Atmospheric Environment 83 (2014) 254-259

Contents lists available at ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv



Short communication

A contribution to solve the atmospheric diffusion equation with eddy diffusivity depending on source distance



CrossMark

ATMOSPHERIC ENVIRONMENT

Davidson Martins Moreira ^{a,d,*}, Amilton Cravo Moraes ^b, Antonio Gledson Goulart ^c, Taciana Toledo de Almeida Albuquerque ^d

^a Federal University of Southern Border, Environmental Engineering, Rua General Osório, 413D, Caixa Postal 181, CEP: 89802210, Chapecó, Santa Catarina, Brazil

^b Instituto Federal Sul-Rio-Grandense, Praça XX de Setembro 455, CEP: 96020170, Pelotas, RS, Brazil

^c Federal University of Pampa, Avenida Tiaraju, 810, CEP: 97546550, Alegrete, RS, Brazil

^d Federal University of Espírito Santo, Environmental Engineering, Av. Fenrando Ferrari, 514, CEP: 29075910, Vitória, ES, Brazil

ARTICLE INFO

Article history: Received 4 April 2013 Received in revised form 19 October 2013 Accepted 21 October 2013

Keywords: Eddy diffusivity Analytical model Atmospheric boundary layer

ABSTRACT

An integral solution of the atmospheric diffusion equation considering wind speed as a function of vertical height and eddy diffusivity as a function of both downwind distance from the source and vertical height is presented. The near-source dispersion problem is investigated comparing a vertical eddy diffusivity function of distance from the source against their asymptotic limit. The results suggest that the inclusion of the memory effect as modeled by Taylor's theory, improves the description of the turbulent transport process of atmospheric effluent released by a low continuous source in convective conditions.

© 2013 Elsevier Ltd. All rights reserved.

1. Introduction

In the last years, special attention has been given to the issue of searching analytical solutions for the advection-diffusion equation in order to simulate the pollutant dispersion in the Atmospheric Boundary Layer (ABL). In fact, the mathematical modeling has been an important tool in all scientific areas, including environmental problems in the atmosphere, water and soil. However, a little attention has been given to the atmospheric problems to find analytical solution of this equation for eddy diffusivity as a function of both downwind distance (x) from the source and the vertical height (z) above the ground, mainly due to the mathematical complexity problem involved. We are aware of the analytical solutions existence in the literature, but for specific and particular problems. Among them, we mention the works of Rounds (1955). Smith (1957), Scriven and Fisher (1975), Demuth (1978), van Ulden (1978), Nieuwstadt and de Haan (1981), Sharan et al. (1996), Lin and Hildemann (1997), Wortmann et al. (2005), Sharan and Modani (2006), Sharan and Kumar (2009). In all of these analytical models, the wind speed is either a power law or logarithmic profile of vertical height and similarly the eddy diffusivity has been assumed either a power law or a parabolic profile of z or a function of downwind distance from the source. However, none of these provides a systematic approach to find the solution with the generalized functional forms of wind speed and eddy diffusivity. At this point, it is important to mention that a solution of the advection-diffusion equation can be written either in integral form and series formulations, with the main property that both solutions are equivalent (Moreira et al., 2010). Furthermore, analytical solutions are very important to understand and describe the physical phenomenon, since they are able to take into account all the parameters of a problem and investigate their influence. Besides, an analytical solution is useful to evaluate the performances of sophisticated numerical dispersion models, which numerically solves the advection-diffusion equation, giving results that can be compared not only with experimental data but also, in an easy way, with the solution itself, to check numerical errors.

Focusing our attention in this direction, the novelty of this work relies on the solution semi-analytically of two-dimensional advection—diffusion equation considering a realistic eddy diffusivity depending on the x and z variables in an air pollution problem. We step forward regarding previous works (Moreira et al.,

^{*} Corresponding author. Federal University of Southern Border, Environmental Engineering, Rua General Osório, 413D, Caixa Postal 181, CEP: 89802210, Chapecó, Santa Catarina, Brazil.

E-mail addresses: davidson@pq.cnpq.br (D.M. Moreira), acm2@pelotas.ifsul.edu. br (A.C. Moraes), antonio.goulart@gmail.com (A.G. Goulart), taciana.albuquerque@ ufes.br (T.T.deA. Albuquerque).

