ON THE ANALYTICAL SOLUTION OF THE ADVECTION-DIFFUSION EQUATION WITH TIME VARIABLE EDDY DIFFUSIVITY COEFFICIENT FOR POLLUTANT RELEASE IN ATMOSPHERE

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Abstract. *In these work we present new simulations for the three-dimensional GILTT solution. incorporating in the diffusive model the dependence of the eddy diffusivities on the temporal variable. To solve this kind of problem the Adomian Decomposition Method is used together with the GILTT method. Applying the Adomian decomposition method we reduce the advection-diffusion equation with time dependence of eddy diffusivity to a recursive set of diffuse equations which are straightly solved by the GILTT method. The motivation for such procedure comes from the fact that the resultant recursive problem can be straightly solved by the GILTT method. Simulations and comparisons with experimental data are presented.*

Keywords: *advection-diffusion equation, analytical solution, integral transform*

1. INTRODUCTION

The advection-diffusion equation has been largely applied in the field of air pollution as well, heat and mass transfer problems. Exists a vast literature regarding the issue of numerical solution, but the analytical approaches are scarce and only for specialized problems of pollutant dispersion simulation in atmosphere, where strong assumptions regarding the eddy diffusivity coefficient and wind profile, except for some stationary problems. Rounds (1955), Smith (1957), Scriven and Fischer (1975), Demuth (1978), van Ulden (1978), Nieuwstadt and de Haan (1981), Tagliazucca et al. (1985), Tirabassi (1989), Tirabassi and Rizza (1994), Sharan et al., (1996), Lin and Hildemann (1997), Tirabassi (2003) have derived solutions with constant wind and eddy diffusivity coefficients, where coefficients vary alone or with height, Sharan and Gupta (2002) and Sharan and Modani (2006) have derived solutions considering that the eddy vary linearly with downwind distance from the source, Sharan and Pramod (2009) considered that the eddy vary as a product of power law of height and a integrable function of x.

In the last decade emerged in literature the GILTT approach (Generalized Integral Laplace Transform Technique) whose main feature relies on the analytical solution of transformed GITT (Generalized Integral Transform Technique) solutions (Cotta and Mikhailov, 1997) by the Laplace Transform technique. This methodology has been largely applied in the topic of simulations of pollutant dispersion in the atmospheric boundary layer (Moreira et al., 2006, 2009). Recently was developed a semi-analytical solution for the 3D advection-diffusion equation combining the GILTT with the Advection-Diffusion Multilayer method called GIADMT (Costa et al., 2006, Vilhena et al., 2008). This solution is based on a discretization of the atmospheric boundary layer in N sub-layers where in each sub-layer the advection-diffusion equation is solved by the Laplace transform technique, considering an average value for the eddy diffusivity and wind speed profiles. In 2009 appeared in the literature the three-dimensional GILTT solution (3D-GILTT) (Buske et al. 2009, 2010, 2011). The idea of solution is the application of the integral transform in the y-direction and then the resultant two-dimensional problem solution following the previous works. No approximation is made along the solution derivation so that is an exact solution except for the round-off error. It is important to outline that both the GIADMT and 3D-GILTT methods does not take into account the temporal variation of the eddy-diffusivity coefficient.

In this work we step forward presenting new simulations for more realistic scenarios incorporating in the diffusive model the dependence of the eddy diffusivities on the temporal variable. To reach this goal we consider temporal variation for the eddy diffusivity coefficient in the three-dimensional advection-diffusion equation. To solve this kind of problem the Adomian Decomposition Method (Adomian, 1984, 1988, 1994) is used together with the GILTT method. Applying the decomposition method we reduce the advection-diffusion equation with time dependence of eddy diffusivity to a recursive set of diffuse equations. The motivation for such procedure comes from the fact that the resultant recursive problem can be straightly solved by the GILTT method. Showing the existence of the solution, the Cauchy-Kowalewsky theorem (Courant and Hilbert, 1989) guarantees the uniqueness. To our knowledge, analytical solution for this kind of problem doesn't exist in the literature. Simulations and comparisons with experimental data are presented. This new methodology is a promising result because it may be used for quantitative and qualitative estimations of pollutant distribution. Finally, we can say that the computer code for these solutions can be used for a fast screening of concentration distribution from a given source and as an auxiliary tool in the control of critical events related to air quality.

To reach this goal, we outline the paper as follows: in section 2, we report the derivation of the solution for the three-dimensional advection-diffusion equation in Cartesian geometry. In section 3 the time-dependent eddy-diffusivity coefficient is given. At section 4 preliminary numerical results and the comparison with the experimental data are presented, and finally in section 5, is discussed the principal aspects of this method and conclusions.

