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Calculation of Iodine-131 Concentration inNeutral and Stable ConditionsUsing Three - Dimensions Advection-DiffusionEquation

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ABSTRACT

A new model was proposedby using separation of variables to solve the diffusion equation in three dimensions, considering that the eddy diffusivity depends on the vertical height z. Comparisons between calculated, observed and previous data in neutral and stable conditions were carried out. Model performances were evaluated using observed data and another model. Results show that both models performance well in calculating activity concentrations with different degree of accuracy. From the statistical evaluations in neutral and stable conditions, one finds that the two models are inside a factor of two with observed data. Regarding NMSE and FB, the correlation for the present model is well with observed data than the previous work. We can conclude that our model shows more accuracy in neutral and stable cases than the previous work.

Keywords: Advection-Diffusion Equation, Separation of Variables, Eddy Diffusivity, dispersion models

1- INTRODUCTION

There is a wide variety of air dispersion models, ranging from the conceptuallyand computationally simple to very demand models. In general, dispersion models arepotentially more accurate as the models become more fundamental and hencecomputationally more intensive. It is important to note that the atmosphere is turbulent and chaotic. Consequently,pollutant concentrations are not constant even when the source and the weather areconstant. A dispersion model can be considered as successful when the average concentration predicted by the model is close to and within a factor of 2 of the actual average concentration and also when a very similar distribution between the observed and predicted concentrations isobtained. The dispersion models based on the analytical solution of the advection-diffusion equation bears significant importance since all the influencing parameters are expressed in themathematically closed form by Alex (2014), Thongmoon et al. (2007) and Atul Kumar et al. (2012). The most general of these solutions is three dimensional, valid for both surface and elevated releases, and allows the velocity and vertical eddydiffusivity profiles to vary independently as power-law functions by Chen and Liu (2011), Marrouf et al. (2013) and Sharan and Modani (2006).

The analytical solution of the atmospheric diffusion equation contains different shapes depending on Gaussian and non-Gaussian solutions. Advection-diffusion equation is one of the most important partial differential equations and observed in a wide range of different applications. The advection-diffusion equation is solved in three dimensions space (x,y,z) using separation of variables technique to evaluate pollutant concentration per emission rate, taking eddy diffusivities of pollutants and mean wind speed in neutral case by Liu and Hildemann (1996), Singh and Tanaka (2000), Kumar Pramod (2010) and Khaled Essa and Sawsan Elsaid (2015).

In this paper, we derived 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 aGaussian 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 under neutral and stable conditions.Statistical measurementshad been utilized in the comparison between the computedand measured concentrations. The results of this study are discussed and presented in tables and illustrative figures.

2- MATHEMATICAL MODEL

The partial differential equation describing advection-dispersion can be written as:

$$u\frac{\partial c(x,y,z)}{\partial x}=\frac{\partial}{\partial y}(k_y\frac{\partial c(x,y)}{\partial y})+\frac{\partial}{\partial z}(k_z\frac{\partial c(x,y)}{\partial z})(1)$$

The eddy diffusivity “k” and wind speed profile “u” must be taken into consideration dependson the height variable (z)for thesolution of the advection–diffusion equation. Therefore, to solve this kind of problem by aseparation technique, a stepwise approximation of these coefficientsmust be performed. The height z_i of the Planetary boundary layer (PBL) was discrete into N sub-intervals in such manner that inside each sub-region, k (z) and u(z) assume respectively the following average valuesAsan (2015) and Buske et al. (2012):

$$k_n = \frac{1}{z_{n+1} - z_n} \int_{z_n}^{z_{n+1}} k_n(z)dz$$

$$u_n = \frac{1}{z_{n+1} - z_n} \int_{z_n}^{z_{n+1}} u(z)dz$$

For n=1: N.