^{1352-2310/\$ -} see front matter © 2013 Elsevier Ltd. All rights reserved. http://dx.doi.org/10.1016/j.atmosenv.2013.10.045

 $-2tan^{-1}$

2005a,b), that include integral and series solutions of the advection—diffusion equation considering the average value for the eddy diffusivity in the *x* direction. In the current work, it was not considered this assumption. Therefore, it is possible to investigate the memory effect in turbulent dispersion process without approximations in the *x* direction, representing an advance the knowledge of near-source process. To reach this goal, we outline the paper as follows: in Section 2 the turbulent parameterization assumed in this work is presented; in Section 3, we report the derivation of the solution for the advection—diffusion equation with eddy diffusivities depending on *x* and *z* variables; in Section 4, results with numerical simulations are reported; finally, in Section 5, we present the conclusions.

2. Parameterizations

In many studies, in order to obtain analytical solutions of the advection—diffusion equation, the eddy diffusivities can be specified as linear functions of downwind distance based on Taylor's (1921) statistical theory of diffusion for smaller travel times. That is,

$$K_x = \alpha U x; \ K_y = \beta U x \text{ and } K_z = \gamma U x$$
 (1)

where α , β and γ represent turbulence parameters and vary with the atmospheric stability. These parameters can be identified as squares of turbulence intensities using Taylor's statistical theory of diffusion (Arya, 1995).

In this work, we step forward regarding analytical solutions, considering the turbulence parameterization scheme suggested by Degrazia et al. (2001) and Goulart et al. (2004), that is depending on x and z variables. In terms of the convective scaling parameters, the eddy diffusivity can be formulated as:

$$K_{\alpha} = w_* h \frac{0.09 c_i^{1/2} \psi^{1/3} (z/h)^{4/3}}{\left(f_{\rm m}^*\right)_i^{4/3}} \int_0^\infty \frac{\sin\left(\frac{7.84 c_i^{1/2} \psi^{1/3} \left(f_{\rm m}^*\right)_i^{2/3} Xn'}{(z/h)^{2/3}}\right)}{(1+n')^{5/3}} \frac{\mathrm{d}n'}{n'}$$
(2)

where w_* is the convective velocity scale ($\alpha = x,y,z$), z is height above the ground, ψ is the nondimensional molecular dissipation rate functions associated to buoyancy productions, $(f_m^*)_i$ is the reduced frequency of the convective spectral peak and $c_i = \alpha_i \alpha_u (2\pi\kappa)^{-2/3}$ with $\alpha_u = 0.5 \pm 0.05$ and $\alpha_i = 1, 4/3, 4/3$ for u, vand w components, respectively, and X is a nondimensional time, since it is the ratio of travel time x/u and the convective timescale h/w^* . For more details regarding vertical eddy diffusivity see the works of Degrazia et al. (2001) and Goulart et al. (2004).

For the sake of comparison, we report numerical simulation for the solution of the advection—diffusion equation assuming the eddy diffusivity K(z) proposed by Degrazia et al. (1997), that represent asymptotic limit of the Eq. (2):

$$K_{z} = 0.22w_{*}h\left(\frac{z}{h}\right)^{1/3}\left(1-\frac{z}{h}\right)^{1/3}\left[1-\exp\left(-\frac{4z}{h}\right)\right.$$
$$\left.-0.0003\exp\left(\frac{8z}{h}\right)\right]$$
(3)

Furthermore, employed in the convective conditions (mixedlayer), we also compare with the parameterization suggested by Brost et al. (1988):

 $K_z = k w_* z (1 - z/h) \tag{4}$

where *k* is the von Karman constant (~ 0.4).

The formulae used for evaluating mean wind speed are those of similarity (Panofsky and Dutton, 1984):

$$u = \frac{u_*}{k} \left[\ln \frac{z}{z_0} - \Psi_m \left(\frac{z}{L} \right) \right]$$
(5)

where u^* is the scale velocity relative to mechanical turbulence, k the von Karman constant, L is the Monin-Obukhov length, z_0 roughness length and Ψ_m is the stability function expressed as:

$$\begin{split} \Psi_m \Big(\frac{z}{L}\Big) \ &= \ ln \Big(\frac{1+A^2}{2}\Big) + ln \Big(\frac{1+A}{2}\Big) \end{split}$$

with $A = (1 - 15z/L)^{1/4}$. The similarity expression is utilized of within the surface layer (above the wind velocity is considered constant with height).

The eddy diffusivity (2), as a function of downwind distance, is dependent of z and gives a description of turbulent dispersion near, intermediate and far from fields of a source in the ABL (the memory effect of turbulent transport is considered).