2. SOLUTION OF THE ADVECTION-DIFFUSION EQUATION

In the sequel we derive the advection-diffusion equation for the simulation of pollutant releasing in the atmospheric boundary layer assuming Fickian closure of the turbulence. We must recall that this equation is derived combining the continuity equation ruled by the conservation law with the Fickian closure of turbulence. Indeed, we write the advection-diffusion equation in cartesian geometry like Blackadar (1997):

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z} = \frac{\partial}{\partial x}\left(K_x \frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial \bar{c}}{\partial z}\right) \tag{1}$$

subjected to the following boundary and initial conditions:

$$K_z \frac{\partial \bar{c}}{\partial z} = 0 \quad \text{at } z = 0, h \tag{1a}$$

$$K_y \frac{\partial \bar{c}}{\partial y} = 0 \quad \text{at } y = 0, L_y \tag{1b}$$

$$K_x \frac{\partial \bar{c}}{\partial x} = 0 \quad \text{at } x = 0, L_x \tag{1c}$$

$$c(x, y, z, 0) = 0 \quad \text{at } t = 0 \tag{1d}$$

Here we replace the source term by a source condition quoted as:

$$\bar{u}c(0, y, z, t) = Q\delta(y - y_0)\delta(z - H_s) \tag{1e}$$

We must notice that $\bar{c}$ denotes the mean concentration of a passive contaminant (g/m^3) and $\bar{u}$, $\bar{v}$ and $\bar{w}$ are the Cartesian components of the mean wind (m/s) in the directions x ($0 < x < L_x$), y ($0 < y < L_y$) and z ($0 < z < h$). Q is the emission rate (g/s), h the height of the atmospheric boundary layer (m), H_s the height of the source (m), L_x and L_y are the limits in the x and y-axis and far away from the source (m) and δ represents the Dirac delta function. The source position is at x = 0, y = y_0 and z = H_s.

In order to solve the problem (1), taking advantage of the well-known solution of the two-dimensional problem with advection in the x-direction by the GILTT method (Moreira et al., 2009), we initially apply the integral transform technique in the y variable. For such, we expand the pollutant concentration as:

$$\bar{c}(x, y, z, t) = \sum_{m=0}^{M} \bar{c}_m(x, z, t) Y_m(y) \tag{2}$$

where $Y_m(y)$ are a set of orthogonal eigenfunctions, given by $Y_m(y) = \cos(\lambda_m y)$, and $\lambda_m = \frac{m\pi}{L_y}$ (m=0,1,2,...) are respectively the set of eigenvalues.

To determine the unknown coefficient $\bar{c}_m(x, z, t)$ for m = 0:M we began recasting Eq. (1) applying the chain rule for the diffusion terms. Substituting Eq. (2) in the resulting equation:

$$\sum_{m=0}^{M}\Big(-\frac{\partial \bar{c}_m(x,z,t)}{\partial t} Y_m(y) - \bar{u}\frac{\partial \bar{c}_m(x,z,t)}{\partial x} Y_m(y) - \bar{v}\,\bar{c}_m(x,z,t)\,Y_m{}'(y) - \bar{w}\frac{\partial \bar{c}_m(x,z,t)}{\partial z} Y_m(y) +$$

$$K_x \frac{\partial^2 \bar{c}_m(x,z,t)}{\partial x^2} Y_m(y) + K_x' \frac{\partial \bar{c}_m(x,z,t)}{\partial x} Y_m(y) + K_y\,\bar{c}_m(x,z,t)\,Y_m''(y) + \tag{3}$$

$$+K_y{}'\,\bar{c}_m(x,z,t)\,Y_m{}'(y) + K_z \frac{\partial^2 \bar{c}_m(x,z,t)}{\partial z^2} Y_m(y) + K_z{}' \frac{\partial \bar{c}_m(x,z,t)}{\partial z} Y_m(y)\Big) = 0$$

and taking moments, meaning applying the operator $\int_0^{Ly} Y_n(y)dy$, we obtain the result:

$$\sum_{m=0}^{M}\Big(-\frac{\partial \bar{c}_m(x,z,t)}{\partial t}\int_0^{Ly} Y_m(y)Y_n(y)dy - \bar{u}\frac{\partial \bar{c}_m(x,z,t)}{\partial x}\int_0^{Ly} Y_m(y)Y_n(y)dy +$$
$$-\bar{v}\,\bar{c}_m(x,z,t)\int_0^{Ly} Y_m{}'(y)Y_n(y)dy - \bar{w}\frac{\partial \bar{c}_m(x,z,t)}{\partial z}\int_0^{Ly} Y_m(y)Y_n(y)dy +$$
$$+K_x\frac{\partial^2 \bar{c}_m(x,z,t)}{\partial x^2}\int_0^{Ly} Y_m(y)Y_n(y)dy + K_x'\frac{\partial \bar{c}_m(x,z,t)}{\partial x}\int_0^{Ly} Y_m(y)Y_n(y)dy + \quad (4)$$
$$-\lambda_m^2\,\bar{c}_m(x,z,t)\int_0^{Ly} K_y\,Y_m(y)Y_n(y)dy + \bar{c}_m(x,z,t)\int_0^{Ly} K_y'\,Y_m{}'(y)Y_n(y)dy$$
$$+ K_z\frac{\partial^2 \bar{c}_m(x,z,t)}{\partial z^2}\int_0^{Ly} Y_m(y)Y_n(y)dy + K_z{}'\frac{\partial \bar{c}_m(x,z,t)}{\partial z}\int_0^{Ly} Y_m(y)Y_n(y)dy\Big) = 0$$

Defining the integrals appearing in the above equation like:

$$\int_0^{Ly} Y_m(y)Y_n(y)dy = \alpha_{n,n}\,;\ \int_0^{Ly} Y_m{}'(y)Y_n(y)dy = \beta_{n,n}\,;$$

$$\int_0^{Ly} K_y\,Y_m(y)Y_n(y)dy = \gamma_{m,n}\,;\int_0^{Ly} K_y'\,Y_m{}'(y)Y_n(y)dy = \eta_{m,n}$$

using these definitions we recast Eq. (4) as:

$$\sum_{m=0}^{M}\Big(-\alpha_{n,n}\frac{\partial \bar{c}_m(x,z,t)}{\partial t} - \bar{u}\,\alpha_{n,n}\frac{\partial \bar{c}_m(x,z,t)}{\partial x} - \bar{v}\,\beta_{n,n}\,\bar{c}_m(x,z,t) - \bar{w}\,\alpha_{n,n}\frac{\partial \bar{c}_m(x,z,t)}{\partial z} + K_x\,\alpha_{n,n}\frac{\partial^2 \bar{c}_m(x,z,t)}{\partial x^2} +$$
$$K_x'\,\alpha_{n,n}\frac{\partial \bar{c}_m(x,z,t)}{\partial x} - \lambda_m^2\,\gamma_{m,n}\,\bar{c}_m(x,z,t) + \eta_{m,n}\bar{c}_m(x,z,t) + K_z\,\alpha_{n,n}\frac{\partial^2 \bar{c}_m(x,z,t)}{\partial z^2} + K_z{}'\,\alpha_{n,n}\frac{\partial \bar{c}_m(x,z,t)}{\partial z}\Big) = 0 \quad (5)$$

Without losing generality, we specialize the application for a pollutant dispersion problem in atmospheric boundary layer, assuming that the speeds $\bar{v}$ and $\bar{w}$ takes the null value and we neglect the diffusion component K_x because we assume that the advection is dominant in the x-direction. Further we also consider that K_y has only dependence on the z-direction. After these assumptions, Eq. (5) reads in matrix fashion like:

$$-\begin{bmatrix}1&0&\cdots&0\\0&1&\cdots&0\\\vdots&\vdots&\ddots&\vdots\\0&0&\cdots&1\end{bmatrix}\begin{bmatrix}\frac{\partial \bar{c}_0}{\partial t}\\\frac{\partial \bar{c}_1}{\partial t}\\\vdots\\\frac{\partial \bar{c}_M}{\partial t}\end{bmatrix} - \bar{u}\begin{bmatrix}1&0&\cdots&0\\0&1&\cdots&0\\\vdots&\vdots&\ddots&\vdots\\0&0&\cdots&1\end{bmatrix}\begin{bmatrix}\frac{\partial \bar{c}_0}{\partial x}\\\frac{\partial \bar{c}_1}{\partial x}\\\vdots\\\frac{\partial \bar{c}_M}{\partial x}\end{bmatrix} + K_z\begin{bmatrix}1&0&\cdots&0\\0&1&\cdots&0\\\vdots&\vdots&\ddots&\vdots\\0&0&\cdots&1\end{bmatrix}\begin{bmatrix}\frac{\partial^2 \bar{c}_0}{\partial z^2}\\\frac{\partial^2 \bar{c}_1}{\partial z^2}\\\vdots\\\frac{\partial^2 \bar{c}_M}{\partial z^2}\end{bmatrix} +$$
$$+K_z{}'\begin{bmatrix}1&0&\cdots&0\\0&1&\cdots&0\\\vdots&\vdots&\ddots&\vdots\\0&0&\cdots&1\end{bmatrix}\begin{bmatrix}\frac{\partial \bar{c}_0}{\partial z}\\\frac{\partial \bar{c}_1}{\partial z}\\\vdots\\\frac{\partial \bar{c}_M}{\partial z}\end{bmatrix} - \lambda_m^2 K_y\begin{bmatrix}1&0&\cdots&0\\0&1&\cdots&0\\\vdots&\vdots&\ddots&\vdots\\0&0&\cdots&1\end{bmatrix}\begin{bmatrix}\frac{\partial \bar{c}_0}{\partial z}\\\frac{\partial \bar{c}_1}{\partial z}\\\vdots\\\frac{\partial \bar{c}_M}{\partial z}\end{bmatrix} = 0$$