Then equation (1) becomes:

$$u_n \frac{\partial c_n(x,y,z)}{\partial x} = k_n \frac{\partial^2 c_n(x,y)}{\partial y^2} + k_n \frac{\partial^2 c_n(x,z)}{\partial z^2} \quad (2)$$

Then the general solutionof equation (2) can be written in the form:

$$c_n(x, y, z) = \frac{Q}{u} c_n(x, y) c_n(x, z) \qquad (3)$$

To solve equation(2) can be written in two parts:

The first part in the form:

$$u_n \frac{\partial c_n(x,y)}{\partial x} = k_n \frac{\partial^2 c_n(x,y)}{\partial y^2} \quad (4)$$

Under the boundary conditions in the form:

(i) $c_n(0, y) = \delta(y)$

$(ii) c_n(x, y) = 0 \text{at} x \to \infty, y \longrightarrow \pm\infty$

$(iii) \frac{\partial c_n(x,y)}{\partial y} = 0$ at y=0, L_y

where L_y is large constant value in they-direction. By using separation of variables then:

c_n(x,y)=X(x)Y(y) (5)

Substituting from equation (5) into equation (4) one gets:

$$uY(y) \frac{dX(x)}{\partial x} = k_n X(x) \frac{d^2 Y(y)}{\partial y^2} \quad (6)$$

Dividing equation (6) on X(x) Y(y) k_n one can get:

$$\frac{1}{X(x)}\frac{u_n}{k_n}\frac{dX(x)}{dx} = \frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2} = -\lambda^2 (7)$$

whereλ^2 is constant.

$$\frac{1}{X(x)}\frac{u_n}{k_n}\frac{dX(x)}{dx} = -\lambda^2 (8)$$

$$\frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2} = -\lambda^2 \ (9)$$

To solve equation (8) one can get:

$\frac{dX(x)}{X(x)} = -\frac{k_n}{u_n}\lambda^2 dx$ (10)Integrating equation (10) with respect to "x"

then:

$$\int \frac{dX(x)}{X(x)} = -\frac{k_n(y)}{u_n}\lambda^2 \int dx$$

$$\ln X(x) = -\frac{k_n(y)}{u_n}\lambda^2 x + \ln c_1 \ (11)$$

wherec_1 is the constant of integration.

$$X(x) = c_1\, e^{-\frac{\lambda^2 k_n}{u_n}x} (12)$$

Equation (9) becomes:

$$\frac{d^2Y(y)}{dy^2} + \lambda^2 Y(y) = 0 \ (13)$$

Then the solution of the equation (13) can be written as:

$$Y(y) = c_2\left(e^{-\lambda y}\right) + c_3\left(e^{\lambda y}\right) (14)$$

By using the boundary equation (ii)find c_3=0

$$Y(y) = c_2\left(e^{-\lambda y}\right) (15)$$

Substituting from equations (12) ,(15) in equation (5), one gets:

$$c_n(x,y) = c_4 e^{-\frac{\lambda^2 k_n}{u_n}x} e^{-\lambda y} (16)$$

Where $c_4=c_1c_2$, Applying the boundary condition (i) such that:

$$c_4 e^{-\lambda y} = \delta(y)$$

$$\therefore c_4 = 1$$

Then the equation (16) can be written as:

$$c_n(x,y) = e^{-\frac{\lambda^2 k_n}{u_n}x} e^{-\lambda y} \quad (17)$$

Applying the boundary equation (iii) one can get:

$$\frac{\partial c_n(x,y)}{\partial y} = -\lambda e^{-\frac{\lambda^2 k_n}{u_n}x} e^{-\lambda y} \quad (18)$$

$$\therefore \cos \lambda y = 0$$

$$\lambda L_y = \frac{n\pi}{2}$$

$$\lambda = \frac{n\pi}{2L_y}$$

Then equation (17) can be written as:

$$\boldsymbol{c_n(x,y) = e^{-\frac{n^2\pi^2 k_n}{4u_n L_y{}^2}x} e^{-\frac{n\pi}{2L_y}y}} \quad (19)$$

- <u>The second part in the form</u>:

$$u\frac{\partial c_n(x,z)}{\partial x} = k_n \frac{\partial^2 c_n(x,z)}{\partial z^2} \quad (20)$$

Under the boundary equation in the form:

(a) $c_n(0,z) = \delta(z - h_s)$ where h_s is the stack height

$(b)\frac{\partial c_n(x,z)}{\partial z} = 0$at z=0,h

where h is mixing height. By using the separation of variables then:

$$c_n(x,z)=X(x)Z(z) \quad (21)$$

$$u\, Z(z)\frac{dX(x)}{\partial x} = k_n X(x)\frac{d^2 Z(z)}{\partial z^2} \quad (22)$$

Dividing equation (22) on X(x) Z(z) k, one can get:

$$\frac{1}{X(x)}\frac{u}{k_n}\frac{dX(x)}{dx} = \frac{1}{Z(z)}\frac{d^2Z(z)}{dz^2} = -\beta^2 (23)$$

whereβ^2 is a constant, then equation (23) becomes:

$$\frac{1}{X(x)}\frac{u}{k_n}\frac{dX(x)}{dx} = -\beta^2 (24)$$

$$\frac{1}{Z(z)}\frac{d^2Z(z)}{dz^2} = -\beta^2 (25)$$

To solve equation (24) one can get:

$$\frac{dX(x)}{X(x)} = -\frac{k_n}{u}\beta^2 dx \qquad (26)$$

Integrating equation (26) with respect to x:

$$\int \frac{dX(x)}{X(x)} = -\frac{k_n}{u}\beta^2 \int dx$$

Then the solution can be written as:

$$X(x) = c_5 e^{-\frac{\beta^2 k_n}{u}x} (27)$$

To solve equation (25) one can get:

$$\frac{d^2Z(z)}{dz^2} = -\beta^2 Z(z) \; (28)$$

$$\frac{d^2Z(z)}{dz^2} + \beta^2 Z(z) = 0 \qquad (29)$$

Then the solution of the equation (29) can be written as:

$$Z(z) = c_6 \cos(\beta z) + c_7 \sin(\beta z) (30)$$

Then one used condition (b), one gets:

$$\frac{\partial Z(z)}{\partial z} = -\beta c_6 \sin(\beta z) + \beta c_7 \cos(\beta z)$$

$$\therefore c_7 = 0$$

$Z(z) = c_6 \cos(\beta z)$ (31)By using the equation (27) and equation (31) one can get:

$c_n(x,z) = c_8 e^{-\frac{\beta^2 k_n}{u}x} \cos(\beta z)$ (32)

where $c_8 = c_5\ c_6$

Applying the boundary condition (a) then:

$$c_8 \cos(\beta z) = \delta(z - h_s)$$

$$\therefore c_8 = \frac{1}{\cos(\beta h_s)}$$

Substituting in equation (32), one can get:

$c_n(x,z) = \frac{1}{\cos(\beta h_s)} e^{-\frac{\beta^2 k_n}{u}x} \cos(\beta z)$(33)

Applying the boundary condition (b)then:

$\frac{\partial c_n(x,z)}{\partial z} = \frac{-\beta}{\cos(\beta h_s)} e^{-\frac{\beta^2 k_n}{u}x} \sin(\beta z) = 0$ (34)Equation (34) at z=h can be written as:

$$\frac{-\beta}{\cos(\beta h_s)} e^{-\frac{\beta^2 k_n}{u}x} \sin(\beta h) = 0$$

$$\therefore \sin(\beta h) = 0$$

$$\therefore \beta = \frac{n\pi}{h}$$

Substituting in equation (33), one can get:

$c_n(x,z) = \frac{1}{\cos\left(\frac{n\pi}{h} h_s\right)} e^{-\frac{n^2\pi^2 k_n}{uh^2}x} \cos\left(\frac{n\pi}{h} z\right)$ (35)

Substituting from equations (19) and (35) in equation (3),one can get:

$$c_n(x,y,z) = \frac{Q}{u}\left(e^{-\frac{n^2\pi^2 k_n}{4u_n L_y{}^2}x} e^{-\frac{n\pi}{2L_y}y}\right)\left[\frac{1}{\cos\left(\frac{n\pi}{h}h_s\right)} e^{-\frac{n^2\pi^2 k_n}{uh^2}x} \cos\left(\frac{n\pi}{h}z\right)\right] (36)$$

