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THREE-DIMENSIONAL ANALYTICAL SOLUTION OF THE ADVECTION-DIFFUSION EQUATION FOR AIR POLLUTION DISPERSION

M. FARHANE[✉1], O. ALEHYANE[2] and O. SOUHAR[1]

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Abstract

We develop a new analytical solution of a three-dimensional atmospheric pollutant dispersion. The main idea is to subdivide vertically the planetary boundary layer into sub-layers, where the wind speed and eddy diffusivity assume average values for each sub-layer. Basically, the model is assessed and validated using data obtained from the Copenhagen diffusion and Prairie Grass experiments. Our findings show that there is a good agreement between the predicted and observed crosswind-integrated concentrations. Moreover, the calculated statistical indices are within the range of acceptable model performance.

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1. Introduction

Atmospheric pollution is always a serious problem. Regions with high pollutant concentrations have negative effects such as the reduction of respiratory resistance against bacterial and viral infections. Therefore, inhabitants of these regions could be more frequently infected in case of epidemics. Recently, many studies have established that atmospheric pollution is one of the favourable factors that can facilitate the propagation of COVID-19. Furthermore, it was found that breathing polluted air may worsen the effects of COVID-19 and can lead to hospitalization and subsequent death [24]. For these reasons, models for the atmospheric processes of the unstructured

[1]Faculty of Sciences El Jadida, LIMA Laboratory, Department of Mathematics, Chouaib Doukkali University, El Jadida, Morocco; e-mail: farhane.m@ucd.ac.ma, souhar.o@ucd.ac.ma
[2]Faculty of Sciences El Jadida, MF Laboratory, Department of Mathematics, Chouaib Doukkali University, El Jadida, Morocco; e-mail: alehyane.o@ucd.ac.ma

temporal and spatial variability of pollutants have been developed and discussed in the literature [5, 12, 14, 16, 19, 22, 23]. Unfortunately, all of these explicit models were obtained only for particular or simplified formulations of the wind speed profile and eddy diffusivity of the three-dimensional parabolic second-order advection–diffusion equation. These simplifications will limit the analysis of the results, since the wind speed profile and eddy diffusivity are the most important factors in the transport and diffusion of contaminants in the air.

The main objective of this work is to overcome these limitations. The idea is to divide the planetary boundary layer (PBL) into a multi-layer domain, such that for each sub-layer, the eddy diffusivity and wind speed assume average values. The analytical solution of the advection–diffusion equation is obtained by using the Fourier transform and the technique of separation of variables that leads to the Sturm–Liouville problem [2]. Finally, to better approach the dominant parameters of the dispersion of pollutants, the following parameterizations are adopted:

(i) the Deaves and Harris wind speed profile [7];
(ii) the vertical eddy diffusivity coefficient is assumed to be an explicit function of both downwind distance and vertical height which are expressed under convective conditions [8];
(iii) the lateral eddy diffusivity coefficient as a function of both downwind distance and vertical height [3, 14].

We begin our paper with a general formulation of the atmospheric dispersion of pollutants in the atmospheric boundary layer as described in Section 2. Then we explore the explicit solution in Section 3. Discussion and numerical results are presented in Section 4 and a conclusion is given in the last section.

2. General problem formulation

The turbulent dispersion of pollutants in the PBL is governed by the advection–diffusion equation

$$\frac{\partial C}{\partial t} + \nabla.(\mathbf{U_w}\, C) = \nabla.(D\,\nabla C) + S, \tag{2.1}$$

where $\mathbf{U_w} = (U, V, W)^T$ is the wind speed vector (m/s) representing the components U, V and W in the east-west, north-south and vertical directions, respectively; D is the molecular diffusion coefficient; S is the source term; and ∇ is the gradient operator.

By use of the time average and fluctuation values, $U = u + u'$, $V = v + v'$, $W = w + w'$ and $C = c + c'$, the wind speed vector $\mathbf{U_w}$ is expressed as

$$\mathbf{U_w} = \overline{\mathbf{U_w}} + \mathbf{U_w}' \quad \text{with} \quad \overline{\mathbf{U_w}} = (u, v, w)^T \quad \text{and} \quad \mathbf{U_w}' = (u', v', w')^T.$$