3. The mathematical scheme

It is well-known that analytical solutions can be expressed either as integral form or series formulation (Moreira et al., 2010). Taking into account the equivalence of these solutions, in this study we report, for the first time, the results attained by an integral solution considering eddy diffusivity depending on z and x variables (without average values in the x direction as in previous works). The reason for this choice comes from the fact that among the semi-analytical and analytical methods available in the literature, this approach is the only one to solve pollutant dispersion problems for a broader class of problems and a variety of physical scenarios with any restriction to spatial characteristics of wind and eddy diffusion coefficients.

For a Cartesian coordinate system in which the *x* direction coincides with that one of the average wind, the steady state advection—diffusion equation is written as (Arya, 1995):

$$u\frac{\partial\overline{c}}{\partial x} = \frac{\partial}{\partial x}\left(K_x\frac{\partial\overline{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial\overline{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial\overline{c}}{\partial z}\right)$$
(6)

where \overline{c} denotes the average concentration, u is the mean wind speed in x direction and K_x , K_y and K_z are the eddy diffusivities. The cross-wind integration of Eq. (6) (neglecting the longitudinal diffusion) leads to (Moreira and Vilhena, 2009):

$$u(z)\frac{\partial\overline{c^{y}}}{\partial x} = \frac{\partial}{\partial z}\left(K_{z}(x,z)\frac{\partial\overline{c^{y}}}{\partial z}\right)$$
(7)

subject to the boundary conditions of zero flux at the ground and ABL top and a source with emission rate Q at height H_s :

$$K_z \frac{\partial c^y}{\partial z} = 0 \text{ at } z = z_0, h$$
(8)

$$u\overline{c^{y}}(0,z) = Q\delta(z-H_{s}) \text{ at } x = 0$$
(9)

where now $\overline{c^y}$ represents the average cross-wind integrated concentration. Bearing in mind the dependence of the K_z coefficient and wind speed profile u on variable z, the height h of an ABL is

2

discretized in *N* sub-intervals in such a manner that inside each interval assume average values in this direction.

At this moment, it is important to mention that the eddy diffusivity represented by Eq. (2) can be write as $K(x,z) = g(z) \cdot f(x,z)$, where g(z) (or a constant) is a dimensional function $[L^2T^{-1}]$ and f(x,z) is a nondimensional function. Therefore, the solution of problem (7) is reduced to the solution of *N* problems of the type:

$$\overline{u}_n \frac{\partial \overline{c_n^y}}{\partial x} = \overline{g}_n \cdot \overline{f}_n(x) \frac{\partial^2 \overline{c_n^y}}{\partial z^2} \quad z_n \le z \le z_{n+1}$$
(10)

for n = 1: *N*, where $\overline{c_n^y}$ denotes the concentration at the *n*th subinterval, and,

$$\overline{u}_{n} = \frac{1}{z_{n+1} - z_{n}} \int_{z_{n}}^{z_{n+1}} u(z) dz$$
(11)

$$\overline{g}_{n} = \frac{1}{z_{n+1} - z_{n}} \int_{z_{n}}^{z_{n+1}} g(z) dz$$
(12)

$$\overline{f}_{n}(x) = \frac{1}{z_{n+1} - z_{n}} \int_{z_{n}}^{z_{n+1}} f(x, z) dz$$
(13)

The proposed integral solution of the advection—diffusion equation with K(x,z) do not have in literature. Recently, Kumar and Sharan (2010) proposed a series solution where is assumed the function $K(x,z) = g(z) \cdot f(x)$ (considering two separate functions). It is important to mention that our hypothesis in K(x,z) is more general.

To obtain the solution of Eq. (10), we make a change of variables (Crank, 1979). Let us introduce a new time variable x^* defined by the transformation as,

$$x^* = \int_0^x \overline{f}_n(x') \mathrm{d}x' \tag{14}$$

The dimension of x^* is same as x [L], so it is referred to as a new space variable. Because $\overline{f}_n(x) > 0$, the function $x \to x^*$ is an increasing function of x, vanishing in x = 0. Thus, the nature of the condition at x = 0 does not change in the new domain.