which clearly leads to the ensuing set of M + 1 two-dimensional diffusion equations:

$$\frac{\partial \bar{c}_m(x,z,t)}{\partial t} + \bar{u}\frac{\partial \bar{c}_m(x,z,t)}{\partial x} = \frac{\partial}{\partial z}\Big(K_z\frac{\partial \bar{c}_m(x,z,t)}{\partial z}\Big) - \lambda_m^2\,K_y\,\bar{c}_m(x,z,t) \quad (6)$$

In this work we consider that the eddy diffusivity in the z variable has time dependence (i.e. $K_z(z,t)$), so is not possible apply the Laplace transform technique to Eq. (6) reducing the transient problem to a stationary problem like in the previous works that used the GILTT method. To solve the problem with time dependence of eddy diffusivity the Adomian Decomposition Method is used together with the GILTT method. Applying the Adomian decomposition method we reduce the advection-diffusion equation with time dependence of eddy diffusivity to a recursive set of diffuse equations. The motivation for such procedure comes from the fact that the resultant recursive problem can be straightly solved by the GILTT method.

The decomposition method is an efficient procedure for solving analytically linear and non-linear differential equations with the advantage that it provides a direct scheme for solving the problem without the need for linearization or transformations. The decomposition procedure permits to cast the solution into a convergent series by using the necessary number of iterations and then rewrite the linear or non-linear problem in a system of recursive linear problems whose solution is known. In the sequel we briefly present the idea of the solution derivation considering the decomposition method.

Considering in problem (6) that $K_z(z,t)$ is rewritten like $K_z(z,t) = k_z(z,t) + \bar{k}_z(z)$ where $\bar{k}_z(z) = \frac{\int_0^t K_z(z,t)dt}{t}$, we have the following equation to solve:

$$\frac{\partial \bar{c}_m(x,z,t)}{\partial t} + \bar{u}\,\frac{\partial \bar{c}_m(x,z,t)}{\partial x} = \frac{\partial}{\partial z}\left(\bar{k}_z(z)\,\frac{\partial \bar{c}_m(x,z,t)}{\partial z}\right) + \frac{\partial}{\partial z}\left(k_z(z,t)\,\frac{\partial \bar{c}_m(x,z,t)}{\partial z}\right) - \lambda_m^2\, K_y\, \bar{c}_m(x,z,t) \tag{7}$$

Initially, following the decomposition method, we pose that the concentration can be expanded in a truncated series like:

$$\bar{c}_m(x,z,t) = \sum_{l=0}^{L} \bar{c}_{m,l}(x,z,t) \tag{8}$$

Replacing Eq. (8) in Eq. (7) we obtain one equation and (L+1) unknowns $\{\bar{c}_{m,l}(x,z,t)\}$. So, we are in position to construct a recursive set of diffusive equations whose solution is known. Obviously this construction is not unique. The recursive set chosen is:

$$\begin{cases} \frac{\partial \bar{c}_{m,0}(x,z,t)}{\partial t} + \bar{u}\,\frac{\partial \bar{c}_{m,0}(x,z,t)}{\partial x} - \frac{\partial}{\partial z}\left(\bar{k}_z(z)\,\frac{\partial \bar{c}_{m,0}(x,z,t)}{\partial z}\right) + \lambda_m^2\, K_y\, \bar{c}_{m,0}(x,z,t) = 0 \\ \frac{\partial \bar{c}_{m,1}(x,z,t)}{\partial t} + \bar{u}\,\frac{\partial \bar{c}_{m,1}(x,z,t)}{\partial x} - \frac{\partial}{\partial z}\left(\bar{k}_z(z)\,\frac{\partial \bar{c}_{m,1}(x,z,t)}{\partial z}\right) + \lambda_m^2\, K_y\, \bar{c}_{m,1}(x,z,t) = S_1(x,z,t) \\ \vdots \\ \frac{\partial \bar{c}_{m,L}(x,z,t)}{\partial t} + \bar{u}\,\frac{\partial \bar{c}_{m,L}(x,z,t)}{\partial x} - \frac{\partial}{\partial z}\left(\bar{k}_z(z)\,\frac{\partial \bar{c}_{m,L}(x,z,t)}{\partial z}\right) + \lambda_m^2\, K_y\, \bar{c}_{m,L}(x,z,t) = S_L(x,z,t) \end{cases} \tag{9}$$