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The application of the Reynolds averaging rules to the vertical mass flow, $\mathbf{U_w}\ C$, leads to [6]

$$\overline{\mathbf{U_w}\ C} = \overline{\mathbf{U_w}}\ c + \overline{\mathbf{U_w}'\ c'} \quad \text{with} \quad \overline{\mathbf{U_w}'\ c'} = (\overline{u'c'}, \overline{v'c'}, \overline{w'c'})^T. \tag{2.2}$$

It turns out that turbulent diffusion can be described with Fick's laws of diffusion as follows [22]:

$$\overline{u'c'} = -K_x \frac{\partial c}{\partial x}, \quad \overline{v'c'} = -K_y \frac{\partial c}{\partial y}, \quad \overline{w'c'} = -K_z \frac{\partial c}{\partial z},$$

where K_x, K_y and K_z are the eddy diffusivity components along the x-, y- and z-directions, respectively.

Note that in a turbulent boundary layer where advection is occurring, K will be larger than D and eddy diffusion will dominate solute transport. In this case, the molecular diffusion coefficient $\nabla.(D\ \nabla C)$ is then to be replaced by an eddy or turbulent diffusivity. The source term could be eliminated from equation (2.1), and should be added to the boundary conditions as a delta function. At the point $(0, 0, H_s)$, there is a source rejecting the pollutant with a continuous flow Q,

$$u\ c(0, y, z) = Q\delta(y)\delta(z - H_s),$$

where H_s is the source height. By application of the Reynolds averaging and the divergence operator to equation (2.2), equation (2.1) may be written as

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}\overline{u'c'} - \frac{\partial}{\partial y}\overline{v'c'} - \frac{\partial}{\partial z}\overline{w'c'} - \overline{U_w}.\nabla c. \tag{2.3}$$

In the remainder of this paper, the following assumptions are considered:

(a) the steady state condition (that is, $\partial c/\partial t = 0$);
(b) the two terms $v(\partial c/\partial y)$ and $w(\partial c/\partial z)$ are neglected since the x-axis coincides with the wind flow average, therefore the wind velocity components w and v are less important; and
(c) the turbulent diffusion in the direction of the mean wind is neglected compared to the advection transport mechanism, that is,

$$u\frac{\partial c}{\partial x} >> \frac{\partial}{\partial x}\left(K_x \frac{\partial c}{\partial x}\right).$$

These assumptions lead to the steady-state advection–diffusion equation defined as $0 < x < L_x$, $-L_y < y < L_y$ and $0 < z < H_{\text{mix}}$,

$$u(z)\frac{\partial c}{\partial x} = \frac{\partial}{\partial y}\left(K_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right),$$

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which is subject to the boundary conditions:

$$\begin{aligned} &\lim_{L_y \longrightarrow \infty} K_y(x,z)\,\frac{\partial c}{\partial y} = 0, \quad K_z(x,z)\,\frac{\partial c}{\partial z} = 0 \quad \text{at } z = z_0, \quad \text{and} \\ &K_z(x,z)\,\frac{\partial c}{\partial z} = 0 \quad \text{at } z = H_{\text{mix}}, \end{aligned} \tag{2.4}$$

where z_0 is the surface roughness length and H_{mix} is the PBL height.

We consider that the eddy diffusivities have the following separable formulations:

$$K_y(x,z) = \zeta_y(x)\, u(z), \tag{2.5}$$

$$K_z(x,z) = \xi(x)\, \varphi_z(z). \tag{2.6}$$

We vertically divide the PBL into H intervals, such that for each one, the eddy diffusivity and wind speed assume average values. For $h = 1, \ldots, H$,

$$u_h = \frac{1}{z_h - z_{h-1}} \int_{z_{h-1}}^{z_h} u(s)\, ds, \tag{2.7}$$

$$\varphi_{z_h} = \frac{1}{z_h - z_{h-1}} \int_{z_{h-1}}^{z_h} \varphi_z(s)\, ds. \tag{2.8}$$

Using the formulations of K_y and K_z in equations (2.5) and (2.6), equation (2.3) can be written as

$$u_h \frac{\partial c_h}{\partial x} = \zeta_y(x)\, u_h \frac{\partial^2 c_h}{\partial y^2} + \xi(x)\, \varphi_{z_h} \frac{\partial^2 c_h}{\partial z^2} \tag{2.9}$$

with u_h and φ_{z_h} (given by equations (2.7) and (2.8)) as constants. Equation (2.9) is subject to the first boundary conditions of equation (2.4) on the one hand, and on the other hand, the continuity of both the concentration and the flux at the interface level is applied. For $h \in \{2, \ldots, H\}$,

$$\begin{cases} \varphi_{z_1} \dfrac{\partial c_1(x,y,z_0)}{\partial z} = 0, \quad \varphi_{z_H} \dfrac{\partial c_H(x,y,z_H)}{\partial z} = 0, \\ c_{h-1}(x,y,z_{h-1}) = \ c_h(x,y,z_{h-1}), \\ \varphi_{z_{h-1}} \dfrac{\partial c_{h-1}(x,y,z_{h-1})}{\partial z} = \varphi_{z_h} \dfrac{\partial c_h(x,y,z_{h-1})}{\partial z}. \end{cases}$$