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

$$D = e^{-\beta\frac{x}{u}}$$

whereβ is the radioactive decay constant.Then equation of the concentration (36) can be written as:

$$c_n(x,y,z) = \frac{Q}{u}\left(\boldsymbol{e}^{-\frac{n^2\pi^2k_n}{4u_nLy^2}x}\boldsymbol{e}^{-\frac{n\pi}{2L_y}y}\right)\left[\frac{1}{\cos\left(\frac{n\pi}{h}h_s\right)}e^{-\frac{n^2\pi^2k_n}{uh^2}x}\cos\left(\frac{n\pi}{h}z\right)\right]e^{-\beta\frac{x}{u}}(37)$$

where the eddy diffusivity are taken in the form:

$k_n = k_0u_*\frac{z}{(1+\frac{5z}{l})}$ in stable condition

$k_n = k_0u_*z$in neutral conditionwhere k_0 is the Von- Karman constant (k_0~0.4) and "L" is a Monin-Obukhov length scale.

3- VALIDATION

The resulting analytical solution is used to calculate the concentration of Iodine-131 (I-131). Data used was obtained from the experiments conducted to collect air samples under neutral and stable conditions. 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 of I-131 has the value 9.95x10^{-7} per second. The roughness length of the area was 6 cmby Khaled Essa (2009) and IAEA (1980).The meteorological conditions and the observed concentrations during the experiments are presented in tables 1, 2 and 3.

Table 1. Summary of meteorological conditions during the experiments

Exp.	u_{27}(m/s)	AtmosphericStability	L(m)	u_*(m/s)	Mixing height (m)

1	**5.80**	**D**	∞	**0.67**	**2680**
2	**3.80**	**E**	**55**	**0.50**	**209**

4- RESULTS AND DISCUSSION

Concentrations of Iodine I-131 below the plume centerline and at a sample height C (x, 0, 0.7 m) were calculated in theneutral and stable atmosphere by using the new model Equation (37). The results are presented in tables (2and 3). The comparison between the measured and predicted concentrations of I-131 in stable and neutral cases is represented graphically in Figs. (1 and 2).

Table2. Observed and predicted concentrations of I-131 in stable condition

Distance (m)	Observed (Bq/m^3)	Predicted (Bq/m^3)	Previous (Bq/m^3)
100	0.25	0.22	0.09
110	0.26	0.23	0.08
120	0.28	0.23	0.07
130	0.28	0.22	0.07
140	0.27	0.23	0.06
150	0.26	0.22	0.06
160	0.25	0.22	0.06
170	0.21	0.22	0.05

180	0.19	0.23	0.05
190	0.16	0.16	0.05
200	0.11	0.09	0.04
300	0.04	0.05	0.03
400	0.01	0.02	0.02

Table3. Observed and predicted concentrations of I-131 in neutral condition

Distance (m)	Observed (Bq/m^3)	Predicted (Bq/m^3)	previous (Bq/m^3)
100	4.1	4.04	6.12
110	3.8	3.80	5.58
120	3.8	3.50	5.12
130	3.7	3.40	4.74
140	3.4	3.30	4.41
150	3.2	3.17	4.12
160	3.1	3.06	3.87
170	3	2.97	3.65
180	2.9	2.89	3.45
190	2.7	2.80	3.28
200	2.4	2.70	3.12
300	1.4	2.30	2.12
400	0.5	1.00	1.62