The problem, together with their source and boundary conditions, in new space variable becomes:

$$\overline{u}_n \frac{\partial \overline{c_n^y}}{\partial x^*} = \overline{g}_n \frac{\partial^2 \overline{c_n^y}}{\partial z^2}$$
(15)

for n = 1:NL, where NL denotes the number of sub-layers and $\overline{c_n^y}$ the concentration at the *n*th sub-layer. Besides which, two boundary conditions are imposed at $z = z_0$ and *h* (ABL height) given by Eq. (8) together with the continuity conditions for the concentration and flux of concentration at the interfaces,

$$c_n^{\nu} = c_{n+1}^{\nu} \quad n = 1, 2, \dots (N-1)$$
$$K_n \frac{\partial \overline{c_n^{\nu}}}{\partial z} = K_{n+1} \frac{\partial \overline{c_{n+1}^{\nu}}}{\partial z} \quad n = 1, 2, \dots (N-1)$$

..

must be considered, in order to be possible to uniquely determine the 2N arbitrary constants appearing in the solution of the set of problems (15). For more details about this, see the work of Moreira et al. (2006). Now, applying the Laplace transform in Eq. (15) results:

$$\frac{d^2}{dz^2}\,\widehat{c}_n(s,z) - \frac{\overline{u}_n s}{\overline{g}_n}\,\widehat{c}_n(s,z) = -\frac{\overline{u}_n}{\overline{g}_n}\overline{c}_n^y(0,z) \tag{16}$$

where $\widehat{c}_n(s,z) = L_p\{\overline{c_n^y}(x^*,z); x^* \to s\}$, which has the well-know solution:

$$\widehat{c}_{n}(s,z) = A_{n}e^{-R_{n}z} + B_{n}e^{R_{n}z} + \frac{Q}{2R_{a}}\left(e^{-R_{n}(z-H_{s})} - e^{R_{n}(z-H_{s})}\right)$$
(17)

where

$$R_n = \sqrt{\frac{\overline{u}_n s}{\overline{g}_n}}$$
 and $R_a = \sqrt{\overline{u}_n s \overline{g}_n}$

The concentration is obtained inverting numerically the transformed concentration:

$$\overline{c_{n}^{\nu}}(x^{*},z) = \frac{1}{2\pi i} \int_{i-\gamma\infty}^{i+\gamma\infty} e^{sx^{*}} \left(A_{n}e^{\left[\left(\sqrt{\frac{\sin}{\overline{s}_{n}}} \right)z \right]} + B_{n}e^{-\left[\left(\sqrt{\frac{\sin}{\overline{s}_{n}}} \right)z \right]} + \frac{Q}{2\sqrt{s\overline{u}_{n}\overline{g}_{n}}} \left\{ e^{-\left[\left(\sqrt{\frac{\sin}{\overline{s}_{n}}} \right)(z-H_{s}) \right]} - e^{\left[\left(\sqrt{\frac{\sin}{\overline{s}_{n}}} \right)(z-H_{s}) \right]} \right\} H(z-H_{s}) \right\} ds$$

$$(18)$$

where $H(z-H_s)$ is the Heaviside function. The integration constants A_n and B_n are previously determined by solving the linear system resulting from the application of the boundary and interfaces conditions.

At this point, we need a method for the Laplace transform inversion. Because all methods have limitations, we emphasize the utilization of more than one algorithm to invert a transform. It is important to mention that Laplace transforms are powerful tools used primarily to solve differential equations. The principal difficulty in using them is finding their inverses. Unless the transform is given in a table, an integration must be performed in the complex plane (Bromwich's integral) to find the inverse. Despite the power of complex analysis, this analytical technique often fails and Bromwich's integral finally must be numerically integrated. Below, we show two alternatives to obtain the inversion, where the more simple method is the Gaussian quadrature scheme. However, the second alternative is a more robust method. It was our option to use in this work the Fixed-Talbot method in the simulations.

a) Gaussian Quadrature scheme (GQ):

$$\overline{c_n^{\gamma}}(x^*,z) = \sum_{k=1}^{M^*} \frac{p_k}{x^*} a_k \left[A_n e^{\left[\left(\sqrt{\frac{p_k \overline{u}_n}{x^* \overline{g}_n}} \right) z \right]} + B_n e^{-\left[\left(\sqrt{\frac{p_k \overline{u}_n}{x^* \overline{g}_n}} \right) z \right]} \right] \\ + \frac{Q}{2\sqrt{\frac{p_k}{x^*} \overline{u}_n \overline{g}_n}} \left\{ e^{-\left[\left(\sqrt{\frac{p_k \overline{u}_n}{x^* \overline{g}_n}} \right) (z - H_s) \right]} \\ - e^{\left[\left(\sqrt{\frac{p_k \overline{u}_n}{x^* \overline{g}_n}} \right) (z - H_s) \right]} \right\} H(z - H_s) \right]$$
(19)

where a_k and p_k are the weights and roots of the Gaussian quadrature scheme tabulated in Stroud and Secrest (1966) and M^* is the

number of the quadrature points. In this method the parameter *s* is replaced by p_k/x^* .

b) Fixed-Talbot scheme (FT):