3. Analytical solution

We start this section by applying Fourier transform to equation (2.9). Let $\hat{c}_h^{\omega}(x,z)$ denote the Fourier transformation of c_h with respect to y. Then,

$$\hat{c}_h^{\omega}(x,z) = \int_{-\infty}^{+\infty} c_h(x,y,z)\, e^{-2i\pi\omega y}\, dy, \quad h \in \{1, \ldots, H\},$$

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which gives

$$u_h\left[\frac{\partial \hat{c}_h^\omega}{\partial x} + (2\pi)^2\omega^2\zeta_y(x)\hat{c}_h^\omega\right] = \xi(x)\ \varphi_{z_h}\ \frac{\partial^2 \hat{c}_h^\omega}{\partial z^2}, \quad z \in [z_{h-1}, z_h].$$

Let

$$\chi_h^\omega(x,z) = \hat{c}_h^\omega(x,z)\exp\left((2\pi)^2\ \omega^2 \int_0^x \zeta_y(s)\,ds\right), \tag{3.1}$$

then

$$\frac{\partial \chi_h^\omega}{\partial x} = \left[\frac{\partial \hat{c}_h^\omega}{\partial x} + (2\pi)^2\omega^2\zeta_y(x)\hat{c}_h^\omega\right]\ \exp\left((2\pi)^2\ \omega^2 \int_0^x \zeta_y(s)\,ds\right).$$

By multiplying both sides of equation (3.1) by

$$\exp\left((2\pi)^2\ \omega^2 \int_0^x \zeta_y(s)\,ds\right)$$

and, since u_h and φ_{z_h} are constants for each interval, we show easily that for all $h \in \{1, \ldots, H\}$,

$$u_h\frac{\partial \chi_h^\omega}{\partial x} = \xi(x)\ \varphi_{z_h}\ \frac{\partial^2 \chi_h^\omega}{\partial z^2}, \quad z \in [z_{h-1}, z_h]. \tag{3.2}$$

We proceed in the same way with the boundary conditions, and find

$$\begin{cases} \varphi_{z_1}\ \dfrac{\partial \chi_1^\omega(x,z_0)}{\partial z} = 0, & \\ \begin{cases} \chi_{h-1}^\omega(x,z_{h-1}) = \chi_h^\omega(x,z_{h-1}), \\ \varphi_{z_{h-1}}\ \dfrac{\partial \chi_{h-1}^\omega(x,z_{h-1})}{\partial z} = \varphi_{z_h}\ \dfrac{\partial \chi_h^\omega(x,z_{h-1})}{\partial z}, \end{cases} & h \in \{2, \ldots, H\} \\ \varphi_{z_H}\ \dfrac{\partial \chi_H^\omega(x,z_H)}{\partial z} = 0. & \end{cases}$$

The solution of equation (3.2) is assumed to be in the form

$$\chi_h^\omega(x,z) = \sum_{n=0}^{\infty} G_{h,n}^\omega(x)\ P_{h,n}(z), \quad h \in \{1, \ldots, H\}.$$

This separated form gives two ordinary differential equations to be solved:

$$\frac{d\ G_{h,n}^\omega}{dx} + \gamma_n^2\ \xi(x)\ G_{h,n}^\omega = 0, \tag{3.3}$$

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and

$$\varphi_{z_h} \frac{d^2 P_{h,n}}{dz^2} + \gamma_n^2 u_h P_{h,n} = 0, \tag{3.4}$$

where γ_n is a separation constant.

The first-order ordinary differential equation (3.3) has the solution

$$G_{h,n}^{\omega}(x) = \mu_n(\omega) \exp\Big(- \gamma_n^2 \int_0^x \xi(s)\, ds\Big),$$

where μ_n is an arbitrary function depending on ω.