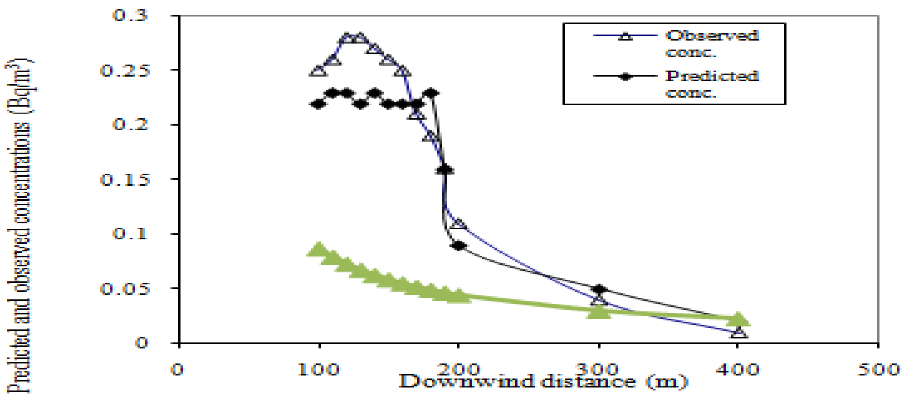

Fig. 1. Comparison between the predicted and observed I-131 concentrations

below the plume centerline in thestable case via downwind distance.

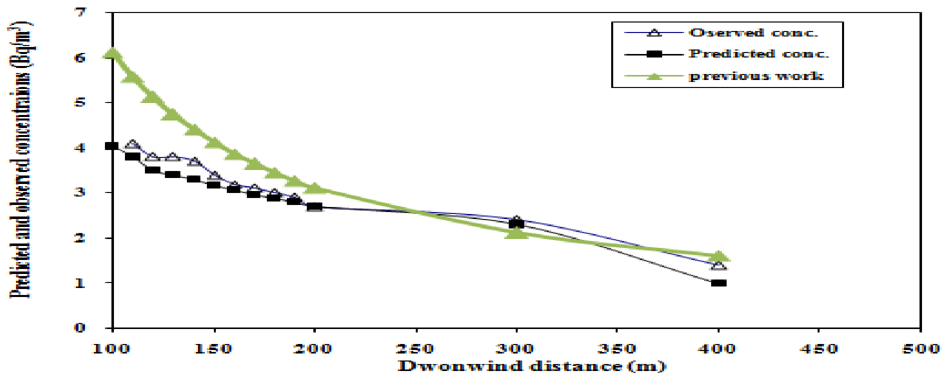

Fig. 2. Comparison between predicted and observed I-131 concentrations

below the plume centerline in theneutralcase via downwind distance.

From tables (2, 3) and figures (1, 2) we can conclude thatthere is good agreement between predicted andobserved concentrations in neutral and stable cases more than the previous work by Essa et al. (2016).

Figures (1& 2) show the predicted concentration with the observed concentration via the downwind distance in stable and neutral case respectively.

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

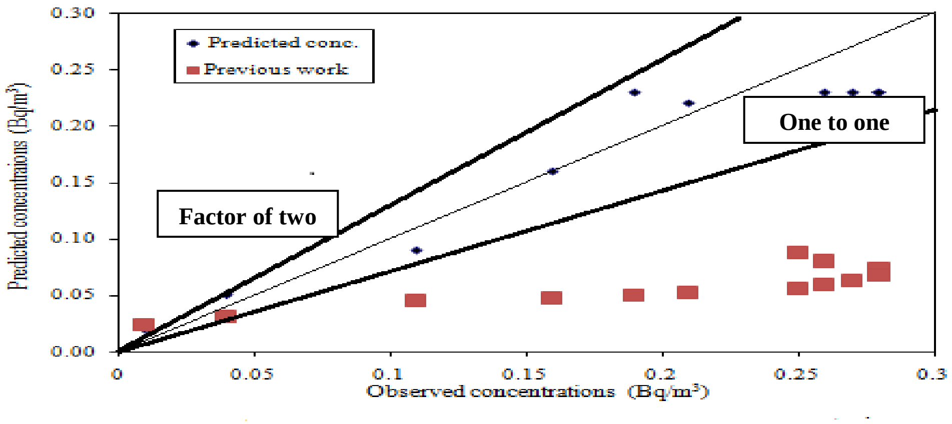

Fig 3. Scatter diagram of observed and predicted concentrations by the new model in stable case.

