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Studying the effect of vertical variation of wind speed and eddy diffusivity on the advection-diffusion equation

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ABSTRACT

The three dimensional steady state advection-diffusion equations have been solved analytically to simulate the dispersion of contaminants in the atmospheric boundary layer (ABL). The solution is based on the assumption that the concentration distribution of pollutants in the crosswind direction has a Gaussian distribution. The analytical solution has been obtained by taking into account the dependence of the vertical eddy diffusivity and the wind speed on the vertical height z. The derived solution has been applied to calculate the concentration of Iodine-131 using data collected from the experiments performed to collect air samples around a Research Reactor. Statistical measures were applied to evaluate the performance of the derived model. The results are discussed and presented in tables and illustrative figures.

Keywords: Air pollution modeling; eddy diffusivity; power law profile, crosswind integrated concentration; Model evaluation.

1. INTRODUCTION

The atmospheric advection- diffusion equation (e.g., Seinfeld 1986) has long been used to describe the transport of pollutant in a turbulent atmosphere. Its analytical solution is of fundamental importance in understanding and describing physical phenomena (Pasquill and Smith 1983). The analytical solution has many advantages over numerical solution, since all parameters appear explicitly in the solution, so, their effect can be easily investigated (Nieuwstadt, 1980). The analytical solution is used to examine the accuracy and performance of the numerical solutions (Runca and Sardei, 1975; Liu and Seinfeld, 1975; Runca, 1982; Khaled SM Essa et al. 2015). An analytical solution that has received much attention and has been studied extensively is the Gaussian plume model. This model assumed that wind speed and turbulence diffusion coefficients are invariant with height. The Gaussian model was modified to include source depletions.

In this paper we present an analytical treatment of the steady state three dimensional advection-diffusion equations under the assumption that the concentration distribution of pollutants in the crosswind direction has Gaussian shape. Also, it is assumed that the vertical eddy diffusivity and the wind speed were specified as functions of height above the ground. A power-law profile is used to describe the variation of vertical eddy diffusivity and wind speed with height. The plume depletion due to radioactive decay of the pollutant is taken into consideration. The resulting analytical solution has been applied to estimate the concentration of I-131 by using data collected from the experiments conducted to collect air samples around the Research Reactor. Statistical measures have been utilized in the comparison between the computed and measured concentrations. The results of this study are discussed and presented in tables and illustrative figures.

2. THE ANALYTICAL SOLUTION

The steady state advection- diffusion equation that describes the dispersion of contaminants in a turbulent boundary layer reads

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

where C(x,y.z) is the average pollutant concentration, S represents the source term, R is the removal term, u, v, w and K_x, K_y, K_z are the components of wind and eddy diffusivity coefficient along the x, y and z directions, respectively.

On using the following assumptions;

1- The mean wind blowing along the x axis, so that v = w = 0,

2- The x transport by the mean flow is greatly outweighs the eddy flux in that direction, that is

$$u\frac{\partial C}{\partial x}\succ\succ\frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right), \tag{2}$$

There is no source and removal of contaminants, i.e., S = 0 and R = 0. Equation (1) reduced to

$$u\frac{\partial C}{\partial x}=\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) \tag{3}$$

By assuming the Gaussian concentration distribution in the crosswind direction (Huang, 1979; Irwin et al., 2007), the solution of Eq. (3) in a three dimensional can be written as:

$$C(x,y,z) = C(x,z)\frac{1}{\sqrt{2\pi}\,\sigma_y} e^{-\frac{y^2}{2\sigma_y^2}} \quad (4)$$

where, C(x,z) is the crosswind integrated concentration and σ_y is the standard deviation of the concentration distribution in the crosswind direction.

The crosswind integration of Eq. (3) from -∞ to + ∞ leads to:

$$u\frac{\partial C(x,z)}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C(x,z)}{\partial z}\right) \quad (5)$$

where

$$C(x,z) = \int_{-\infty}^{+\infty} C(x,y,z)dy \quad (6)$$

The mathematical formulation of C(x,z) is obtained by solving Eq.(5) taking into account the vertical variation of both the wind speed u and the vertical eddy diffusivity K_z with the vertical height z above the ground. In this study we have used a power law profile to describe the variation of u and K_z with height in the boundary layer (Britter, et al., 2003) as:

$$u(z) = az^n, \qquad a = u_1/z_1^n \quad (7)$$

$$K_z(z) = c\,z^m, \qquad c = K_{z1}/z_1^m \quad (8)$$

where, z_1 is the reference height where the wind speed u_1 and the eddy diffusivity K_{z1} are measured, a, c are dimensional coefficients. The values of the profile exponents' m, n depend on the atmospheric stability and the nature of the underlying surface. Within the constant stress region near the surface, powers for velocity and diffusivity must sum to unity (m + n =1).