It is a more robust inversion method and this formula is general in FT method, where we can approximate the value of the integral by using the trapezoidal rule with step size π/M , obtained in the work of Abate and Valkó (2004):

$$\overline{c_n^{\mathbf{y}}}(\mathbf{x}^*, z) = \frac{r}{M} \left[\frac{1}{2} \overline{c_n^{\mathbf{y}}}(r, z) e^{r\mathbf{x}^*} + \sum_{k=1}^{M-1} \operatorname{Re} \left[e^{\mathbf{x}^* S(\theta_k)} \overline{c_n^{\mathbf{y}}}(s(\theta_k), z) (1 + i\tau(\theta_k)) \right] \right]$$
(20)

where

$$s(\theta_k) = r\theta(\cot\theta + i), \quad -\pi < \theta < +\pi$$

 $\tau(\theta_k) = \theta_k + (\theta_k \cot \theta_k - 1) \cot \theta_k$

$$\theta_k = \frac{k\pi}{M}$$

and r is a parameter based on numerical experiments and M is the number of terms in the summation.

Both GO and FT methods have only one free parameter: M^* . which is the number of the quadrature points in the GO method and *M*, which is the number of terms in the summation in the FT method. Both algorithms provide increasing accuracy as M^* and M increases. Because all methods have limitations, we emphasize the utilization of more than one algorithm to invert a transform. Since numerical Laplace inversion techniques are not exact, and often depend on the choice of a free parameter that is unknown a priori, it is advantageous to either use more than one inversion technique or perform experimentation and study the effect of the free parameter on the solution. In recent years, numerical transform inversion has become recognized as an important technique in operations research, notably for calculating probability distributions in stochastic and deterministic models (Abate and Valkó, 2004). The significance of numerical Laplace inversion is obvious from the big range of applications. Well-known in engineering, Laplace transformation methods are also used in order to solve differential and integral equations and to assist when other numerical methods are applied.

Concerning the issue of stepwise approximation, it is important to get in mind that the stepwise approximation of a continuous function converges to the continuous function when the stepwise of the approximation goes to zero. For this method, it is only necessary to choose the number of the sub-layers in an appropriate manner, by taking the smoothness of the functions K and u into account. Therefore, this model preserves the beauty of an analytical solution without compromising the accuracy of wind speed and eddy diffusivity to compute the cross-wind integrated concentrations.

In summary, for a better understanding of the reader, the implementation of the algorithm for computing the solution consists on the following steps: stepwise approximation of the eddy diffusivity and wind speed in the *z* direction; change of variable in the *x* direction; the Laplace transform application to the advection—diffusion equation in the transformed variable; semi-analytical solution of the linear ordinary equation set resulting in the Laplace transform inversion, using the FT scheme.

4. Comparison with experimental data

In order to illustrate the aptness of the discussed formulation to simulate contaminant dispersion in the ABL, we evaluate the performance of the discussed solutions against experimental ground-level concentration using the Prairie Grass dispersion experiments, which allow us to validate the results encountered by the solution. The Prairie Grass experiment was realized in O'Neill, Nebraska, 1956. The pollutant (SO₂) was emitted without buoyancy at a height of 0.5 m and it was measured by samplers at a height of 1.5 m in five downwind distances (50, 100, 200, 400, 800 m). The Prairie Grass site was flat with a roughness length of 0.6 cm. The results for twenty convective $(-h/L^{-1} > 10)$ experiments are presented. For more details see the work of Nieuwstadt (1980).

Table 1 presents some performance measurements obtained using the well-known statistical evaluation procedure described by Hanna (1989). The statistical index FB indicates whether the predicted quantities underestimate or overestimate the observed ones. The statistical index NMSE represents the quadratic error of the predicted quantities in relation to the measured data. The best results are indicated by values nearest to 0 in NMSE, FB, and FS (Fractional Standard), and nearest to 1 in COR (CORrelation coefficient) and FA2 (FActor of 2).

These results are compared with those obtained from a K(z)(asymptotic limit, Eq. (3), and Brost et al., 1988, Eq. (4)), and are shown in Table 1. In general, the concentrations are close to those observed within a factor of 2 of 86% and correlation of 98% for K(x,z)scheme, including the best NMSE. The scheme K(z), represented by asymptotic limit of Eq. (2), predicts the concentrations with a factor of 2 of 74% and correlation of 97% and, the scheme K(z) of Brost et al. (1988), a factor of 2 of 53% and correlation of 92%, with poor NMSE of 1.46. In this case, it is possible to note that the model reproduces very well the observed concentration using K(x,z). Besides that, we observe from Fig. 1 that the model reproduces better the concentrations closer to the source (higher concentrations). The discrepancies increase for larger distances (lower concentrations), where the plume penetrates the free convection layer, rapidly decreasing the concentration (Nieuwstadt, 1980). The Prairie Grass experiment used sulfur dioxide gas. However, we understand now that many of these tracers were subject to significant removal due to deposition, which was not included in this model (Gryning et al., 1983).