where we have the following notation for the term S_L :

$$S_L(x,z,t) = \frac{\partial}{\partial z}\left(k_z(z,t)\,\frac{\partial \bar{c}_{m,L-1}(x,z,t)}{\partial z}\right) \qquad \text{for } l = 1{:}L \tag{10}$$

The solutions of the homogeneous equations (9) are easily obtained by the standard procedure of the GILTT approach for eddy diffusivity depending on height (Moreira et al., 2006, 2009). Moreover, it is important to emphasize that the first problem of the recursive set (9) satisfies the initial, boundary and source conditions by Eqs. (1a-e), while the remaining problems satisfy homogeneous conditions. Once the set of problems (9) is solved, the solution for problem (1) is well determined using Eq. (8). The result accuracy is then controlled by the number of terms in the series summation of the solution.

3. TIME DEPENDENT EDDY DIFFUSIVITY

In order to illustrate the suitability of the discussed formulation to simulate contaminant dispersion in the atmospheric boundary layer, we evaluate the performance of the new solution against experimental ground-level concentration. To do this we have to introduce a boundary layer parameterization. In the atmospheric diffusion problems the choice of a turbulent parameterization represents a fundamental aspect for the contaminants dispersion modeling. From a physical point of view a turbulence parameterization is an approximation to nature in the sense that we are putting in mathematical models an approximated relation that in principle can be used as a surrogate for the natural true unknown term. The reliability of each model strongly depends on the way as turbulent parameters are calculated and related to the current understanding of the atmospheric boundary layer (Mangia et al., 2002)

The present parameterization is based on the Taylor statistical diffusion theory and a turbulent kinetic energy spectral model to derive parameters that express the capability of dispersion in a atmospheric boundary layer dominated by convective turbulence. The derivation of the time-dependent eddy diffusivity coefficient gives a algebraic expression for the eddy diffusivity as suggested by Degrazia (2002):

$$K_z = \frac{0.583 w_* h c_w \psi^{2/3} (z/h)^{4/3} T^* \left[0.55 (z/h)^{2/3} + 1.03 c_w^{1/2} \psi^{1/3} \left(f_m^*\right)_w^{2/3} T^*\right]}{\left[0.55 (z/h)^{2/3} \left(f_m^*\right)_w^{1/3} + 2.06 c_w^{1/2} \psi^{1/3} \left(f_m^*\right)_w T^*\right]^2} \tag{11}$$

where *n'* is non-dimensional frequency, T^* is the non-dimensional time ($T^* = \frac{t\, w_*}{\bar{u}\, h}$), w_* is the convective velocity scale, $c_w=0.36$, $(f_m^*)_w$ is the normalized frequency of the spectral peak namely:

$$(f_m^*)_w = \frac{z}{(\lambda_m)_w} = 0.55\left(\frac{z}{h}\right)\left[1 - \exp\left(-\frac{4z}{h}\right) - 0.0003\exp\left(\frac{8z}{h}\right)\right]^{-1} \tag{12}$$

for the vertical component. Further, $(\lambda_m)_w = 1.8h[1 - \exp(-4z/h) - 0.0003\exp(8z/h)]$ is the value of the spectral peak of vertical wavelength.

For the eddy diffusivity in the y-direction we used the following expression:

$$K_y = \frac{\sqrt{\pi}\,\sigma_v}{16\left(f_m\right)_v q_v} \tag{13}$$

with $\sigma_v^2 = \frac{0.98 c_v}{\left(f_m\right)_v^{2/3}}\left(\frac{\psi_\varepsilon}{q_v}\right)^{2/3}\left(\frac{z}{h}\right)^{2/3} w_*^2$; $q_v = 4.16\frac{z}{h}$; $\left(f_m\right)_v = 0.16$ and $\psi_\varepsilon^{1/3} = \left[\left(1-\frac{z}{h}\right)^2\left(-\frac{z}{L}\right)^{-2/3} + 0.75\right]^{1/2}$. More, *k* is the von Karman constant (*k* = 0.4), σ_v is the Eulerian standard deviation of the longitudinal turbulent velocity, q_v is the stability function, ψ_ε is the non-dimensional molecular dissipation rate function and $\left(f_m\right)_v$ is the peak wavelength of the turbulent velocity spectra.