Equation (5) is subject to the following boundary conditions:

(a) The ground is assumed to be completely reflects the diffusing material, i.e.

$$K_z \frac{\partial C(x,z)}{\partial z} = 0 \quad \text{at} \quad z = 0 \quad (9)$$

(b) The contaminant is not able to penetrate the top of the mixing layer of height h, i.e.

$$K_z \frac{\partial C(x,z)}{\partial z} = 0 \quad \text{at} \quad z = h \quad (10)$$

(c) The law of conservation of the flux of pollutant can be written as:

$$uC(0,z) = Q\delta(z-h) \quad (11)$$

where Q is the emission rate and δ (.) is the Dirac delta function

Substituting by Eqs. (7 and 8) into Eq, (5), yields:

$$\frac{\partial C}{\partial x} = \frac{c}{a} m\, z^{m-n-1} \frac{\partial C}{\partial z} + \frac{c}{a} z^{m-n} \frac{\partial^2 C}{\partial z^2} \qquad (12)$$

Using the separation of variables technique:

$$C(x, z) = \varphi(x)\, \psi(z) \qquad (13)$$

which transforms Eq. (12) into two ordinary differential equations?

The first equation is:

$$\frac{1}{\varphi} \frac{d\varphi}{dx} = -\lambda^2 \qquad (14)$$

and its solution has the form:

$$\varphi(x) = A_o e^{-\lambda^2 x} \qquad (15)$$

where, $-\lambda^2$ is a separation constant and A_o is an integration constant.

The second equation is:

$$z^2 \frac{d^2\psi}{dz^2} + m\, z \frac{d\psi}{dz} + \frac{a}{c} \lambda^2 z^{n-m+2} \psi = 0 \qquad (16)$$

On using the transformations

$$t^2 = z^{n-m+2} \qquad (17)$$

and

$$\psi(z) = t^{\mu} G(t) \qquad (18)$$

Eq. (16) becomes as:

$$t^2 \frac{d^2 G}{dt^2} + t \frac{dG}{dt} + (\eta^2 t^2 - \mu^2) G = 0 \qquad (19)$$

which is the Bessel equation of order μ where,

$$\mu = \frac{1-m}{n-m+2}\,; \qquad \eta = \frac{\sqrt{a/c}\ \lambda}{(n-m+2)/2} \qquad \text{and} \quad n-m+2 \neq 0 \qquad (20)$$

The general solution of Eq, (19) is given by:

$$G(t) = A_1 J_\mu(\eta t) + A_2 J_{-\mu}(\eta t) \tag{21}$$

where J_μ and $J_{-\mu}$ are Bessel's function of the first kind and A_1 and A_2 are arbitrary constants.

Returning to the original variables, the general solution of Eq.(16) can be written as:

$$\psi(z) = z^{\frac{1-m}{2}} \left[A_1 J_\mu(\eta z^{\frac{1-m}{2\mu}}) + A_2 J_{-\mu}(\eta z^{\frac{1-m}{2\mu}}) \right] \tag{22}$$

Applying the boundary condition Eq.(9) at z = 0 on the above equation, yields $A_1 = 0$, and Eq. (22) becomes as:

$$\psi(z) = A_2\, z^{\frac{1-m}{2}} J_{-\mu}(\eta z^{\frac{1-m}{2\mu}}) \tag{23}$$

Application of the boundary condition Eq.(10) at z = h on Eq.(23) yields:

$$J_{-\mu+1}(\eta h^{(n-m+2)/2}) = 0 \tag{24}$$

which can be written as:

$$J_{-\mu+1}(A\lambda\, h^{(n-m+2)/2}) = 0, \qquad A = \frac{2\sqrt{a/c}}{n-m+2} \tag{25}$$

On putting $\lambda = \lambda_j$, (j = 1,2,......), one gets:

$$J_{-\mu+1}(A\lambda_j\, h^{(n-m+2)/2}) = 0 \tag{26}$$

So, the values of λ_j can be determined from the zeroes of Eq. (26)

