Simulation of Pollutant Dispersion in the Atmosphere under Unstable Conditions Using an Analytical Solution

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Abstract. *Analytical solutions of equations are of fundamental importance in understanding and describing physical phenomena. In this work we present the solution of the two-dimensional advection-diffusion equation in Cartesian geometry by the GILTT approach, considering that the eddy diffusivity and the vertical wind profile depends on the z variable. To carry more information of the original problem, a Sturm-Liouville problem given by Bessel functions is used as basis in the solution. Numerical simulations and comparisons with experimental data are presented.*

1. Introduction

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 and it easy to obtain the asymptotic behavior of the solution, which is usually difficult to generate through numerical calculations. 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.

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). We mention the works of Rounds (1955), Smith (1957), Scriven and Fischer (1975), Demuth (1978), van Ulden (1978), Nieuwstadt (1980), Nieuwstadt and de Haan (1981), Tagliazucca et al. (1985), Tirabassi (1989), Koch (1989), Tirabassi and Rizza (1994), Sharan et al., (1996), Lin and Hildemann (1997), Sharan and Modani (2005, 2006). These solutions are valid for very specialized practical situations with restrictions on wind and eddy diffusivities vertical profiles. To solve the advection-diffusion equation for more realistic physical scenario appeared in the literature the ADMM (Advection Diffusion Multilayer Method) approach (Moreira et al. (2006), Costa et al. (2006)), valid for any eddy diffusivity and wind profile depending on the height. The main idea relies on the discretisation of the ABL in a multilayer domain, assuming in each layer that the eddy diffusivity and wind profile take averaged values. The resulting advection-diffusion equation in each layer is then solved by the Laplace Transform technique. A more general methodology, that skips the multilayer discretisation of the height z appearing in the ADMM approach, is known in the literature as GILTT (Generalized Integral Laplace Transform Technique) approach. The main idea of this methodology comprehends the steps: expansion of the concentration in series of eigenfunctions attained from an auxiliary problem, replacing this equation in the advection-diffusion equation and taking moments, we come out with a matrix ordinary differential equation that is then solved analytically by the Laplace Transform technique (Moreira et al. (2009), Buske et al. (2011, 2012)). Similar solutions were proposed by Kumar e Sharan (2010) and Guerreiro et al. (2012).

To reach our objective, we begin presenting the solution of the two-dimensional advection-diffusion equation in Cartesian geometry by the GILTT approach, considering that the eddy diffusivity and the vertical wind profile depends on the z variable (is important to remember that the eddy diffusivity can depend also on time and space as in the articles of Moreira et al. (2009) and Vilhena et al. (2012)). Traditionally, the GILTT approach uses as basis eigenfunctions given in terms of cosine functions. Here, a new Sturm-Liouville problem will be considered, carrying more information of the original problem. In this case, the eigenfunctions are given by Bessel functions. Once we construct the general solution, numerical simulations and future perspectives of this methodology are presented.

2. The advection-diffusion equation and the GILTT method

The advection-diffusion equation of air pollution in the atmosphere is essentially a statement of conservation of the suspended material and it can be written as:

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z} = -\frac{\partial \overline{u'c'}}{\partial x} - \frac{\partial \overline{v'c'}}{\partial y} - \frac{\partial \overline{w'c'}}{\partial z} + S \tag{1}$$

where $\bar{c}$ denotes the average concentration of a passive contaminant (g/m^3), $\bar{u}$, $\bar{v}$, $\bar{w}$ are the mean wind (m/s) components along the axis x, y and z, respectively and S is the source term. The terms $\overline{u'c'}$, $\overline{v'c'}$ and $\overline{w'c'}$ represent, respectively, the turbulent fluxes of contaminants (g/sm^2) in the longitudinal, crosswind and vertical directions.