4. NUMERICAL RESULTS

In order to illustrate the aptness of the discussed formulation to simulate contaminant dispersion in the atmospheric boundary layer, we evaluate the performance of the discussed solutions against experimental centerline concentrations using the Copenhagen dispersion experiment. This experiment was carried out in the northern part of Copenhagen, described by Gryning and Lyck (1984). It consisted of tracer released without buoyancy from a tower at a height of 115 m, and collection of tracer sampling units at the ground-level positions at the maximum of three crosswind arcs. The sampling units were positioned at two to six kilometers from the point of release. The site was mainly residential with a roughness length of the 0.6 m. Table 1 summarizes the meteorological conditions of the Copenhagen experiment where L is the Monin-Obukhov length, h is the height of the convective boundary layer, w_* is the convective velocity scale and u_* is the friction velocity.

Table 1: Meteorological conditions of the Copenhagen experiment.

Expt	$\bar{u}\,(115m)$ *(ms^{-1})*	$\bar{u}\,(10m)$ *(ms^{-1})*	u_* *(ms^{-1})*	*L (m)*	w_* *(ms^{-1})*	*h (m)*
1	3.4	2.1	0.36	-37	1.8	1980
2	10.6	4.9	0.73	-292	1.8	1920
3	5.0	2.4	0.38	-71	1.3	1120
4	4.6	2.5	0.38	-133	0.7	390
5	6.7	3.1	0.45	-444	0.7	820
6	13.2	7.2	1.05	-432	2.0	1300
7	7.6	4.1	0.64	-104	2.2	1850
8	9.4	4.2	0.69	-56	2.2	810
9	10.5	5.1	0.75	-289	1.9	2090

The wind speed profile used in the simulations is described by a power law expressed as follows (Panofsky and Dutton, 1988):

$$\frac{\overline{u_z}}{\overline{u_1}} = \left(\frac{z}{z_1}\right)^n \qquad (14)$$

where $\overline{u}_z$ and $\overline{u}_1$ are the mean wind speeds horizontal to heights z and z_1 and n is an exponent that is related to the intensity of turbulence (Irwin, 1979), that is, n = 0.1 in unstable conditions.

Figure 1 presents a plotter of the K_z(z,t) for three different times (t = 500, 1500, 2500s) using the experiment 8 of Copenhagen. Figure 2 shows the scatter diagram of the centerline ground-level observed concentrations versus the simulated by the 3D-GILTT model, normalized by the emission rate and using two points in the time Gaussian Quadrature inversion (Moreira et al., 2006; Stroud and Secrest, 1966)). In the scatter diagram analysis, closer the data are form the 45 degree line, better are the results. The lateral lines indicate a factor of two (FA2), i.e, if all the obtained data are between these lines we have a FA2 equal to 1 (maximum value). Having a look to the scatter diagram presented in Fig. 2 we promptly realize that the 3D-GILTT model reproduces satisfactorily the observed concentrations for these points of quadrature.

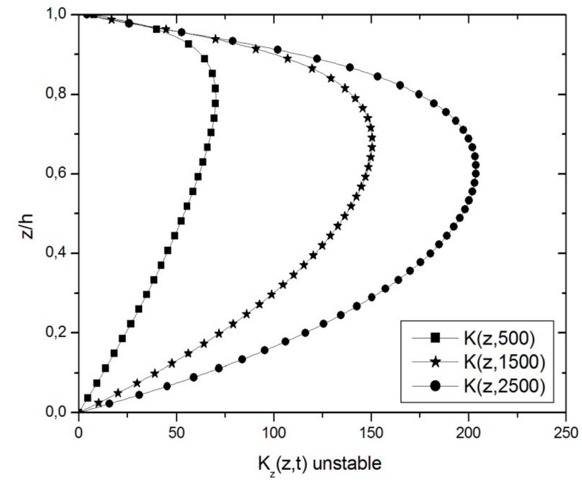

Figure 1 – Plot of the K_z(z,t) for three different times (t = 500, 1500, 2500s) using the experiment 8 of Copenhagen

