Evaluation of analytical solution of advection diffusion equation in three dimensions

Khaled S. M. Essa1 | Ahmed M. Mosallem1 | Ahmed S. Shalaby2

1Mathematics and Theoretical Physics Department, NRC, Atomic Energy Authority, Cairo, Egypt
2Department of Physics, Faculty of Science, Beni-Suef University, Beni Suef, Egypt

Correspondence
Ahmed M. Mosallem, Mathematics and Theoretical Physics Department, NRC, Atomic Energy Authority, Cairo, Egypt.
Email: ahmedmetwally77@hotmail.com

Abstract
Three-dimensional advection–diffusion equation with steady state was evaluated from continuous point source taking the vertical and crosswind eddy diffusivities as power law of vertical height and downwind distance with constant wind speed to get the concentration in three dimensions. Separation of variables technique and Hankel transform were used to calculate this equation. The proposed analytical solution was compared with diffusion experiment of radioactive Iodine-135 ($^{135}$I) in unstable condition at Inshas, Cairo, Egypt. A good agreement achieved between calculated and observed concentration support our proposed model.

KEYWORDS
Hankel transform, radioactive iodine-135, separation of variables technique, unstable conditions

1 | INTRODUCTION

The solution of the atmospheric diffusion equation contains different shapes which depends on Gaussian and non-Gaussian plume models. This equation is one of the most important partial differential equations that had wide range of different applications. The advection–diffusion equation is evaluated in three dimensions space (x, y, z) using separation of variables technique to estimate pollutant concentration per emission rate, taking eddy diffusivities of pollutants and mean wind speed in neutral case as were given before by Lin and Hildemann (1996), Singh and Tanaka (2000), Kumar and Sharan (2010), and Essa et al. (2015).

Gaussian models based on solutions of advection–diffusion equation derived by Hanna Steven et al. (1982), Berland (1991), Essa et al. (2007), and Essa and Fouad (2011) assuming that the eddy diffusivity and wind speed are constants. Demuth (1978), Tirabassi (1989), and Lin and Hildemann (1996) solved advection–diffusion equation by assuming that an eddy diffusivity and wind speed are given as power law. Sharan and Manish (2006) used the separation of variables technique to solve the advection–diffusion equation taking eddy diffusivity as a linear function in downwind distance and wind speed as a power law. Marrouf et al. (2015) solved the advection–diffusion equation taking eddy diffusivity and wind speed as power law. Sharan and Kumar (2009) and Goyal and Kumar (2011) got on analytical solution of two-dimensional advection–diffusion equation using separation of variables technique, taking the vertical eddy diffusivity as a power law of vertical height and downwind distance, also taking the wind speed as a power law profile.

Essa et al. (2019a) got a normalized crosswind integrated concentration by solving the steady state three-dimensional advection–diffusion equation using Fourier...
transform taking vertical eddy diffusivity as a linear function of downwind distance and constant wind speed. Also, Essa et al. (2019b) solved the same problem by assuming that the vertical eddy diffusivity is a linear function of vertical height as well as a power law. Semi-analytical model for coupled multispecies advective-dispersive transport subject to rate-limited sorption has been studied by Chen et al. (2011). Aly and Kalla (1999) used Hankel transformation to express the pollutant concentration in terms of a given flux of dust from the ground surface to the atmosphere. Essa et al. (2020) evaluated the advection–diffusion equation with variable vertical eddy diffusivity and wind speed using Hankel transform.

The Hankel transform is an integral transform which expresses any given function \( f(z) \) as the weighted sum of an infinite number of Bessel functions of the first kind \( J_n(sz) \). It is also known as the Fourier-Bessel transform. It uses Bessel functions to transform from one coordinate to another. When we are dealing with problems that show circular symmetry, Hankel transform may be very useful. Because the Hankel transform is the two-dimensional Fourier transform of a circularly symmetric function, it plays an important role in the present calculations. In this paper, we use the Hankel transform and the separation of variables technique to solve the three-dimensional steady-state advection–diffusion equation. Taking the vertical eddy diffusivity as a power law of vertical height and the crosswind eddy diffusivity as a function of downwind distance and constant wind speed to find the concentration in three dimensions. A comparison is done between the proposed solution model and diffusion experiment of radioactive \(^{138}\)I in unstable condition at Inhas, Cairo, Egypt. The proposed model shows a well agreement with the observed concentrations.