Equation (3.4) represents a Sturm–Liouville problem. Solutions of such problem form an eigenfunction basis of the form

$$P_{h,n}(z) = \alpha_{h,n} \cos(\lambda_{h,n} z) + \beta_{h,n} \sin(\lambda_{h,n} z), \tag{3.5}$$

where $\lambda_{h,n} = \gamma_n \sqrt{(u_h/\varphi_{z_h})}$.

Equation (3.5) satisfies the following boundary conditions:

$$\begin{cases} \varphi_{z_1} \dfrac{d\, P_{1,n}(z_0)}{dz} = 0, & (3.6) \\ \begin{cases} P_{h-1,n}(z_{h-1}) = P_{h,n}(z_{h-1}), \\ \varphi_{z_{h-1}} \dfrac{d\, P_{h-1,n}(z_{h-1})}{dz} = \varphi_{z_h} \dfrac{d\, P_{h,n}(z_{h-1})}{dz}, \end{cases} \quad h \in \{2, \ldots, H\} & (3.7) \\ \varphi_{z_H} \dfrac{d\, P_{H,n}(z_H)}{dz} = 0. & (3.8) \end{cases}$$

To calculate the expression of $P_{h,n}$, it comes down to calculate the values of $\alpha_{h,n}$ and $\beta_{h,n}$, on each of the sub-layer $[z_{h-1}, z_h], h \in \{1, \ldots, H\}$.

By solving the recursive system resulting from substitution of equation (3.5) in equations (3.6)–(3.8), we obtain respectively the formulations of $\alpha_{h,n}$ and $\beta_{h,n}$. More specifically, we have the following.

For the first sub-layer, $\alpha_{1,n}$ and $\beta_{1,n}$ satisfy the equation

$$\alpha_{1,n} \sin(\lambda_{1,n} z_0) - \beta_{1,n} \cos(\lambda_{1,n} z_0) = 0,$$

from which we can take $\beta_{1,n} = \sin(\lambda_{1,n} z_0)$, so that $\alpha_{1,n} = \cos(\lambda_{1,n} z_0)$, which means

$$P_{1,n}(z) = \cos(\lambda_{1,n}(z - z_0)).$$

For the last sub-layer (H^{th} sub-layer),

$$\alpha_{H,n} = \cot(\lambda_{H,n} z_H)\, \beta_{H,n}.$$

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Additionally for the intermediate sub-layers,

$$\alpha_{h,n} = \frac{\varphi_{z_h}\lambda_{h,n} - \varphi_{z_{h-1}}\lambda_{h-1,n}}{2\varphi_{z_h}\lambda_{h,n}}\Big[\Big\{\cos((\lambda_{h,n}+\lambda_{h-1,n})z_{h-1}) + \frac{\varphi_{z_h}\lambda_{h,n} + \varphi_{z_{h-1}}\lambda_{h-1,n}}{\varphi_{z_h}\lambda_{h,n} - \varphi_{z_{h-1}}\lambda_{h-1,n}} \times \cos((\lambda_{h,n}-\lambda_{h-1,n})z_{h-1})\Big\}\alpha_{h-1,n} + \Big\{\sin((\lambda_{h,n}+\lambda_{h-1,n})z_{h-1}) - \frac{\varphi_{z_h}\lambda_{h,n} + \varphi_{z_{h-1}}\lambda_{h-1,n}}{\varphi_{z_h}\lambda_{h,n} - \varphi_{z_{h-1}}\lambda_{h-1,n}}\sin((\lambda_{h,n}-\lambda_{h-1,n})z_{h-1})\Big\}\beta_{h-1,n}\Big],$$

and

$$\beta_{h,n} = \frac{\varphi_{z_h}\lambda_{h,n} - \varphi_{z_{h-1}}\lambda_{h-1,n}}{2\varphi_{z_h}\lambda_{h,n}}\Big[\Big\{\sin((\lambda_{h,n}+\lambda_{h-1,n})z_{h-1}) + \frac{\varphi_{z_h}\lambda_{h,n} + \varphi_{z_{h-1}}\lambda_{h-1,n}}{\varphi_{z_h}\lambda_{h,n} - \varphi_{z_{h-1}}\lambda_{h-1,n}} \times \sin((\lambda_{h,n}-\lambda_{h-1,n})z_{h-1})\Big\}\alpha_{h-1,n} - \Big\{\cos((\lambda_{h,n}+\lambda_{h-1,n})z_{h-1}) - \frac{\varphi_{z_h}\lambda_{h,n} + \varphi_{z_{h-1}}\lambda_{h-1,n}}{\varphi_{z_h}\lambda_{h,n} - \varphi_{z_{h-1}}\lambda_{h-1,n}}\cos((\lambda_{h,n}-\lambda_{h-1,n})z_{h-1})\Big\}\beta_{h-1,n}\Big].$$

