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GROUND LEVEL CONCENTRATIONS ON AREA SOURCES

1.   Analytical and numerical solutions of the steady state two-dimensional differential equation were obtained by separation and finite difference methods respectively. The solution can be used to calculate ground level concentration of air pollutant over an area source at an urban area.

The methods are applied to calculate sulphur dioxide concentrations distribution over 2-hours period in Nashville, Tennessee, USA. Our calculating concentrations are found to agree well with the observations than other methods using statistical technique.

2.   Study of advection and diffusion of emitted pollutants from area sources are very important because of bearing its direct effect on calculating dispersion of containment of urban area. Air dispersion model based on its analytical solution had several advantages over numerical models because all of the parameters are explicitly expressed in mathematical form.

Analytical solutions are useful for examining the accuracy and performance of the numerical models through studies of the analytical solution that allows valuable insight to be gained regarding the behaviour of a system [Runca 1982 and Essa *et al.*, (2007)].

An analytical solution has received more attention in the Gaussian plume equation, which assumes that wind speed and turbulent eddies are invariant with height. A simple Gaussian profile is not found in the vertical direction for a ground – level or an elevated release and unstable conditions (Nieuw-Stadt and Van Ulden (1978), Gryning *et al.*, (1983) and Briggs (1985). A new approach to simulate the pollutant dispersion in the planetary boundary layer is estimated by Wortmann *et al.* (2005) and Essa *et al.*, (2007). A semi analytical model for the tritium dispersion simulation in the planetary boundary layer from the Angra I nuclear power plant is estimated by Moreira *et al.*, (2005). In the work we derive a simple solution of the steady state diffusion equation which describes advection in the direction of the wind and diffusion in the vertical direction using separation and finite difference methods. These methods have been giving solutions which agree well with observed concentration of sulphur dioxide.

3.   Under steady state condition, the ambient concentration $C(x, z)$ of contaminant at a point (x, z) of the

atmospheric advection–diffusion equation under several hypothesis is written in the form (Essa *et al.*, 2006).

$$u(z)\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left[K(z)\frac{\partial C}{\partial z}\right] \qquad (1)$$

where u is the mean wind velocity and K is turbulent diffusion coefficient. Diffusion in the x and y directions is neglected. It is assumed that the pollutants are emitted as steady flux at the ground surface $z = 0$ *i.e.*,

$$K(z)\frac{\partial C}{\partial z} = -Q \qquad \text{at } z = 0 \qquad (2)$$

where Q is the source strength that assumed to be constant with downwind distance x. It is assumed that there is no concentration over mixing height $h(x)$:

$$C(x, z) = 0 \qquad \text{at} \quad z \ge h(x) \qquad (3)$$

Consequently, there is no flux over the mixing height, *i.e.*,

$$\frac{\partial C}{\partial z} = 0 \qquad \text{at} \quad z \ge h(x) \qquad (4)$$

It is further assumed that at the top of the boundary layer the concentration varies smoothly in the x direction, *i.e.*,

$$\frac{\partial C}{\partial x} = 0 \qquad \text{at} \quad z = h(x).$$

Using the above condition, we get:

$$\frac{\partial^2 C}{\partial z^2} = 0 \qquad \text{at} \quad z = h(x) \qquad (5)$$

The wind velocity in neutral case and the diffusion coefficient may be written (Hanna *et al.*, 1982) in the empirical form:

$$u(z) = \frac{u_*}{k_v}\left[\ln\frac{z}{z_0}\right], \qquad K(z) = k_0 + k_1\left(\frac{z}{z_0}\right)^n$$

At the ground surface $K = k_o$, the diffusion coefficient should be non zero at the point of emission for vertical diffusion, u_* is the friction velocity, k_v is Von-Kaman constant = 0.4, z_0 is the roughness height, and k_1 is

the value of the eddy diffusivity at reference height. Boundary conditions (Eqns. 3 to 5) are satisfied if we assume the concentration C as a polynomial of third degree. Let us assume the solution of Eqn. 1 can be written in the separation form as:

$$C(x, z) = g(x)\left(1 - \frac{z}{h}\right)^3 \qquad (6)$$

Using condition (Eqn. 2), we get,

$$\frac{\partial C}{\partial z} = 3g(x)\left(1 - \frac{Z}{h(x)}\right)^2\left(\frac{1}{-h(x)}\right)$$

since $K(z)\dfrac{\partial C}{\partial z} = -Q$ at $z = 0$ then

$$g(x) = \frac{h(x)Q}{3k_0} \qquad (7)$$

In the pervious equation, the depth of the pollutant layer $h(x)$ is unknown. An expression for $h(x)$ is obtained by integrating Eqn. 1 from 0 to h with respect to z, using Eqn. 2. Further integrating it over x, assuming that $g(x_0) = 0$, *i.e.*, $h(x_0) = 0$ and $u_* = 0.4$ in neutral case, we get

$$(x - x_0) = \frac{h^2}{12k_0}\left[\ln\left(\frac{h}{z_0}\right) - \frac{25}{12}\right] \qquad (8)$$