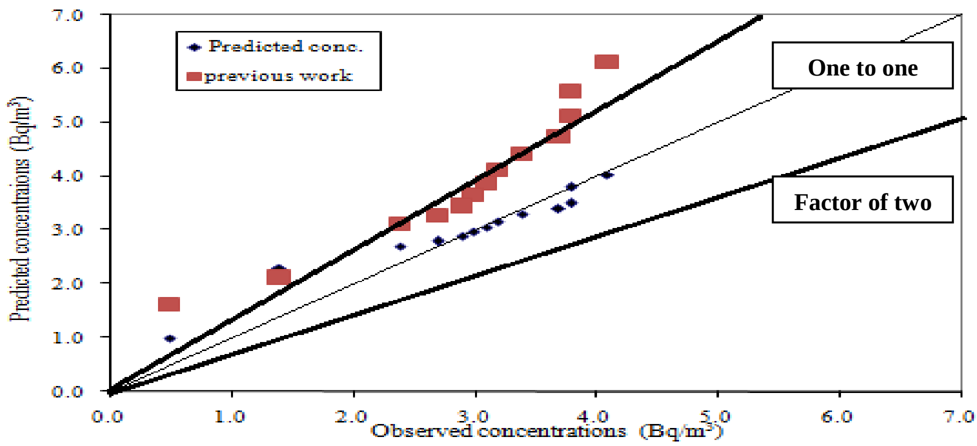

Fig 4. Scatter diagram of observed and predicted concentrations by the new model in neutral case.

4- MODEL EVALUATION STATISTICS

Now, the statistical method is presented and comparison between predicted and observed results as offered by Hanna (1989) [17]. The following standard statistical performance measures that characterize the agreement between prediction (C_p=C_{pred}/Q) and observations (C_o=C_{obs}/Q):

$$\text{Fraction Bias (FB)} = \frac{(\overline{C_o} - \overline{C_p})}{[0.5(\overline{C_o} + \overline{C_p})]}$$

$$\text{Normalized Mean Square Error (NMSE)} = \frac{\overline{(C_p - C_o)^2}}{\overline{(C_p C_o)}}$$

$$\text{Correlation Coefficient (COR)} = \frac{1}{N_m}\sum_{i=1}^{N_m}(C_{pi} - \overline{C_p}) \times \frac{(C_{oi} - \overline{C_o})}{(\sigma_p \sigma_o}$$

$$\text{Factor of Two (FAC2)} = 0.5 \le \frac{C_p}{C_o} \le 2.0$$

where σp and σ_o are the standard deviations of predicted C_p and observed C_o concentration respectively. Here the over bars indicate the average over all measurements. A perfect model would have the following idealized performance: NMSE = FB = 0 and COR= FAC2 = 1.0.

Table 4: Statistical evaluation of thepresent model and previous work in stable condition.

Models (stable condition)	NMSE	FB	COR	FAC2
Present	**0.03**	**0.09**	**0.96**	**1.02**
Previous work *	**0.11**	**-0.30**	**0.88**	**1.00**

*(Essa et al. 2016)

Table 5: Statistical evaluation of thepresent model and previous work in theneutral condition.

Models (neutral condition)	NMSE	FB	COR	FAC2
Present	0.01	-0.02	0.97	1.12
Previous work*	2.29	1.12	0.81	1.00

*(Essa et al. 2016)

From the statistical evaluations in neutral and stable conditions, one finds that the two models are inside a factor of two with observed data. Regarding NMSE and FB, the correlation for the present model is well with observed data than the previous work.

CONCLUSIONS

A new model was proposedby using separation of variables to solve the diffusion equation in three dimensions, considering that the eddy diffusivity depends on the vertical height z. Comparisons between calculated, observed and previous data in neutral and stable conditions were carried out. Model performances were evaluated using observed data and another model. Results show that two calculated models performance well with the observed concentrations with different degree of accuracy. From the statistical evaluations in neutral and stable conditions, one finds that the all models are inside a factor of two with observed data. Regarding NMSE and FB, the correlation for the present model is well with observed data than the previous work. We can conclude that our model shows more accuracy in neutral and stable conditions than the previous work.

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