The eigenvalues $\gamma_n,\ n \in \mathbb{N}^*$ of this problem are real and discrete, and the eigenfunctions are mutually orthogonal. The orthogonality relation developed by Mikhailov and Ozisik [17] for this class of (self-adjoint) problems with respect to the density u_h on each interval $[z_{h-1}, z_h], h \in \{1, \ldots, H\}$ leads to

$$\sum_{h=1}^{H} \int_{z_{h-1}}^{z_h} u_h\, P_{h,m}(s)\, P_{h,n}(s)\, ds = \|P_{h,m}\| \,.\, \|P_{h,n}\| \,.\, \delta_{m,n},$$

where $\delta_{m,n}$ is the Kronecker symbol. Then, we can write

$$\|P_{H,n}\|^2 = \sum_{h=1}^{H} \int_{z_{h-1}}^{z_h} u_h\, (P_{h,n}(s))^2\, ds$$
$$= \begin{cases} \displaystyle\sum_{h=1}^{H} u_h(z_h - z_{h-1}), & \text{when } \gamma_n = 0,\\ \displaystyle\sum_{h=1}^{H} \frac{u_h}{2\,\lambda_{h,n}}[\sin(\lambda_{h,n}(z_h - z_{h-1}))\{(\alpha_{h,n}^2 - \beta_{h,n}^2)\cos(\lambda_{h,n}(z_h + z_{h-1})) & \\ +2\alpha_{h,n}\beta_{h,n}\sin(\lambda_{h,n}(z_h + z_{h-1}))\} + \lambda_{h,n}(\alpha_{h,n}^2 + \beta_{h,n}^2)(z_h - z_{h-1})], & \text{when } \gamma_n \neq 0. \end{cases}$$

The eigenvalues of each sub-layer can be obtained by integrating equation (3.4) on each of the intervals $[z_{h-1}, z_h],\ h \in \{1, \ldots, H\}$, taking into account the boundary conditions equations (3.6)–(3.8). However, the eigenfunctions $P_{H,n}$ form a complete set, so χ_H^ω can be developed as

$$\chi_H^\omega(x,z) = \sum_{n=0}^{\infty} a_n \exp\Big(-\gamma_n^2 \int_0^x \xi(s)\,ds\Big) P_{H,n}(z).$$

Then, the coefficients a_n are given by

$$a_n = \frac{1}{\|P_{h,n}\|^2} \sum_{\ell=1}^{H} \int_{z_{\ell-1}}^{z_\ell} u_\ell \chi_\ell^\omega(0,z)\, P_{\ell,n}(z)\,dz = \begin{cases} \dfrac{Q}{\sum_{h=1}^{H} u_h(z_h - z_{h-1})}, & \text{when } \gamma_n = 0, \\ \dfrac{Q}{\|P_{h,n}\|^2} \sum\limits_{\ell=1}^{H} P_{\ell,n}(H_s), & \text{when } \gamma_n \neq 0. \end{cases}$$

The inverse Fourier transform of

$$\exp\Big((2\pi)^2\,\omega^2 \int_0^x \zeta_y(s)\,ds\Big)$$

is given by

$$\frac{1}{2\sqrt{\pi \int_0^x \zeta_y(s)\,ds}} \exp\Big(-\frac{y^2}{4\int_0^x \zeta_y(s)\,ds}\Big).$$

Consequently,

$$c_H(x,y,z) = \frac{Q}{2\sqrt{\pi \int_0^x \zeta_y(s)\,ds}} \exp\Big(-\frac{y^2}{4\int_0^x \zeta_y(s)\,ds}\Big) \times \sum_{n=0}^{\infty} \exp\Big(-\gamma_n^2 \int_0^x \xi(s)\,ds\Big) \frac{P_{H,n}(z)}{\|P_{H,n}\|^2} \Big(\sum_{h=1}^{H} P_{h,n}(H_s)\Big). \tag{3.9}$$