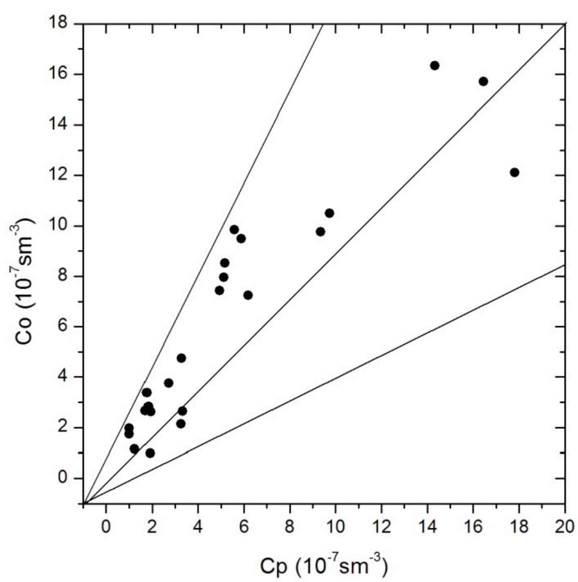

Figure 2 – Observed (Co) and predicted (Cp) scatter plot of centerline concentration using the Copenhagen dataset. Data between dotted lines correspond to ratio Co/Cp∈[0.5,2].

In Tab. 2 we compare the experimental findings with the model predictions by the proposed procedure. From the comparison one observes a reasonable agreement among the model and the experimental data. On the other hand in Tab. 3, we indicate the numerical convergence of the new approach. The convergence analysis shows that few terms in the series solution, represent an analytical solution with spurious errors. As expected we realize a faster numerical convergence far from the source, in the sense that we got a prescribed accuracy with a few terms of series summation. You must also notice that μ_l denotes the components of the series solution.

Table 2: Concentrations of nine runs with various positions of the Copenhagen experiment and model prediction by the 3D-GILTT approach with time dependence of eddy diffusivity.

Run	***Distance (m)***	***Observed*** *($10^{-7}s.m^{-3}$)*	***Predictions*** *($10^{-7}s.m^{-3}$)*
1	1900	10.5	9.73
1	3700	2.14	3.26
2	2100	9.85	5.57
2	4200	2.83	1.83
3	1900	16.33	14.33
3	3700	7.95	5.12
3	5400	3.76	2.72
4	4000	15.71	16.44
5	2100	12.11	17.82
5	4200	7.24	6.19
5	6100	4.75	3.28
6	2000	7.44	4.93
6	4200	3.47	1.76
6	5900	1.74	1.00
7	2000	9.48	5.88
7	4100	2.62	1.95
7	5300	1.15	1.23
8	1900	9.76	9.34
8	3600	2.64	3.33
8	5300	0.98	1.91
9	2100	8.52	5.16
9	4200	2.66	1.70
9	6000	1.98	1.00

In the further we use standard statistical indices in order to compare the quality of the two approaches. Note that we present the two analytical model approaches, since the earlier one was found to be acceptable in comparison to other approaches found in the literature and both give a solution in closed form. Table 2 present some performances evaluations of the model results using the statistical evaluation procedure described by Hanna (1989) and defined in the following way:

NMSE (normalized mean square error) = $\overline{(C_o - C_p)^2} \big/ \overline{C_p}\,\overline{C_o}$,

FA2 = fraction of data (%, normalized to 1) for $0.5 \le (C_p / C_o) \le 2$,

COR (correlation coefficient) = $\overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} \big/ \sigma_o \sigma_p$,

FB (fractional bias) = $\overline{C_o} - \overline{C_p} \big/ 0.5(\overline{C_o} + \overline{C_p})$,

FS (fractional standard deviations) = $(\sigma_o - \sigma_p) \big/ 0.5(\sigma_o + \sigma_p)$,

where the subscripts o and p refer to observed and predicted quantities, respectively, and the overbar indicates an averaged value. The statistical index FB says if the predicted quantities underestimate or overestimate the observed ones. The statistical index NMSE represents the model values dispersion in respect to data dispersion. The best results are expected to have values near to zero for the indices NMSE, FB and FS, and near to 1 in the indices COR and FA2. The statistical indices point out that a reasonable agreement is obtained between experimental data and the 3D-GILTT model.

Table 3: Numerical convergence of the 3D-GILTT model with time dependence of eddy diffusivity for each distance of the 9 experiments of Copenhagen.