The general solution of Eq. (5) can be written as:

$$C(x,z) = B\left[z^{\frac{1-m}{2}} J_{-\mu}(\eta z^{\frac{1-m}{2\mu}}) \right] e^{-\lambda^2 x} \tag{27}$$

Application of the boundary condition Eq. (11) on Eq. (27) and by using the following integration (Gradshteyn and Ryzhik, 2007)

$$\int_0^\infty x^\beta J_\nu(bx)dx = 2^\beta b^{-\beta-1} \frac{\Gamma\{(1+\nu+\beta)/2\}}{\Gamma\{(1+\nu-\beta)/2\}} \qquad [-\mathrm{Re}\,\nu - 1 \prec \mathrm{Re}\,\beta \prec 0.5,\ \ b \succ 0] \tag{28}$$

gives:

$$B = \frac{Q}{ah^{(n+(1-m)/2)}} \left[\frac{\mu}{1-m} \left(\frac{2}{\eta}\right)^{\beta+1} \frac{\Gamma\{(1-\mu+\beta)/2\}}{\Gamma\{(1-\mu-\beta)/2\}} \right]^{-1} \tag{29}$$

where Γ is the gamma function and

$$\beta = \frac{2\mu}{1-m} - 1 \tag{30}$$

The general solution of Eq. (3) takes the form:

$$C(x,y,z) = \frac{QB_1}{\sqrt{2\pi}\,\sigma_y\, ah^{(n+(1-m)/2)}} z^{\frac{1-m}{2}} J_{-\mu}(A\lambda\, z^{\frac{1-m}{2\mu}})\, e^{-\lambda^2 x}\, e^{-\frac{y^2}{2\sigma_y^2}} \tag{31}$$

where,

$$B_1 = \left[\frac{\mu}{1-m}\left(\frac{2}{A\lambda}\right)^{\beta+1} \frac{\Gamma\{(1-\mu+\beta)/2\}}{\Gamma\{(1-\mu-\beta)/2\}}\right]^{-1} \tag{32}$$

Plume depletion by radioactive decay

The radioactive decay will reduce the concentrations of a short-lived radionuclide as it disperses downwind; the modified concentration can be obtained by multiplying the initial source strength, Q, by the following depletion factor (IAEA, 1982):

$$F_r = e^{-\lambda_r \frac{x}{u}} \tag{33}$$

where, λ_r is the radioactive decay constant of the radionuclide with the units of reciprocal time, and represents the fraction of the radionuclides that decay per unit time.

Description of statistical measures

The commonly statistical measures used for model evaluation were chosen for the present study are (Fariba and Hanadi, 2004 and Davidson et al., 2005):

(1) The normalized mean square error is defined as

$$NMSE = \overline{(C_p - C_o)^2} / \overline{C_p} \times \overline{C_o} \tag{34}$$

where C_o and C_p are the observed and predicted concentrations, respectively. It gives information on the overall deviations between the predicted and observed concentrations. A good model should have NMSE value close to zero.

(2) The correlation coefficient

$$R = \overline{(C_o - \overline{C}_o)(C_p - \overline{C}_p)} / \sigma_o \sigma_p \tag{35}$$

where σ_o and σ_p are the standard deviations of the observed and predicted concentrations, respectively. The value of R lies between 0 and 1 and for good performance of a model it should be close to unity.

(3) The fractional bias is given by

$$FB = 2(\overline{C}_o - \overline{C}_p)/(\overline{C}_o + \overline{C}_p) \quad (36)$$

This provides information on the tendency of the model to overestimate or underestimate the observed concentrations. It has a value of zero for an ideal model and varies between -2 and 2. The model over predicts if FB < 0.

(4) Factor of two and factor of five:

$$FAC2 = \text{fraction of data (\%) for which } 0.5 \le C_p/C_o \le 2 \quad (37)$$

$$FAC5 = \text{fraction of data (\%) for which } 0.2 \le C_p/C_o \le 5 \quad (38)$$

The value of FAC2 and FAC5 should be close to unity for good model performance.