The crosswind-integrated concentration $c_H^y(x,z)$ is obtained by integrating equation (3.9) with respect to y from $-\infty$ to $+\infty$, which yields

$$c_H^y(x,z) = Q \sum_{n=0}^{\infty} \exp\Big(-\gamma_n^2 \int_0^x \xi(s)\,ds\Big) \frac{P_{H,n}(z)}{\|P_{H,n}\|^2} \sum_{h=1}^{H} P_{h,n}(H_s). \tag{3.10}$$

4. Validation and experimental data

The wind speed profile $u(z)$ is parameterized using the model of Deaves and Harris [7]. This model is extrapolated using experimentally measured wind speed profiles. The advantage of this profile over other ones is that it extends the accurate representation of the logarithmic law to a small height, and through better accuracy

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for the logarithmic and power law models to a moderate height,

$$u(z) = \frac{u_*}{k}\left[\ln\left(\frac{z+z_0}{z_0}\right) + 5.75\left(\frac{z}{H_{\mathrm{mix}}}\right) - 1.88\left(\frac{z}{H_{\mathrm{mix}}}\right)^2 - 1.33\left(\frac{z}{H_{\mathrm{mix}}}\right)^3 + 0.25\left(\frac{z}{H_{\mathrm{mix}}}\right)^4\right],$$

where H_{mix} is the PBL height. The modified form of the vertical eddy diffusivity coefficient K_z, given in equation (2.6), is adopted from [8], where the functional

$$\varphi_z(z) = 0.22\, H_{\mathrm{mix}}\, w_* \left(\frac{z}{H_{\mathrm{mix}}}\left(1 - \frac{z}{H_{\mathrm{mix}}}\right)\right)^{1/3}\left(1 - \exp\left(-\frac{4\,z}{H_{\mathrm{mix}}}\right) - 0.0003\, \exp\left(\frac{8\,z}{H_{\mathrm{mix}}}\right)\right),$$

where w_* is the convective velocity. The integrable correction dimensionless function in equation (2.6) is defined in terms of the along-wind length scale L_1 as follows [18]:

$$\xi(x) = 1 - \exp\left(-\frac{x}{L_1}\right). \tag{4.1}$$

The length L_1 is given in terms of u, φ_z and σ_w as [18]

$$L_1 = \frac{1}{\sigma_w^2(H_s)}\, u(H_s)\, \varphi_z(H_s),$$

where σ_w is the vertical turbulent intensity. Note that there exist many expressions of σ_w; we adopt here the expression given by Hanna *et al.* [13]:

$$\sigma_w = 0.96\, w_*\left(\frac{3\,z}{H_{\mathrm{mix}}} + \frac{|L|}{H_{\mathrm{mix}}}\right)^{1/3},$$

where L is the Monin–Obukhov length [21]. The Monin–Obukhov length is a parameter used in atmospheric dispersion having the dimension of a length, and describes the atmospheric stability states according to their sign, that is, L is negative (positive) for an unstable (stable) situation whereas $|L| >> 1$ indicates neutral situation [21].

Note that when $L_1 \to 0$, the term $\exp(-x/L_1)$ becomes negligible in equation (4.1), and K_z depends only on z (that is, $K_z \equiv \varphi_z$ in equation (2.6)).

The lateral eddy diffusivity is given by Huang [14]:

$$K_y(x, z) = \frac{1}{2}\, u(z)\frac{d\,\sigma_y^2(x)}{dx}, \tag{4.2}$$

where σ_y is the standard deviation in the crosswind direction (depends only on x). By identifying equations (2.5) and (4.2), we obtain

$$\zeta_y(x) = \frac{1}{2}\,\frac{d\,\sigma_y^2(x)}{dx}.$$

The model presented as equation (3.10) is assessed and validated using data sets obtained from the Copenhagen diffusion and Prairie Grass experiments.

The Copenhagen experiments were realized in the northern part of Copenhagen between 12/09/1978 and 19/07/1979 as described by Gryning et al. [10] and Gryning and Lyck [11]. They were carried out using the tracer sulphur hexafluoride (SF6), which was realized without buoyancy from a tower at a height of $H_s = 115\ m$, the roughness length was $z_0 = 0.6\, m$. The remaining required parameters for these experiments are given in [10, 11].

The Prairie Grass experiments were realized in O'Neil, Nebraska between 03/07/1956 and 30/08/1956 and well detailed by Nieuwstadt [20] and the data downloaded from http://www.harmo.org/jsirwin (see [1]). They were carried out using the tracer sulphur dioxide (SO_2), realized without buoyancy from a tower at a height of $H_s = 1.5\ m$, the roughness length was $z_0 = 0.006\, m$. All necessary data for these experiments are given in [1, 20].