2 | MATHEMATICAL TREATMENT

The advection–diffusion equation can be written as:

\[
\frac{1}{u} \frac{\partial C(x,y,z)}{\partial x} = \frac{\partial}{\partial y} \left( k_y \frac{\partial C(x,y,z)}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial C(x,y,z)}{\partial z} \right)
\]  

(1)

where \( C(x,y,z) \) is the concentration of pollutants (g/m\(^3\)) or (Bq/m\(^3\)), \( k_y \) and \( k_z \) are the crosswind and vertical eddy diffusivities, respectively, wind speed profile “\( u \)” is constant. Taking \( k_y \) as a function of downwind distance and constant wind speed, \( k_z \) as a function of both power law of vertical height and downwind distance to solve the advection–diffusion equation in three dimensions using separation of variable technique as follows: One assumes that:

\[
k_y(x,z) = \beta xu
\]

(2a)

\[
k_z(x,z) = \gamma xz^n, \quad z \neq 0
\]

(2b)

where \( x \) is downwind distance, \( \beta \) and \( \gamma \) are constants which are measured at reference height and “\( n \)” is a parameter depends on stability conditions (Irwin, 1979). Then Equation (1) becomes:

\[
\frac{1}{x} \frac{\partial C}{\partial x} = \beta \frac{\partial^2 C}{\partial y^2} + \gamma \frac{\partial}{\partial z} \left( z^n \frac{\partial C}{\partial z} \right)
\]

(3)

Equation (3) is solved under the boundary conditions as follows:

\[
k_z \frac{\partial C}{\partial z} = 0, \quad \text{at } z = 0, h
\]

(4a)

\[
k_y \frac{\partial C}{\partial y} = 0, \quad \text{at } y = 0, L_y
\]

(4b)

\[
uC(x,y,z) = Q\delta(y)\delta(z - h) \quad \text{at } x = 0
\]

(4c)

\[
C(x,y,z) \rightarrow 0 \quad \text{as } x \rightarrow \infty
\]

(4d)

where \( h \) is the mixing height (m), \( L_y \) is a large distance in the crosswind direction, \( h \) is a stack height, and \( \delta \) is a Dirac delta function. Assuming the general solution of Equation (3) in the form:

\[
C(x,y,z) = \varphi(x,y)\psi(x,z)
\]

(5)

Substituting Equation (5) in Equation (3) and dividing on \( \varphi(x,y)\psi(x,z) \), one can get:

\[
\frac{1}{x} \frac{\partial \varphi}{\partial x} + \frac{1}{x\varphi} \frac{\partial \varphi}{\partial x} = \frac{\beta}{\varphi} \frac{\partial^2 \varphi}{\partial y^2} + \frac{\gamma}{u\psi} \frac{\partial}{\partial z} \left( z^n \frac{\partial \psi}{\partial z} \right)
\]

(6)

subdividing Equation (6) into the following two equations as follows:

\[
\frac{1}{x\varphi} \frac{\partial \varphi}{\partial x} = \frac{\beta}{\varphi} \frac{\partial^2 \varphi}{\partial y^2}
\]

(7a)

\[
\frac{1}{x\varphi} \frac{\partial \varphi}{\partial x} = \frac{\gamma}{u\psi} \frac{\partial}{\partial z} \left( z^n \frac{\partial \psi}{\partial z} \right)
\]

(7b)
2.1 First equation of the model

Equation (7a) can be solved with different methods like separation of variable and generalized integral transform methods (Chen et al., 2019). Here, we use the separation of variable method to solve it by assuming that:

\[ \psi(x,y) = \chi_l(x)\eta_l(y) \]  

(8)

Substituting Equation (8) in Equation (7a) and dividing on \( \chi_l(x)\eta_l(y) \), one gets:

\[ \frac{1}{\chi_l(x)} \frac{\partial \chi_l(x)}{\partial x} - \frac{\beta}{\eta_l(y)} \frac{\partial^2 \eta_l(y)}{\partial y^2} = -\lambda_l^2 \]  

(9a)

where \( \lambda_l^2 \) is a constant of separation. Then we get on the differential equations as follows:

\[ \frac{\partial \chi_l}{\partial x} = -\lambda_l^2 \chi_l \]  

(10a)

\[ \frac{\partial^2 \eta_l(y)}{\partial y^2} = \frac{-\lambda_l^2}{\beta} \eta_l \]  

(10b)

The solution of Equations (10a) and (10b) has the form:

\[ \chi_l(x) = c_1 e^{-\frac{\lambda_l^2}{\beta} x^2} \]  

(11a)

\[ \eta_l(y) = c_2 \cos\left(\frac{\lambda_l y}{\sqrt{\beta}}\right) + c_3 \sin\left(\frac{\lambda_l y}{\sqrt{\beta}}\right) \]  