3. RESULTS AND DISCUSSION

The resulting analytical solution is used to calculate the concentration of Iodine-131 (I-131) emitted from a Research Reactor. The data used was obtained from the experiments conducted to collect air samples around the Reactor under neutral and stable conditions. The samples were collected at a height of 0.7 m above the ground. The emissions were released from a stack of height 27 m.. The decay constant λr of I-131 has the value 9.95×10^{-7} per second. The roughness length of the area around the Reactor was 0.6 m (Khaled, 2009).

The meteorological conditions and the observed concentrations during the experiments are taken from Khaled, (2009) and presented in Tables 1, 3 and 4. The values of the lateral dispersion parameter σ_y were computed using the Briggs formulae in urban conditions, see Table 2.

Table 1. Summary of meteorological conditions during the experiments (Khaled, 2009).

Exp.	u_{10} (m/s)	$\Delta T/\Delta z$ ($^oC/100$)	Atmospheric stability	L (m)	u_* (m/s)	u_{27} (m/s)	mixing height (h) (m)
1	4.8	-0.52	D	∞	0.67	5.80	2680
5	1.9	-0.12	E	55	0.50	3.80	209

Table 2. Formulas recommended by Briggs (1973) for σ_y (x) and σ_z (x); $10^2 < x < 10^4$ m

Atmospheric stability	σ_y (x) (m)	σ_z (x) (m)
D	$0.16x\,(1+0.0004x)^{-1/2}$	$0.14x\,(1+0.0003x)^{-1/2}$
E and F	$0.11x\,(1+0.0004x)^{-1/2}$	$0.08x\,(1+0.00015x)^{-1/2}$

Table 3. Observed and predicted concentrations of I-131 in stable condition

distance (m)	Observed conc. (Bq/m^3)	Predicted conc. (Bq/m^3)
100	0.25	0.09
110	0.26	0.08
120	0.28	0.07
130	0.28	0.07
140	0.27	0.06
150	0.26	0.06
160	0.25	0.06
170	0.21	0.05
180	0.19	0.05
190	0.16	0.05
200	0.11	0.04
300	0.04	0.03
400	0.01	0.02

The concentrations of Iodine I-131 below the plume centerline and at a sample height C (x, 0, 0.7 m) in Bq./ m^3 were calculated in neutral and stable atmosphere by using the new model Eq. (31). The results are presented in Tables (3 and 4). The comparisons between the measured and predicted concentrations of I-131 in stable and neutral cases are represented graphically as in Figs. (1 and 2).

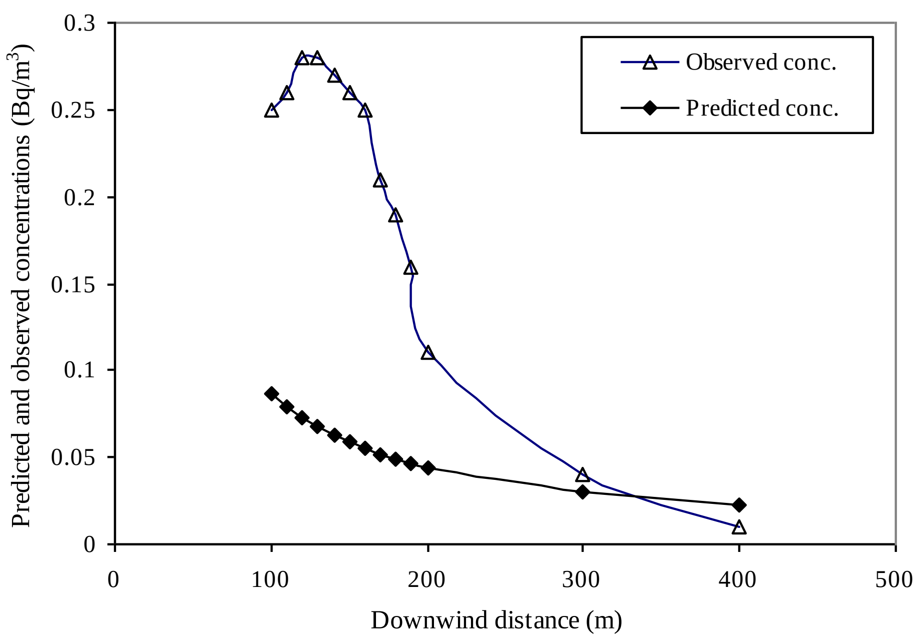

Fig. 1. Comparison between the predicted and observed I-131 concentrations below the plume centerline in stable case.