For the practical implementation of the analytical solution, we have discretized the PBL into 2 and 4 sub-layers. For the 2-sub-layers case, the discretization is

$$dz_1 = \frac{7(H_{\text{mix}} - z_0)}{13} \quad \text{and} \quad dz_2 = \frac{6(H_{\text{mix}} - z_0)}{13};$$

and for the 4-sub-layers case, the discretization is

$$dz_1 = \frac{3(H_{\text{mix}} - z_0)}{15}, \quad dz_2 = \frac{3(H_{\text{mix}} - z_0)}{15}, \quad dz_3 = \frac{7(H_{\text{mix}} - z_0)}{15},$$

$$\text{and} \quad dz_4 = \frac{2(H_{\text{mix}} - z_0)}{15}.$$

The quality and performance of models are usually presented by drawing a scatter diagram using predicted and observed values. Figure 1 represents a scatter diagram between observed and predicted crosswind-integrated concentrations for the two formulations of the vertical diffusivity and the number of sub-layers in the PBL (when $H = 2$ and $H = 4$) for the Copenhagen (top panel) and the Prairie Grass (bottom panel) experiments. The figure shows a good agreement between the predicted and observed values which seem to be a good parameterization of the model. An immediate visualization inspection of the overall model performance shows that the observed crosswind-integrated concentration tended to be slightly larger than those predicted. The quantitative evaluation of models is usually made through statistical performance analysis that is presented and widely used in many works. The statistical indices which we will use here are defined as [4]: the normalized mean square error ($NMSE$), the mean relative square error ($MRSE$), the correlation coefficient (COR), the fractional bias (FB), the fractional standard deviations (FS), the geometric mean bias (MG), the geometric mean variance (VG) and the factor of two ($FAC2$). The perfect models would have $NMSE = MRSE = FB = FS = 0$ and $COR = MG = VG = FAC2 = 1$ [4]. The satisfied numerical results given in Figure 1 are re-affirmed from the values of statistical performance measures summarized in Table 1. The calculated values are mostly within the range of acceptable model performance for both formulations of the vertical eddy diffusivity. Furthermore, Table 1 indicates that similar results are obtained compared to other analytical procedures, previously published in the literature [9, 12, 15, 19].

