3012
0.8	.7035	.6769	.7201	.4750	.3545	.2014
0.9	.6664	.6365	.6852	.4094	.2738	.1016
1.0	.6294	.5961	.6502	.3438	.1932	.0018

At a = .5 km
H = 1 km;
At t = 60 sec.
k = .001 km/gm/sec.= $1.0 \times 10^{-3} \times$ km/gm/sec.

Table 2. The concentration distribution at different radius values and different height where t = 60 sec. and k = $1.0x10^{-3}$ km/gm/sec.

z \ r → (z ↓)	0.0	0.1	0.2	0.3	0.4	0.5
0.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.1	.9307	.9288	.9307	.9157	.9087	.9000
0.2	.8614	.8577	.8614	.8315	.8174	.8001
0.3	.7922	.7865	.7921	.7473	.7261	.7002
0.4	.7229	.7154	.7228	.6631	.6348	.6003
0.5	.6537	.6443	.6536	.5789	.5435	.5003
0.6	.5844	.5731	.5843	.4947	.4522	.4004
0.7	.5152	.5020	.5150	.4105	.3609	.3005
0.8	.4459	.4309	.4457	.3263	.2696	.2006
0.9	.3767	.3597	.3765	.2421	.1783	.1006
1.0	.3074	.2886	.3072	.1578	.0870	.0007

REFERENCES

Kakamari, Khaleel Ahmed G., 2001. Ph.D. Thesis in Bangalore University.

Khan, Sujit Kumar, 1992. Ph.D. Thesis in Bangalore University.

Rainville, E.D., 1960. Special Functions, McMillan.

Seinfeld, John H., 1986. Atmospheric chemistry and physics of air pollution, John Wiley & Sons.

Saxena, V.P., Juneja, A., Aslan, Z. and Durkanoglu, F., 2001. Modelling of horizontal dispersion of pollutants in the atmosphere with wind: A Core Study in the Proc. of Sec Int. Symp. on Air Quality Management Urban, Regional and Globol Scales, Istanbul – Turkey, 403-409.

Saxena, V.P., Jat, H.S., Miri, Praveen and Juneja, A, 2003-A. Pollution distribution in an urban atmosphere with vertical emittence : A Mathematical Study in the Proc. of Sec. National Conference on Urban air Pollution Issues & Managements, Surat (Gujarat), India, 3.12-3.19.

Saxena, V.P., Jat, H.S., Miri, Preveen and Juneja, A., 2003-B. Mathematical modelling of air pollution in urban atmosphere with surface deposition. Proc of Sec. National Conference on Urban Air Pollution Issues and Management, Surat (Gujarat), India, 3.3-3.11.

Saxena, V.P., and Juneja, A., 2003, Numerical study of air pollution in annular regions with point source. Proc. of Sec. 26th NATO/CCMS Int. Technical Meeting on Air Pollution Modelling and its Application, Istanbul Technical University, Istanbul – Turkey, 568.

Tokgozlu, A., Saxena, V.P., Ocak, S. and Erturk, F., 2001. Transient concentration distribution of pollutants over Isparta Proc. of Sec. Int. Symp. on Air Quality Management Urban, Regional and Globol scales, Istanbul – Turkey, 396-402.