Table 4. Observed and predicted concentrations of I-131 in neutral condition

distance (m)	Observed conc. (Bq/m^3)	Predicted conc. (Bq/m^3)
100	4.1	6.12
110	3.8	5.58
120	3.8	5.12
130	3.7	4.74
140	3.4	4.41
150	3.2	4.12
160	3.1	3.87
170	3	3.65
180	2.9	3.45
190	2.7	3.28
200	2.4	3.12
300	1.4	2.12
400	0.5	1.62

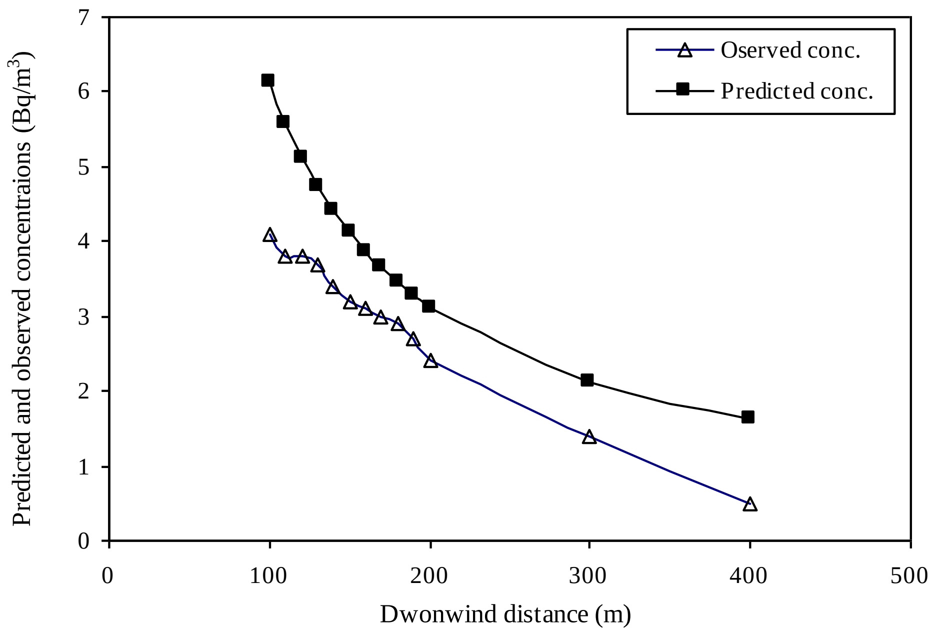

FIg.2. Comparison between the predicted and observed I-131 concentrations below the plume centerline in neutral case.

A scatter diagram between the predicted concentrations by the new model and the corresponding observations under stable and neutral cases is shown in Figs. (3 and 4), respectively.

To evaluate the performance of the new model statistical analysis is made on the observed and predicted concentrations under stable and neutral conditions. Table 5 shows the results of the statistical analysis has been made to evaluate the performance of the present model.

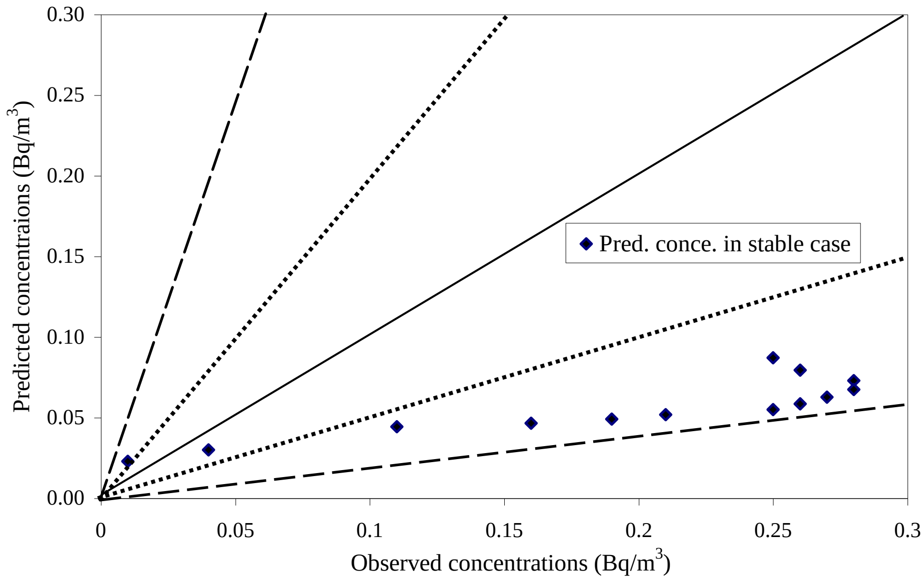

Fig. 3. Scatter diagram of observed and predicted concentraions by the new model in stable case. Dotted lines indicate a factor of two, dashed lines a factor of five, solid line is the one-to one line.