(11b)

where \( c_1, c_2, \) and \( c_3 \) are constants. Applying the conditions Equation (4b) on Equation (11b) at \( y = 0 \) and \( L_y \), one can get \( c_3 = 0 \) and \( \lambda_l = \frac{i\pi}{L_y} \). The solution of Equation (7) can be written in the form:

\[ \psi(x,y) = \sum_{l=0}^{\infty} \chi_l(x)\eta_l(y) = \sum_{l=0}^{\infty} B_l e^{-\frac{1}{\beta} x^2} \cos\left(\frac{\pi l y}{L_y}\right) \]  

(12)

where \( B_l = c_1 c_2 \), using the boundary condition, Equation (4c) and Equation (5), we find:

\[ \frac{u}{Q} \psi(0,z) = \delta(z-h_s) \]  

(13a)

\[ \psi(0,y) = \delta(y) \]  

(13b)

Applying condition Equation (13b) then: \( B_l = \frac{1}{L_y}, B_0 = \frac{1}{L_y} \).

Then, the solution of Equation (7a) becomes:

\[ \psi(x,y) = \sum_{l=0}^{\infty} \chi_l(x)\eta_l(y) = \frac{1}{L_y} + \sum_{l=1}^{\infty} \frac{2}{L_y} e^{-\frac{1}{\beta} x^2} \cos\left(\frac{\pi l y}{L_y}\right) \]  

(14)

2.2 Second description model

Now Equation (7b) can be rewritten in the form:

\[ z^\gamma \frac{d^2 \psi}{dz^2} + nz^{n-1} \frac{d\psi}{dz} - u \frac{\partial \psi}{\partial x} = 0 \]  

(15)

One takes substitution (Essa et al., 2019) as follows:

\[ \psi(x,z) = \rho^m \omega(x,\rho), \quad \rho = \frac{z^{\frac{1}{2}}}{} \quad \text{and} \quad m = \frac{1-n}{2-n} \]  

(16)

Then, Equation (15) becomes:

\[ \frac{d^2 \omega}{d\rho^2} + \frac{1}{\rho} \frac{d\omega}{d\rho} - \frac{m^2}{\rho^2}\omega - \frac{4u(1-m)^2}{\gamma x} \frac{\partial \omega}{\partial x} = 0 \]  

(17)

The Hankel transform for any given function \( f(z) \) takes the form (Aly and Kalla, 1999):

\[ \mathcal{H}_m \{ f(z) \} = \tilde{f}(s) \equiv \int_0^\infty f(z) J_m(sz) z \, dz \]

Which for:

\[ \Delta_m f(z) \equiv \frac{d^2 f(z)}{dz^2} + \frac{1}{z} \frac{df(z)}{dz} - \left(\frac{m}{z}\right)^2 f(z) \]

Leads to:

\[ \mathcal{H}_m \{ \Delta_m f(z) \} \equiv -s^2 \tilde{f}(s) \]

Where \( J_m(sz) \) represents Bessel function of the first kind of order \( m \). By applying this transformation on Equation (17), one can get:

\[ -s^2 \tilde{\omega}(s) - \frac{4u(1-m)^2}{\gamma x} \frac{\partial \omega}{\partial x} = 0 \]  

(18)

Then:

\[ \tilde{\omega}(x,s) = A \exp \left[ -\frac{\gamma x^2 s^2}{8u(1-m)^2} \right] \]  

(19)
By substituting in Equation (16) and using the condition of Equation (13a), one gets:

$$\bar{\phi}(0, s) = \frac{Qh_s}{2(1-m)u} I_m \left( \frac{sh_s}{\gamma x} \right) = A$$

(20)

then the solution Equation (19) will be:

$$\bar{\phi}(x, s) = \frac{Qh_s}{2(1-m)u} I_m \left( \frac{sh_s}{\gamma x} \right) \exp \left[ -\frac{\gamma x^2 s^2}{8u(1-m)^2} \right]$$

(21)

Taking the inverse Hankel transformation, one gets:

$$\phi(x, \rho) = \frac{Qh_s}{2(1-m)u} \int_0^\infty I_m \left( \frac{sh_s}{\gamma x} \right) \exp \left[ -\frac{2u(1-m)^2 \left( \frac{h_s^2}{\gamma x^2} + \rho^2 \right)}{\gamma x^2} \right]$$

$$\times I_m \left( \frac{4uh (1-m)^2 \left( \frac{h_s^2}{\gamma x^2} + \rho \right)}{\gamma x^2} \right)$$

(22)

where $I_m$ is the modified Bessel function of the first kind of order $m$.