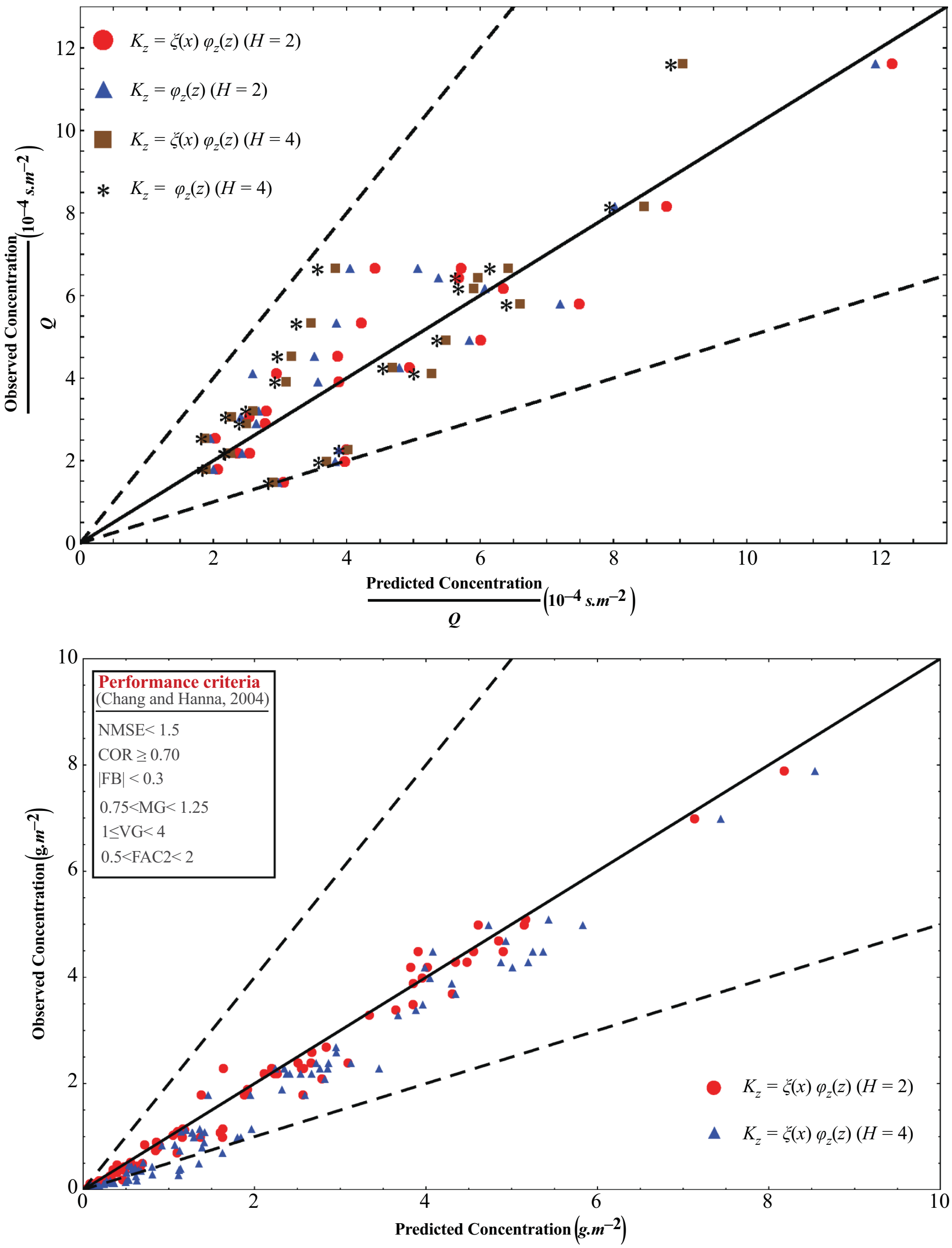

FIGURE 1. Scatter plot of observed and predicted crosswind-integrated concentrations of the Copenhagen (top panel) and the Prairie Grass experiments (bottom panel). The solid line is a one-to-one line ($y = x$) and dotted lines correspond to a factor of two (that is, $y = 0.5x$ and $y = 2x$).

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TABLE 1. Statistical measures for the Copenhagen and Prairie Grass experiments.

Models	NMSE	MRSE	COR	FB	FS	MG	VG	FAC2
Copenhagen experiments								
$K_z = \xi(x)\varphi_z(z)$ $(H = 2)$	0.0533	0.0533	0.8657	−0.0135	0.0018	0.9660	1.0885	1.096
$K_z = \varphi_z(z)$ $(H = 2)$	0.0660	0.0660	0.8498	0.0432	0.03897	1.0235	1.1007	1.055
$K_z = \xi(x)\varphi_z(z)$ $(H = 4)$	0.0768	0.0768	0.8308	0.0543	0.1686	1.0273	1.1022	0.9235
$K_z = \varphi_z(z)$ $(H = 4)$	0.0892	0.0890	0.8274	0.0973	0.2065	1.0726	1.1124	0.8882
[9] $(H = 2)$	0.08	–	0.86	−0.02	0.05	–	–	1.0
[9] $(H = 4)$	0.1	–	0.82	0.1	0.04	–	–	0.92
[15]	0.069	–	–	−0.009	0.051	0.996	1.055	1.009
Prairie Grass experiments								
$K_z = \xi(x)\varphi_z(z)$ $(H = 2)$	0.0210	0.0209	0.9809	−0.0503	−0.0108	0.9018	1.0645	0.9807
$K_z = \xi(x)\varphi_z(z)$ $(H = 4)$	0.0613	0.0608	0.9763	−0.1809	−0.0514	0.8616	1.3228	0.9373
[19]	0.25	–	0.92	0.03	0.20	–	–	0.68
[12]	0.04	–	0.96	−0.09	0.13	–	–	0.79

5. Conclusion

The solution of the three-dimensional steady-state atmospheric diffusion equation was developed taking into account more realistic formulations of the wind speed profile and two formulations of the vertical eddy diffusivity. The convergence was numerically validated using data sets obtained from the Copenhagen and Prairie Grass experiments. The results showed that predicted and observed values were in good agreement and the calculated statistical indices were mostly within the range of acceptable model performance. The findings of the current study show that the current model could be an interesting approach for an accurate prediction of the atmospheric dispersion of pollutants and may be appropriate for other continuous flows.

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