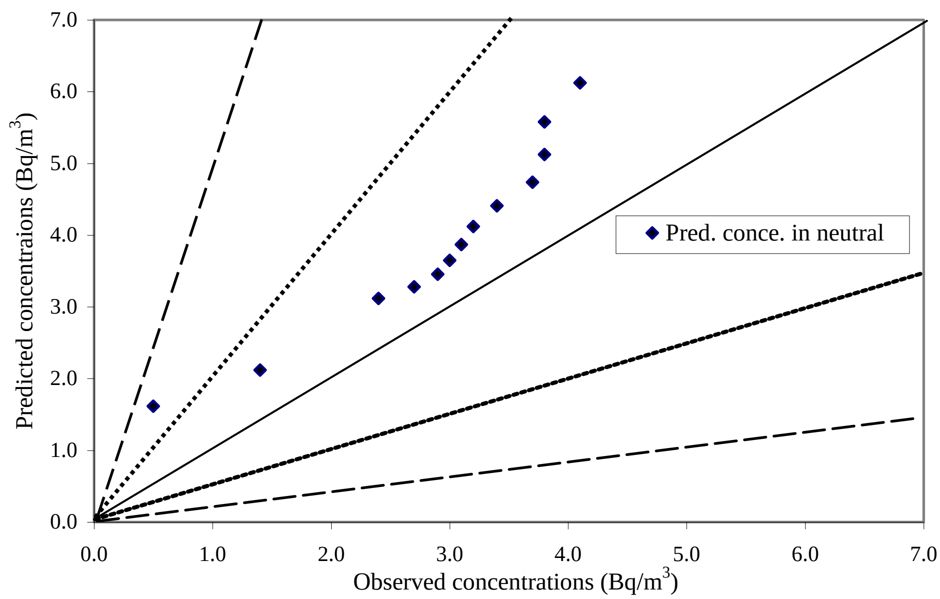

Fig. 4. Scatter diagram of observed and predicted concentrations by the new model in neutral case. Dotted lines indicate a factor of two, dashed lines a factor of five, solid line is one- to -one line.

Table 5. Statistical evaluation of the new model performance in neutral and stable conditions.

stability	R	NMSE	FB	FAC2	FAC5
E	0.81	2.29	1.12	0.08	1.00
D	0.88	0.11	-0.30	0.92	1.00

Tables (3 and 4) and Figs (1 and 2) show a very good agreement between the measured and predicted concentrations by the new model in neutral case and a less agreement in stable case.

Figures (3 and 4) and Table 5 reveal that the model over predicts the observed concentrations in neutral case and under predicts in stable case.

The statistical measures in Table 5 point out that a very good agreement is obtained between concentrations observed and predicted by the new model in neutral conditions, with NMSE and FB values nearest zero, R (0.88), 92% of the predicted concentrations within the factor of two and all the predicted values within the factor of five. In stable atmosphere the statistical indices indicate a less agreement between observed and predicted values.

4. SUMMARY AND CONCLUSIONS

An analytical solution of the three dimensional advection- diffusion equation has been obtained where, the vertical eddy diffusivity and the wind speed are taken to be dependent on the vertical height z. The solution is based on the assumption that the concentration distribution of pollutants in the crosswind direction has a Gaussian shape. The resulting solution have been applied to calculate the concentration of I-131 using data collected from the diffusion experiments conducted around a Research Reactor. Statistical analysis was performed on the observed and predicted concentrations to evaluate the performance of the derived models. The results of this study have been discussed and presented in tables and illustrative figures. The statistical measures depict that the new model presents a better performance in neutral case.

FUTURE ISSUES

The advection diffusion equation is solved using Laplace transform and separation of variables methods to evaluate crosswind integrated of pollutant concentration per emission rate in three dimensions with constant wind speed and eddy diffusivity under steady state.

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