Taking $k_0 = 3\text{m}^2/\text{s}$,

The exact solution of the above equation becomes in the form:

$$h = \exp\left[0.5\,\text{Lambert}\,W\left(-1.1164\frac{(x - x_0)}{z_0^2} + 2.0833\right)\right]z_0$$

where, $\text{Lambert}\,W(x)\ e^{\text{Lambert}\,W(x)} = x$

For one point source, the ground level concentration takes form:

$$g(x) = \frac{Q\exp\left[0.5\,\text{Lambert}\,W\left(-1.1164\frac{(x - x_0)}{z_0^2} + 2.0833\right)\right]z_0}{9} \qquad (9)$$

But for an area source, the ground level concentration is written in the form [Lebedeff and Hameed (1975)], we get:

$$g(x) = \left(\frac{1}{9}\right)\sum_{L=1}^{S}(Q_L - Q_{L-1})z_0$$
$$\exp\left[0.5\,\text{Lambert}\,W\left(-1.1164\frac{(x - x_{L-1})}{z_0^2} + 2.0833\right)\right] \qquad (10)$$

For the numerical integration of equation (1) the Crank-Nicolson scheme has been applied yielding the finite difference form (Mark 1999):

$$\alpha\left[\left(\frac{1}{\alpha} + 2K_j + K_{j+1} - K_{j-1}\right)\right]C_{i+1, j}$$
$$+ \left(2K_j + K_{j+1} - K_{j-1}\right)C_{i+1, j+1}$$
$$- \left(K_{j-1} - K_j\right)\left(\frac{2\Delta zQ}{k_0}\right) = C_{i, j}, \quad j = 1, 2\ldots\ldots N \qquad (11)$$

where $\alpha = \Delta x/4U(\Delta z)^2$, Δx is the horizontal interval between the grid points i and $i + 1$, Δz is the vertical interval between the points j and $j + 1$. A set of n-equations are obtained one for each box of fluid in the $i + 1$ plane, which are solved simultaneously. Then the procedure is to step to the $i + 2$ plane and repeat the process with the known plane $i + 1$.

To illustrate this procedure, consider an array four boxes wide and four boxes high. The set of $n = 16$ simultaneous algebraic equations for the $i + 1$ plane may be written as:

$$[A][C] = [D] \qquad (12)$$

where A is a 16×16 matrix, C is a 16×1 matrix of the unknown concentrations, and D is a 16×1 matrix of the corresponding known concentration fluxes in the I plane plus any source terms.

We used equation (9) to calculate ground level concentration of sulphur dioxide (SO_2) at a given point for one point source. For an area source, we used two equations (10) and (11) using analytical and numerical methods to evaluate ground level concentration.

TABLE 1

Observed and calculated sulphur dioxide concentrations in Nashville are given in pphm.
(part per hundred million) where 1pphm = 2.7×10^{-5} gm^{-3} of SO$_2$

Obs. Sta. No.	Observed	Our analytical	Our numerical	Integral	Old Numerical
19	5.8	7.1	5.7	8.7	5.1
48	13.6	14.1	14.6	17	6.5
52	2.9	5.2	5.3	6.2	0.4
56	6.9	6.8	6.4	8.9	0.9
60	20.9	20.2	18	20	14
82	13.2	14.6	9.7	9.7	4.2
90	4.1	3.6	3.9	6.8	2.7
Correlation Coefficient		0.99	0.96	0.92	0.89

We applied two Eqns. 10 and 11 to calculate the dispersion of SO$_2$ in the atmosphere of Nashvill, Tennessee, USA, over 2-hours period. Source inventory and meteorological data for the problem is taken from Randerson (1970). Measured values of SO$_2$ concentration at seven observation stations are compared with the values calculated by two Eqns. (10) and (11) with others (integral method lebedeff and Hameed 1975 and old numerical method, Randerson 1970). Table 1 shows observed and calculated concentrations, namely, our models for analytical and numerical methods, integral method (Lebedeff and Hameed 1975) and numerical solution of the three–dimensional diffusion (Randerson 1970).

4. The correlation coefficients of the four calculated methods show that our analytical and numerical models using the two Eqns. (10) and (11) respectively yield better results than the other two methods (integral method Lebedeff and Hameed 1975, and old numerical method Randerson 1970).