One of the most widely used closures for Eq. (1), is based on the gradient transport hypothesis (or K-theory) which, in analogy with the Fick's law of molecular diffusion, assumes that turbulence causes a net movement of material down the gradient of material concentration at a rate which is proportional to the magnitude of the gradient (Seinfeld and Pandis (1998)):

$$\overline{u'c'} = -K_x \frac{\partial \bar{c}}{\partial x} \quad ; \quad \overline{v'c'} = -K_y \frac{\partial \bar{c}}{\partial y} \quad ; \quad \overline{w'c'} = -K_z \frac{\partial \bar{c}}{\partial z} \tag{2}$$

where K_x, K_y, K_z are the Cartesian components of eddy diffusivity (m^2/s) in the x, y and z directions, respectively. In the first order closure all the information on the turbulence complexity is contained in the eddy diffusivities.

The Eq. (2), combined with the continuity equation of mass, leads to the advection-diffusion equation. For a Cartesian coordinate system we rewrite the advection-diffusion equation like (Blackadar (1997)):

$$\frac{\partial \bar{c}}{\partial t}+\bar{u}\frac{\partial \bar{c}}{\partial x}+\bar{v}\frac{\partial \bar{c}}{\partial y}+\bar{w}\frac{\partial \bar{c}}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial \bar{c}}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial \bar{c}}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial \bar{c}}{\partial z}\right)+S \qquad (3)$$

The advection-diffusion equation (3) can be solved analytically by the 3D-GILTT approach (Buske et al. (2011, 2012), Vilhena et al. (2012)). Here, for comparison with experimental data we will assume for the advection-diffusion equation (3): stationary conditions, crosswind integrated concentrations and that the advection is much higher than the diffusion in the x-direction. After the simplifications, let us consider the problem:

$$\bar{u}\frac{\partial \overline{c_y}}{\partial x}=\frac{\partial}{\partial z}\left(K_z\frac{\partial \overline{c_y}}{\partial z}\right), \qquad (4)$$

for $0<z<h$ and $x>0$, subject to the boundary conditions of zero flux at the ground and ABL top and a source with emission Q at height H_s ($\overline{u c_y}(0,z)=Q\delta(z-H_s)$ at x = 0). Here $\overline{c_y}$ represents the crosswind integrated concentration, h is the ABL height, K_z is the eddy diffusivity variable with the height z ($K_z=K(z)$), $\bar{u}$ is the longitudinal wind speed ($\bar{u}=\bar{u}(z)$), and δ is the Dirac delta function.

Following the works of Moreira et al. (2009), Buske et al. (2011) and Vilhena et al. (2012) we pose that the solution of problem (4) has the form:

$$\overline{c_y}(x,z)=\sum_{n=0}^{N}\bar{c}_n(x)\Psi_n(z) \qquad (5)$$

where $\Psi_n(z)$ are the eigenfunctions of an associated Sturm-Liouville problem and $\bar{c}_n(x)$ is the transformed concentration.

In the application of the GILTT method, the following auxiliary Sturm-Liouville problem is chosen:

$$\Psi_n''(z)+\lambda_n^2\Psi_n(z)=0 \qquad \text{at} \quad 0<z<h \qquad (6a)$$

$$\Psi_n'(z)=0 \qquad \text{at} \quad z=0, h, \qquad (6b)$$

which has the solution $\Psi_n(z)=\cos(\lambda_n z)$, where $\Psi_n(z)$ are the eigenfunctions and $\lambda_n=n\pi/h$ (*n=0,1,2,...*) are the respective eigenvalues.

Here, a different expansion for the solution of the advection-diffusion equation will be explored. In other words, we propose another Sturm-Liouville problem as the basis generator. The idea of this proposal comes from the fact that the auxiliary problem (6) has the same shape of the ordinary differential equation (relative do z variable) that appears in the solution of Eq. (4) by the method of separation of variables, when the vertical eddy diffusivity is considered constant. This suggests the possibility of using a new auxiliary problem that appears in the solution of Eq. (4) by the method of separation of variables, considering linear vertical eddy diffusivity, $K_z = z$, given by:

$$\Psi_n'(z\ \Psi_n'(z))+\lambda_n^2\Psi_n(z)=0 \qquad \text{at} \quad 0<z<h \qquad (7a)$$

$$\Psi_n'(z)=0 \qquad \text{at} \quad z=0, h, \qquad (7b)$$

which has Bessel functions of first specie and order zero as solution $\Psi_n(z)=J_0(\lambda_n\sqrt{z/h})$, where λ_n (*n=0,1,2,...*) are the positive roots of the Bessel function of first specie and order one, J_1. Problem (7) carries more information from the original problem than the series expansion (5).