We show in Table 2, in order to verify the errors involved due to (i) the number of sub-layers and (ii) numerical inversion, the solution obtained at various points (x = 50,100, 200, 400 and 800 m) for the experiment five of Prairie Grass with L = -28 m, h = 780 m, $w^* = 1.64$ m s⁻¹ and Q = 78 g s⁻¹. We also include a comparison with a numerical solution (finite differences scheme) of Eq. (7).

We observe promptly the numerical convergence of the results encountered for ground-level concentration as function of Δz (vertical discretization) and *M* (number of terms in the summation). As expected, for a source in a very low height (~0.5 m), distances closer to the source require a more fine discretization and greater number of *M* terms to obtain good results. In this work we used $\Delta z = 0.25$ m until 0.1*h* and $\Delta z = 10$ m for sub-layers above, with *M* = 100. The hybrid and numerical techniques match well, particularly in the area close to the source. However, the

Table 1

Statistical indices to evaluate the model performance with three different parameterizations.

Prairie Grass	NMSE	COR	FA2	FB	FS
<i>K</i> (<i>x</i> , <i>z</i>) Eq. (2)	0.06	0.98	0.86	-0.08	0.01
<i>K</i> (<i>z</i>) Eq. (3)	0.17	0.97	0.74	0.04	0.38
<i>K</i> (<i>z</i>) Eq. (4)	1.46	0.92	0.53	0.67	0.86

concentration results of the numerical method are slightly greater than semi-analytical results with increasing of the distance.

In spite of the critical dependence of the solution (for low source case) on the number and choice of the sub-layers as well as the number of terms used in the summation for inverse Laplace transform, we can have confidence in the numerically generated numbers from the semi-analytical solution (*K* and *u* converges to the continuous function when $\Delta z \rightarrow 0$ and we used a robust method for Laplace inversion scheme).

We must remark regarding the numerical methods that besides the domain discretization into a set of discrete points displayed in a grid, all the derivatives in the advection-diffusion equation that are approximated by a finite difference scheme (finite differences, finite elements, etc.). However, stability and convergence are the key and important issues as far as numerical solution is considered. Depending on the scheme, the solution may have oscillation or spike. Hence it will lead to the erroneous conclusions as compared to the real physics. Besides, the numerical methods impose a large number of step calculations used in performing the integration. Hence it is necessary to have stable and convergence solution with the optimized CPU time consumption. This feature also does not appear in the semi-analytical method, because the semi-analytical character of the solution allows us to perform the calculation at any distance. This guarantees the smaller computational time as well the smaller round-off error influence in the accuracy of the results of the hybrid method when compared with the numerical ones, because in practice we find that it demands less mathematical operations. Although to deal with realistic situations, we need to shift to numerical methods, it is helpful to examine first some of the possible analytical solutions to obtain a known framework and test solutions. In this sense, the analytical solutions are useful for a variety of applications, such as: providing approximate analyses of alternative pollution scenarios, conducting sensitivity analyses to investigate the effects of various parameters or processes involved in contaminant transport, extrapolation over large times and distances where numerical solutions may be impractical, serving as screening models or benchmark solutions for more complex



Fig. 1. Scatter diagram of observed (Co) and predicted (Cp) data. Data between the middle diagonal line indicates perfect agreement. Dotted lines indicate a factor of two.

Table 2

Numerical convergence of the solution as function of Δz and M obtained at various points (x = 50,100, 200, 400 and 800 m) and numerical solution results for the experiment five of Prairie Grass.