Fig. 1 Shows that our calculated and numerical concentrations are within a factor of two with the observations concentrations, also the concentrations using integral method Lebedeff and Hameed (1975), but the old numerical method lies in factor of four with the observations concentrations.

The datasets were applied subsequently to the following statistical indices (Hanna 1989) : Nmse (normalized mean square error) $= \overline{\left(C_0 - \overline{C}_p\right)^2} / \, C_0 C_p$; Fa2 = fraction of data (%) for $0.5 \le \left(C_p / C_0\right) \le 2$; Cor (Correlation coefficient) $= \overline{\left(C_0 - \overline{C}_0\right)\left(C_p - \overline{C}_p\right)} / \sigma_0 \sigma_p$; Fb (fractional bias) $= \overline{C}_0 - \overline{C}_p / 0.5\left(\overline{C}_0 + \overline{C}_p\right)$; and
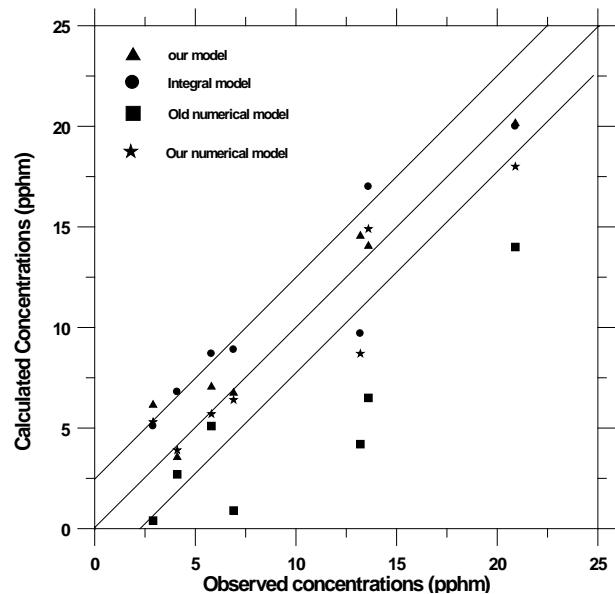

Fig. 1. Comparing between calculated and observed concentrations of sulphur dioxide at Nashville, Tennessee

Fs (fractional standard deviation) $= \left(\sigma_0 - \sigma_p\right) / 0.5\left(\sigma_0 + \sigma_p\right)$ where subscripts 0 and p refer to observed and predicted quantities, respectively, and an over bar indicated an average.

The results of the statistical indices used to evaluate the concentrations of sulfur dioxide are shown in Table 2. The statistical index Fb indices the predicted quantities are underestimate or overestimate the observed ones. The

TABLE 2

Results of statistical indices used to evaluate the model performance

Model	Nmse	Fa 2	Cor	Fb	Fs
Our analytical method	0.01	1.14	0.99	-0.06	0.061
Our numerical method	0.05	1.05	0.96	0.06	0.198
Integral method	0.07	1.36	0.93	-0.14	0.202
Old numerical method	0.69	0.47	0.89	0.66	0.342

statistical index Nmse represents the quadratic error of the predicted quantities in relation to the observed one. Best results are indicated by values nearest 0 in Nmse, Fb and Fs, and nearest 1 in Cor, Fa2. The statistical indices show that a reasonable agreement is obtained between observed and our estimated concentrations than old numerical method (Randerson 1970).

It can be seen from Table 2, that the calculated values of Nmse, Fb and Fs of our analytical and numerical methods are smaller than the corresponding values for the integral and old numerical methods, also the correlation coefficients of our work are greater than the others and near to one. Also from Table 2 both the values of our work and integral method (Lebedeff and Hameed 1975) lie in the factor of two, but the old numerical method (Randerson 1970) lies outside.

Notice that it is difficult to establish statistical significance of indices with such small samples though some marginal improvement are noticed in the Fig. 1 relating to new methods.

5.   Our analytical and numerical models using logarithmic law of the wind speed method give better results with observation values than the integral method using power law of the wind speed (Lebedeff and Hameed 1975) and the numerical methods (Randerson 1970). Also, the correlation coefficients of our models tend to one and greater than others.

A good agreement with our analytical and numerical models results was obtained with the proposed approach that considers the K_z value to vary with the vertical distance.

The logarithmic law of the wind speed gives better results in the surface layer than power law used by (Lebedeff and Hameed 1975).

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M. ABDEL-WAHAB*
KHALED S. M. ESSA
M. EMBABY
SAWSAN E. M. ELSAID

Meteorology and Astronomy Department, Faculty of Science, Cairo University
Mathematics and Theoretical Physics, NRC, Atomic Energy Authority, P. O. 13759, Cairo
(*10 November 2008, Modified 6 May 2009*)
e mail : essa_ksm@yahoo.com