To determine the unknown coefficient $\bar{c}_n(x)$ we replace Eq. (5) in Eq. (3) and applying the operator $\int_0^h (\,)\Psi_m(z)dz$, we come out with the result:

$$\sum_{n=0}^{N} \bar{c}_n\,'(x) \int_0^h u\Psi_n \Psi_m \, dz - \sum_{n=0}^{N} \bar{c}_n(x) \int_0^h \Psi_m \frac{\partial}{\partial z}\left(K_z \frac{\partial \Psi_n}{\partial z} \right) dz = 0 \,. \tag{8}$$

Observe that, using the integration parts technique, we can recast the second integral in Eq. (8) as:

$$\int_0^h \Psi_m \frac{\partial}{\partial z}\left(K_z \frac{\partial \Psi_n}{\partial z} \right) dz = \Psi_m K_z \frac{\partial \Psi_n\,'}{\partial z} - \int_0^h \Psi_m\,' K_z \frac{\partial \Psi_n\,'}{\partial z} dz = -\int_0^h \Psi_m\,' K_z \frac{\partial \Psi_n\,'}{\partial z} dz$$

once $\Psi_m K_z \frac{\partial \Psi_n\,'}{\partial z} = 0$ for both Sturm-Liouville problems considered in this work (Eqs. (6) and (7)). Therefore, Eq. (8) is rewritten as:

$$\sum_{n=0}^{N} \bar{c}_n\,'(x) \int_0^h u\Psi_n \Psi_m \, dz + \sum_{n=0}^{N} \bar{c}_n(x) \int_0^h \Psi_m\,' K_z \frac{\partial \Psi_n\,'}{\partial z} dz = 0 \tag{9}$$

which can be recast in matrix form like:

$$Y^{'}(x) + FY(x) = 0 \,, \tag{10}$$

subject to the initial condition $Y(0) = \bar{c}_n(0)$. Here *Y(x)* is the vector whose components are $\bar{c}_n(x)$ and $F = B^{-1}.E$; $B = \{b_{n,\mathrm{m}}\}$ and $E = \{e_{n,\mathrm{m}}\}$ are the matrices whose entries are, respectively:

$$b_{n,m} = \int_0^h \bar{u}\Psi_n \Psi_m dz \qquad \text{and} \qquad e_{n,m} = \int_0^h \Psi_m\,' K_z \frac{d\Psi_n\,'}{dz} dz \,.$$

The vector Y(0) is obtained from the source condition, by a similar procedure leading to $Y(0) = \bar{c}_n(0) = Q\Psi_m(H_s)B^{-1}$, where B^{-1} is the inverse of matrix *B* given above.

The transformed problem represented by the Eq. (10) is solved analytically following the work of Moreira et al. (2009), by the combined Laplace transform technique and diagonalization of the matrix F ($F = X\,D\,X^{-1}$). By this procedure we come out with the result:

$$\overline{Y(s)} = X(sI + D)^{-1}\, X^{-1} Y(0) \;\;, \tag{11}$$

where $\overline{Y(s)}$ denotes the Laplace Transform of the vector $Y(x)$. Here *D* is the diagonal matrix of eigenvalues of the matrix *F*, *X* is the matrix of the respective eigenfunctions and X^{-1} it is the inverse. The elements of the matrix *(sI + D)* have the form $\{s + d_n\}$ where d_n are the eigenvalues of the matrix F given in Eq. (9). Performing the Laplace transform inversion of Eq. (11), we come out with:

$$Y(x) = X\; G(x)\, X^{-1} Y(0) \;\;, \tag{12}$$

where G(x) is the diagonal matrix with elements $e^{-d_i x}$.

Therefore, the solution for the concentration given by Eq. (5) is now well determined once the vector $\bar{c}_n(x)$ is known. The solution of the problem (4) using as basis eigenfunctions given in terms of cosines and Bessel functions will be called here as GILTTC and GILTTB, respectively.

3. Numerical results

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 different dispersion experiments available in the literature. Below we briefly discuss the Copenhagen and Prairie-Grass dispersion experiments, which allow us to validate the results encountered by the mentioned solutions. The computational code was developed in Fortran.