VD (Δz) and	Cross-wind concentration $\overline{c^{y}}$ (g m ⁻²)						
NTC $(M)^{a}$	x = 50 m	<i>x</i> = 100 m	<i>x</i> = 200 m	<i>x</i> = 400 m	<i>x</i> = 800 m		
$\Delta z = 0.25, M = 10$	3.742	1.844	0.905	0.450	0.230		
$\Delta z=0.25,M=50$	3.111	1.545	0.760	0.380	0.194		
$\Delta z=0.25,M=100$	3.111	1.545	0.760	0.380	0.194		
$\Delta z = 0.5, M = 10$	3.791	1.847	0.904	0.450	0.230		
$\Delta z=0.5,M=50$	3.173	1.552	0.761	0.380	0.194		
$\Delta z = 0.5, M = 100$	3.173	1.552	0.761	0.380	0.194		
$\Delta z=1,M=10$	3.813	1.850	0.904	0.450	0.230		
$\Delta z = 1, M = 50$	3.212	1.559	0.762	0.380	0.194		
$\Delta z = 1, M = 100$	3.212	1.559	0.762	0.380	0.194		
$\Delta z = 2, M = 10$	3.401	1.810	0.903	0.450	0.230		
$\Delta z=2,M=50$	2.763	1.503	0.756	0.379	0.194		
$\Delta z=2,M=100$	2.763	1.503	0.756	0.379	0.194		
$\Delta z=10,M=10$	-0.482	0.506	0.696	0.424	0.228		
$\Delta z=10,M=50$	0.028	0.452	0.554	0.350	0.191		
$\Delta z=10,M=100$	0.028	0.452	0.554	0.350	0.191		
Numerical solution	3.312	2.231	1.425	0.825	0.532		

^a VD (Vertical Discretization) and NTC (Number of Terms for Convergence).

transport processes that cannot be solved exactly, and for validating more comprehensive numerical solutions of the governing transport equations. In contrast to the existing analytical solutions, the analytical solution that is presented here is not limited to the shape of the *u* and *K* profiles, so that it is possible to utilize realistic *u* and *K* profiles.

5. Conclusions

In this work, we present a new integral analytical solution of two-dimensional advection-diffusion equation by using integral transform method considering the eddy diffusivity depending on x and z variables. The model given is general in the sense that it can use any form of parameterization of wind speed u(z) and eddy diffusivity K(x,z) as an explicit function of variables x and z. By analytical we observed that no approximation is made along its derivation, except for the stepwise approximation of the parameters and the Laplace numerical inversion by FT scheme. It is important to mention that analytical solutions are very important to understand and describe the physical phenomenon, since they are able to take into account all the parameters of a problem and investigate their influence. Moreover, we need to remember that air pollution models have two kinds of errors. The first one is due to the physical modeling and another one inherent to the numerical solution of the equation associated to the model. Henceforth, we may affirm that the analytical solution, in some sense, mitigate the error associated to the mathematical model. Therefore, the model errors somehow, restricts to the physical modeling error.

To evaluate the memory effect, which is consistent with the prediction of the Taylor statistical diffusion theory and, therefore, reinforce our confidence in the parameterization (2), a numerical comparison is also made with results that come out of a simulation using the asymptotic vertical eddy diffusivity (Eq. (3)) valid for large diffusion time and the proposed by Brost et al. (1988). The statistical analysis of the results shows a good agreement between the results of the proposed approach using K(x,z) with the experimental ones. Furthermore it is important to emphasize that the results obtained with eddy diffusivity depending on the source distance (Eq. (2)) are better than the ones reached with asymptotic eddy diffusivity (Eq. (3)), valid only for the far field of a low source. The present analysis suggests that the inclusion of the memory effect as modeled by Taylor's theory improves the description of the

turbulent transport process of atmospheric effluent released by a low continuous source.

Acknowledgments

The authors thank CNPq for the partial financial support of this work. The authors also extend special gratitude to the anonymous reviewer for his significant contribution and collaboration in the preparation of the final manuscript.

References

- Abate, J., Valkó, P.P., 2004. Multi-precision Laplace transform inversion. Int. J. Num. Methods Eng. 60, 979–993.
- Arya, S.P., 1995. Modeling and parameterization of near-source diffusion in weak winds. J. Appl. Meteorol. 34, 1112–1122.
- Brost, R.A., Haagenson, P.L., Kuo, Y.H., 1988. The effect of diffusion on tracer puffs simulated by a regional scale Eulerian model. J. Geophys. Res. 93 (D3), 2389– 2404.
- Crank, J., 1979. The Mathematics of Diffusion. Oxford University Press, p. 414.
- Degrazia, G.A., Campos Velho, H.F., Carvalho, J.C., 1997. Nonlocal exchange coefficients for the convective boundary layer derived from spectral properties. Contr. Atmos. Phys. 70 (1), 57–64.
- Degrazia, G.A., Moreira, D.M., Vilhena, M.T., 2001. Derivation of an eddy diffusivity depending on source distance for vertically inhomogeneous turbulence in a convective boundary layer. J. Appl. Meteorol. 40, 1233–1240.
- Demuth, C., 1978. A contribution to the analytical steady solution of the diffusion equation for line sources. Atmos. Environ. 12, 1255–1258.
- Goulart, A.G., Moreira, D.M., Carvalho, J.C., Tirabassi, T., 2004. Derivation of eddy diffusivities from an unsteady turbulence spectrum. Atmos. Environ. 38 (36), 6121–6124.
- Gryning, S.E., van Ulden, A.P., Larsen, S.E., 1983. Dispersion from a continuous ground-level source investigated by a K model. Q. J. R. Meteorol. Soc. 109 (460), 355–364.
- Hanna, S.R., 1989. Confidence limit for air quality models as estimated by bootstrap and jacknife resampling methods. Atmos. Environ. 23, 1385–1395.
- Kumar, P., Sharan, M., 2010. An analytical model for dispersion of pollutants from a continuous source in the atmospheric boundary layer. Proc. R. Soc. Atmos. 466, 383–406.
- Lin, J.S., Hildemann, L.M., 1997. A generalised mathematical scheme to analytically solve the atmospheric diffusion equation with dry deposition. Atmos. Environ. 31, 59–71.