Run	***Terms Adomian decomposition***	$\bar{c}(x,y,z,t)$ ***(10⁻⁷s.m⁻³)***		
1	μ_0	7.76	2.65	
	$\mu_0+\mu_1$	10.04	3.27	
	$\mu_0+\mu_1+\mu_2$	9.73	3.26	
	$\mu_0+\mu_1+\mu_2+\mu_3$	9.73	3.26	
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	9.73	3.26	
2	μ_0	4.76	1.63	
	$\mu_0+\mu_1$	5.70	1.85	
	$\mu_0+\mu_1+\mu_2$	5.58	1.83	
	$\mu_0+\mu_1+\mu_2+\mu_3$	5.57	1.83	
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	5.57	1.83	
3	μ_0	10.14	3.65	1.88
	$\mu_0+\mu_1$	15.21	5.17	2.72
	$\mu_0+\mu_1+\mu_2$	14.38	5.12	2.72
	$\mu_0+\mu_1+\mu_2+\mu_3$	14.33	5.12	2.72
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	14.33	5.12	2.72
4	μ_0	6.33		
	$\mu_0+\mu_1$	16.48		
	$\mu_0+\mu_1+\mu_2$	16.44		
	$\mu_0+\mu_1+\mu_2+\mu_3$	16.44		
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	16.44		
5	μ_0	11.79	4.30	2.26
	$\mu_0+\mu_1$	19.86	6.36	3.30
	$\mu_0+\mu_1+\mu_2$	18.08	6.17	3.28
	$\mu_0+\mu_1+\mu_2+\mu_3$	17.82	6.18	3.28
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	17.82	6.19	3.28
6	μ_0	4.13	1.55	0.89
	$\mu_0+\mu_1$	5.07	1.78	1.01
	$\mu_0+\mu_1+\mu_2$	4.93	1.76	1.00
	$\mu_0+\mu_1+\mu_2+\mu_3$	4.93	1.76	1.00
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	4.93	1.76	1.00
7	μ_0	4.98	1.71	1.09
	$\mu_0+\mu_1$	6.02	1.96	1.23
	$\mu_0+\mu_1+\mu_2$	5.89	1.95	1.23
	$\mu_0+\mu_1+\mu_2+\mu_3$	5.88	1.95	1.23
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	5.88	1.95	1.23
8	μ_0	6.13	2.41	1.37
	$\mu_0+\mu_1$	9.70	3.35	1.91
	$\mu_0+\mu_1+\mu_2$	9.35	3.33	1.91
	$\mu_0+\mu_1+\mu_2+\mu_3$	9.34	3.33	1.91
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	9.34	3.33	1.91
9	μ_0	4.48	1.54	0.92
	$\mu_0+\mu_1$	5.26	1.72	1.01
	$\mu_0+\mu_1+\mu_2$	5.16	1.70	1.00
	$\mu_0+\mu_1+\mu_2+\mu_3$	5.16	1.70	1.00
	$\mu_0+\mu_1+\mu_2+\mu_3+\mu_4$	5.16	1.70	1.00

Table 4: Statistical comparison between the 3D-GILTT model and the Copenhagen dataset.

Model	***NMSE***	***COR***	***FA2***	***FB***	***FS***
3D-GILTT	0.14	0.91	1.00	0.15	-0.07

5. CONCLUSIONS

We presented an analytical approach to solve the three-dimensional advection-diffusion equation using integral transform techniques and the Adomian decomposition method considering temporal variation of the eddy diffusivity coefficient. The Cauchy-Kowalewski theorem guarantees the existence and uniqueness of the solution, because no approximation is made along the solution derivation except for the series truncation of the solution. Therefore, we are confident to underline the novelty of the proposed solution because, to our knowledge, analytical solutions are not found in the literature for this sort of problem with the eddy diffusivity coefficient depending on variables z and t.

Analytical solutions of equations are of fundamental importance in understanding and describing physical phenomena, since they are able to take into account all the parameters of a problem, and investigate their influence. Moreover, when using models, while they are rather sophisticated instruments that ultimately reflect the current state of knowledge on turbulent transport in the atmosphere, the results they provide are subject to a considerable margin of error. This is due to various factors, including in particular the uncertainty of the intrinsic variability of the atmosphere. Models, in fact, provide values expressed as an average, i.e., a mean value obtained by the repeated performance of many experiments, while the measured concentrations are a single value of the sample to which the ensemble average provided by models refer. This is a general characteristic of the theory of atmospheric turbulence and is a consequence of the statistical approach used in attempting to parameterize the chaotic character of the measured data. An analytical solution can be useful in evaluating the performances of numerical model (that solve numerically the advection diffusion equation) that could compare their results, not only against experimental data but, in an easier way, with the solution itself in order to check numerical errors without the uncertainties presented above.

We will step forward checking the new model to other stability conditions, apply to different parameterizations and compare the results with other experimental data sets.

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