The Copenhagen field campaign took place in the suburbs of Copenhagen in 1978, and is 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 (z = 0) 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. The meteorological conditions during the dispersion experiments ranged from moderately unstable to convective.

In the Prairie-Grass experiment, according to Barad (1958), the tracer SO_2 was released without buoyancy at a height of 0.46 m, and collected at a height of 1.5 m at five downwind distances (50, 100, 200, 400 and 800 m) at O'Neill, Nebraska in 1956. The Prairie Grass site was quite flat and much smooth with a roughness length of 0.6 cm. Here we consider the experimental data appearing in the paper of Nieuwstadt (1980).

The choice of the turbulent parameterization represents a fundamental aspect for pollutant dispersion modeling. In terms of the convective scaling parameters, the vertical eddy diffusivity can be formulated as (Degrazia et al. (1997)):

$$\frac{K_z}{w_* h} = 0.22\left(\frac{z}{h}\right)^{1/3}\left(1-\frac{z}{h}\right)^{1/3}\left[1-\exp\left(-\frac{4z}{h}\right)-0.0003\exp\left(\frac{8z}{h}\right)\right] \tag{13}$$

where z is height; h is the thickness of the ABL and w_* is the convective velocity scale.

In our simulations, we use the wind speed profile described by a power law, according Panofsky and Dutton (1984),

$$\frac{\bar{u}_z}{\bar{u}_1} = \left(\frac{z}{z_1}\right)^{\alpha} \tag{14}$$

where $\bar{u}_z$ and $\bar{u}_1$ are the mean wind velocity respectively at the heights z and z_1, while α is an exponent that is related to the intensity of turbulence (Irwin (1979)). For the Copenhagen experiment $\alpha = 0.1$ and for the Prairie-Grass experiment $\alpha = 0.07$.

In Tables 1 and 2 we present some performances evaluations of the model for the Copenhagen and Prairie-Grass experiments, respectively, using the statistical evaluation procedure described by Hanna (1989) and defined as:

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.

For the Copenhagen experiment the statistical indices of Table 1 point out that a good agreement is obtained between experimental data and the GILTT method for both basis, regarding the NMSE, FB and FS values relatively near to zero and COR relatively near to 1. At this point, we can affirm that no significant difference between the models was observed for the high source of the Copenhagen experiment.

Table 1: Statistical indices evaluating the model performance using the Copenhagen experiment.

Model	NMSE	COR	FA2	FB	FS
GILTTC – N=100	0.05	0.91	1.00	-0.01	0.14
GILTTB – N=100	0.05	0.91	1.00	-0.04	0.13

Table 2 shows the performance of the solution for the Prairie-Grass experiment. The statistical indices of the table point out that a reasonable agreement is obtained between experimental data and the GILTT method. It is important to notice that the GILTTB numerically converges much faster than GILTTC (while GILTTB needs 100 eigenvalues, GILTTC needs 300 eigenvalues to reach the same accuracy).

Table 2: Statistical indices evaluating the model performance using the Prairie-Grass experiment.

Model	NMSE	COR	FA2	FB	FS
GILTTC – N=100	0.80	0.83	0.64	0.39	0.56
GILTTC – N=200	0.23	0.92	0.71	0.06	0.33
GILTTC – N=300	0.15	0.95	0.72	-0.01	0.28
GILTTB – N=100	0.11	0.97	0.71	-0.1	0.23

4. Conclusions

In this work, focusing our attention to the task of pollution dispersion simulation in atmosphere, we present analytical solutions in series expansion, solving the two-dimensional advection-diffusion equation by the GILTT approach. By analytical we mean that no approximation is made along its derivation. Analytical solutions 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, we need to remember that air pollution models have two kinds of errors. The first one due 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. As a consequence, the model errors are restricted to the physical modeling error.

For the problems discussed, we promptly realize the very good results achieved, under statistical point of view, by the GILTT method when compared with the experimental data, for the two basis used. For the case of high source no significant difference was observed between GILTTC and GILTTB. However, for the low source, GILTTB numerically converges much faster than GILTTC. We focus our future attention in the direction of the generalization of this solution.

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