- Moreira, D.M., Tirabassi, T., Carvalho, J.C., 2005a. Plume dispersion simulation in low wind conditions in stable and convective boundary layers. Atmos. Environ. 39 (20), 3643–3650.
- Moreira, D.M., Vilhena, M.T., Tirabassi, T., Buske, D., Cotta, R.M., 2005b. Near source atmospheric pollutant dispersion using the new GILTT method. Atmos. Environ. 39 (34), 6290–6295.
- Moreira, D.M., Vilhena, M.T., Tirabassi, T., Costa, C.P., 2006. Simulation of pollutant dispersion in the atmosphere by the Laplace transform: the ADMM approach. Water Air Soil Pollut. 177, 285–297.
- Moreira, D.M., Vilhena, M.T., 2009. In: Air Pollution and Turbulence: Modeling and Applications, 1st ed. CRC Press, Boca Raton, p. 354.
- Moreira, D.M., Vilhena, M.T., Tirabassi, T., Buske, D., Costa, C.P., 2010. Comparison between analytical models to simulate pollutant dispersion in the atmosphere. Int. J. Environ. Waste Manage. 6 (3–4), 327–344.
- Nieuwstadt, F.T.M., 1980. An analytical solution of the time-dependent, onedimensional diffusion equation in the atmospheric boundary layer. Atmos. Environ. 14, 1361–1364.
- Nieuwstadt, F.T.M., de Haan, B.J., 1981. An analytical solution of one-dimensional diffusion equation in a non-stationary boundary layer with an application to inversion rise fumigation. Atmos. Environ. 15, 845–851.
- Panofsky, H.A., Dutton, J.A., 1984. Atmospheric Turbulence. John Wiley & Sons, New York, p. 397.
- Rounds, W., 1955. Solutions of the two-dimensional diffusion equation. Trans. Am. Geophys. Union 36, 395–405.
- Scriven, R.A., Fisher, B.A., 1975. The long range transport of airborne material and its removal by deposition and washout-II. The effect of turbulent diffusion. Atmos. Environ. 9, 59–69.
- Sharan, M., Singh, M.P., Yadav, A.K., 1996. A mathematical model for the atmospheric dispersion in low winds with eddy diffusivities as linear function of downwind distance. Atmos. Environ. 30, 1137–1145.
- Sharan, M., Modani, M., 2006. A two-dimensional analytical model for the dispersion of air pollutants in the atmosphere with a capping inversion. Atmos. Environ. 40, 3469–3489.
- Sharan, M., Kumar, P., 2009. An analytical model for crosswind integrated concentrations released from a continuous source in a finite atmospheric boundary layer. Atmos. Environ. 43, 2268–2277.
- Smith, F.B., 1957. The diffusion of smoke from a continuous elevated point source into a turbulent atmosphere. J. Fluid Mech. 2, 49–76.
- Stroud, A.H., Secrest, D., 1966. Gaussian Quadrature Formulas. Prentice Hall Inc., Englewood Cliffs, NJ, p. 374.
- Taylor, G.I., 1921. Diffusion by continuous movements. Proc. London Math. Soc. 20, 196–212.
- van Ulden, A.P., 1978. Simple estimates for vertical diffusion from sources near the ground. Atmos. Environ. 12, 2125–2129.
- Wortmann, S., Vilhena, M.T., Moreira, D.M., Buske, D., 2005. A new analytical approach to simulate the pollutant dispersion in the PBL. Atmos. Environ. 39, 2171–2178.