From Equations (16) and (14), Equation (5) becomes:

$$C(x, y, z) = \varphi(x, y) \psi(x, z)$$

$$= \frac{Q(2-n)^3 (h_s)^{2n}}{4\pi x^2} \exp \left[ -\frac{u(1-n)^2 (h_s^{-1-n} + z^{-1-n})}{8\pi x^2} \right]$$

$$\times I_{\frac{2n}{2}} \left( \frac{u(1-n)^2 (h_s)^{\frac{2n}{2}}}{4\pi x^2} \right) \sum_{i=0}^{\infty} B_i e^{-\frac{i x}{L_y}} \cos \left( \frac{i \pi}{L_y} y \right)$$

(23)

Finally, the solution in three dimensions can be written in the form:

$$C(x, y, z) = \varphi(x, y) \psi(x, z)$$

$$= \frac{Q(2-n)^3 (h_s)^{2n}}{4\pi x^2} \exp \left[ -\frac{u(1-n)^2 (h_s^{-1-n} + z^{-1-n})}{8\pi x^2} \right]$$

$$\times I_{\frac{2n}{2}} \left( \frac{u(1-n)^2 (h_s)^{\frac{2n}{2}}}{4\pi x^2} \right) \sum_{i=0}^{\infty} B_i e^{-\frac{i x}{L_y}} \cos \left( \frac{i \pi}{L_y} y \right)$$

(24)

3 RESULTS AND DISCUSSION

The measured diffusion data for the comparison were gathered during nine I-135 isotope tracer experiment in moderate wind conditions with unstable conditions at Egyptian Atomic Energy Authority (EAEA), Nuclear Research Center (NRC), Inshas, located at the northern part of Cairo, Egypt at longitude 31°24’ and latitude 30°17’. During each run, the tracer was released from a source that had a height of 43 m and which was working for 24 h. The air samples were collected during half hour intervals at a height of 0.7 m. We collected air samples in a horizontal distance from 98 to 186 m around the source. The study area is flat, dominated by sandy soil with a poor vegetation cover. The air samples collected were analyzed in the Radiation Protection Department, NRC, EAEA, Cairo, Egypt using a high volume air sampler with 220 V /50 Hz bias (ESSA et al., 2005) and (Essa and El-Otaify, 2008). Meteorological data have been provided by measurements done at 10 and 60 m height. Table 2 gives information about the diffusion tests and the wind vectors. In addition, it contains the mixing height ($h$). We require the knowledge of wind speed, wind direction, source strength, and mixing height. Wind speeds are greater than 3 ms$^{-1}$ most of the time even at 10 m level. Further the variation of the wind direction with time is also visible (Essa and El-Otaify, 2008). Thus in the present study, we have adopted dispersion parameters for urban terrain which are based on power law functions. The analytical expressions depend upon downwind distance, vertical distance, and atmospheric stability. The atmospheric stability has been calculated from the Monin-Obukhov length scale (L$^{-1}$) (GOLDER, 1972) dependent on friction velocity, temperature, and surface heat flux. The values of “n” as a function of air stability are taken from Hanna Steven et al. (1982) and presented in Table 1. The observed concentration of I$^{135}$ isotope and the meteorological data during the experiments are taken from Essa et al. (2019) and presented in Table 2. The predicted concentrations by Equation (24) the plume centerline are also presented in Table 2. A comparison between predicted and observed concentrations of radioactive I$^{135}$ via downwind distance in unstable condition at Inshas is shown in Figure 1, also, the relation between predicted and observed concentration data is shown in Figure 2.

One finds that the predicted model is well agreement with observed concentrations data as shown in Figure 1. Also, the predicted concentrations lie inside a factor of two with the observed concentration data as shown in Figure 2.
The statistical method is presented and comparison between predicted and observed results as offered by (Hanna, 1989) are done. The following standard statistical performance measures and characterizes the agreement between predictions \((C_p = C_{pred})\) and observations \((C_O = C_{Obs})\):

\[
\text{Fraction bias (FB)} = \left( \frac{C_O - C_p}{0.5(C_O + C_p)} \right)
\]

\[
\text{Normalized mean square error (NMSE)} = \frac{(C_O - C_p)^2}{C_p^2 + C_O^2}
\]

\[
\text{Correlation coefficient (COR)} = \frac{\sum_{i=1}^{N_m} (C_{pi} - \bar{C}_p) \times (C_{oi} - \bar{C}_o)}{\sigma_p \sigma_o}
\]

\[
\text{Factor of two (FAC2)} = 0.5 \leq \frac{C_p}{C_O} \leq 2.0
\]

where \(\sigma_p\) and \(\sigma_o\) are the standard deviations of predicted \(C_p\) and observed \(C_o\) concentrations, respectively. Over bars refer to the average over all measurements.

A perfect model must have the following performance: NMSE = FB = 0 and COR = FAC2 = 1.0.

**TABLE 2** Meteorological parameters of nine convective experiments in March to May 2006 and concentrations measured at Inshas in unstable condition and the corresponding values predicted by Equation (24)

| Run | Stability class | “H” mixing height (m) | Wind direction (degree) | “u” wind speed (m/s) | Q (Bq) | Downwind distance (m) | Observed conc. (Bq/m³) | Predicted conc. (Bq/m³) |
|-----|----------------|-----------------------|------------------------|---------------------|-------|-----------------------|------------------------|------------------------|
| 1   | A              | 600.85                | 301.1                  | 4                   | 1,028,571 | 100                  | 0.025                  | 0.0296                 |
| 2   | A              | 801.13                | 278.7                  | 4                   | 1,050,000 | 98                   | 0.037                  | 0.0197                 |
| 3   | B              | 973                   | 190.2                  | 6                   | 42,857.14 | 115                  | 0.091                  | 0.0508                 |
| 4   | C              | 888                   | 197.9                  | 4                   | 471,428.6 | 135                  | 0.197                  | 0.2247                 |
| 5   | A              | 921                   | 181.5                  | 4                   | 492,857.1 | 99                   | 0.272                  | 0.3339                 |
| 6   | D              | 443                   | 347.3                  | 4                   | 514,285.7 | 184                  | 0.188                  | 0.1218                 |
| 7   | C              | 1,271                 | 330.8                  | 4                   | 1,007,143 | 165                  | 0.447                  | 0.4159                 |
| 8   | C              | 1,842                 | 187.6                  | 4                   | 1,043,571 | 134                  | 0.123                  | 0.1500                 |
| 9   | A              | 1,642                 | 141.7                  | 4                   | 1,033,929 | 96                   | 0.032                  | 0.0381                 |

**TABLE 1** Power-law exponent “n” of eddy diffusivity as a function of air stability in urban area

|   | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| n | 0.85 | 0.85 | 0.80 | 0.75 | 0.60 | 0.40 |

**FIGURE 1** Variation of predicted and observed concentration (Bq/m³) of I₁³⁵ via downwind distance

**FIGURE 2** A scatter diagram of the observed and predicted concentrations of I₁³⁵
One can easily see from Table 3 that the statistical technique shows that the predicted model agrees well the observed concentration data on regarding to both NMSE and FB which are near to zero, COR and FAC2 are close to one. The predicted concentration data are achieved about 0.98% from observed concentration data.

### 5 | CONCLUSION

Three-dimensional steady state advection–diffusion equation considering a continuous point source with vertical eddy diffusivity as a power law of vertical height and taking the crosswind eddy diffusivity as a function of downwind distance and constant wind speed, was solved using both of separation of variables technique and Hankel transform.

The results were compared with diffusion experiment of radioactive $^{133}$I in unstable condition at Inshas, Cairo, Egypt. We noticed that the predicted concentration data agree very well with the observed ones. Statistical technique shows that the predicted concentration data lie inside a factor of two with the observed data regarding to NMSE and FB which are near to zero, COR and FAC2 which are close to one. This emphasized the good agreement occurred between the predicted concentration data and observed ones. Also, we conclude that the Hankel transformation method has been successfully used to solve the advection diffusion equation in a simple manner due to its simplicity in its applications.

### AUTHOR CONTRIBUTIONS

**khaled essa:** Conceptualization; formal analysis; methodology; writing-review & editing. **Ahmed Mosallem:** Conceptualization; formal analysis; methodology; writing-review & editing. **Ahmed Shalaby:** Conceptualization; formal analysis; methodology; writing-review & editing.

### ORCID

**Ahmed M. Mosallem** [https://orcid.org/0000-0003-4240-5068](https://orcid.org/0000-0003-4240-5068)

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### TABLE 3

| Model    | NMSE | FB   | COR | FAC2 |
|----------|------|------|-----|------|
| Predicted| 0.06 | 0.02 | 0.96| 0.98 |

|Table 3| Statistical evaluation of present model in unstable condition
|**Model**|**NMSE**|**FB**|**COR**|**FAC2**|
|--------|--------|------|-------|--------|
|Predicted| 0.06   | 0.02 | 0.96  | 0.98   |
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