18th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 October 2017, Bologna, Italy

A SOLUTION OF THE TIME-DEPENDENT ADVECTION-DIFFUSION EQUATION

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Abstract: We present an analytical solution that considers time dependence in the wind profile and in the eddy diffusivity. A solution is constructed following the idea of a decomposition method upon expanding the pollutant concentration in a truncated series, thus obtaining a set of recursive equations whose solutions are known. Each equation of this set is solved by the GILTT (Generalized Integral Laplace Transform Technique) method. The solution's ability to represent real situations was checked, comparing model predictions with the OLAD (Over-Land Along-wind Dispersion) experimental data set.

Key words: *Air pollution modelling, advection-diffusion equation, analytical solution, decomposition method*

INTRODUCTION

In the last decade, great progress was made to the issue of searching analytical solutions for the steady-state advection–diffusion equation in order to simulate the pollutant dispersion in the Planetary Boundary Layer (PBL). The solutions were valid only for very specialized practical situations with restrictions on wind and eddy diffusivities vertical profiles. Recently appeared an analytical solution of the steady-state advection-diffusion equation, applying the new GILTT method (Generalized Integral Laplace Transform Technique) that accepts any wind and eddy diffusivity vertical profile. The main idea of this methodology comprehends the following 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 solved analytically by the Laplace Transform technique. For more information, see Moreira et al. (2009). In this paper, we extend these last results presenting a time-dependent three-dimensional solution.

THE TIME-DEPENDENT SOLUTION

The advection-diffusion equation is a deterministic approach to dispersion of pollutants in the atmosphere. It is obtained by mass conservation combined with first order close (K-Theory):

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z} = \frac{\partial}{\partial x}\left(\kappa_x \frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\kappa_y \frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\kappa_z \frac{\partial \bar{c}}{\partial z}\right) \tag{1}$$

Here $\bar{c}$ denotes the mean concentration of a passive contaminant; $\overline{\mathrm{u}}$, $\overline{\mathrm{v}}$ e $\overline{\mathrm{w}}$ are the cartesian components of the mean wind speed in the direction x, y and z, respectively; κ_x, κ_y and κ_z are the eddy diffusivities. For brevity, here, we align the predominant wind direction with the direction of the x coordinate, $\overline{\mathrm{v}} = \overline{\mathrm{w}} = 0$, and equation (1) simplifies to:

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial x}\left(\kappa_x \frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\kappa_y \frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\kappa_z \frac{\partial \bar{c}}{\partial z}\right) \tag{2}$$

The space-time domain is given by $t > 0$, $0 < x < L_x$, $0 < y < L_y$, $0 < z < z_i$ and equation (2) is subject to the following boundary and initial conditions:

$$\kappa_x \frac{\partial \bar{c}}{\partial x} = 0 \text{ em } x = 0 \text{ e } x = L_x;$$
$$\kappa_y \frac{\partial \bar{c}}{\partial y} = 0 \text{ em } y = 0 \text{ e } y = L_y$$
$$\kappa_z \frac{\partial \bar{c}}{\partial z} = 0 \text{ em } z = 0 \text{ e } z = z_i$$
$$\bar{c}(x, y, z, 0) = 0$$

the source condition is:

$$\overline{uc}(0, y, z, t) = Q\delta(y - y_0)\delta(z - H_s)\delta(t - t_0),$$

with Q being the emission rate, z_i the height of the atmospheric boundary layer, H_s the height of the source, L_x and L_y are domain limits in the x and y-direction far from the source and δ represents the Dirac delta function.

In order to construct a time-dependent solution, first we separate time-dependent wind field and time-dependent eddy diffusivity contributions from their time averaged values:

$$\bar{u}(z, t) = \bar{U}(z) + U(z, t), \quad (3a)$$

$$\kappa_x(z, t) = \bar{K}_x(z) + K_x(z, t), \quad (3b)$$

$$\kappa_y(z, t) = \bar{K}_y(z) + K_y(z, t), \quad (3c)$$

$$\kappa_z(z, t) = \bar{K}_z(z) + K_z(z, t), \quad (3d)$$

where $\bar{U}(z)$, $\bar{K}_x(z)$, $\bar{K}_y(z)$ and $\bar{K}_z(z)$ are the time averages. Upon inserting these assumptions in equation (2) yields:

$$\frac{\partial \bar{c}}{\partial t} + \bar{U}\frac{\partial \bar{c}}{\partial x} - \frac{\partial}{\partial x}\left(\bar{K}_x \frac{\partial \bar{c}}{\partial x}\right) - \frac{\partial}{\partial y}\left(\bar{K}_y \frac{\partial \bar{c}}{\partial y}\right) - \frac{\partial}{\partial z}\left(\bar{K}_z \frac{\partial \bar{c}}{\partial z}\right) = -U\frac{\partial \bar{c}}{\partial x} + \frac{\partial}{\partial x}\left(K_x \frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial \bar{c}}{\partial z}\right) \quad (4)$$

According to the idea of the decomposition method (Adomian, 1988) the solution of (4) is written as a truncated expansion:

$$\bar{c}(x, y, z, t) = \sum_{l=0}^{J} c_l(x, y, z, t) \quad (5)$$

These new degrees of freedom for each component may now be used to decompose (4) into a set of advection-diffusion equations, that together form a recursive scheme:

$$\begin{cases} \dfrac{\partial c_0}{\partial t} + \bar{U}\dfrac{\partial c_0}{\partial x} - \dfrac{\partial}{\partial x}\left(\bar{K}_x \dfrac{\partial c_0}{\partial x}\right) - \dfrac{\partial}{\partial y}\left(\bar{K}_y \dfrac{\partial c_0}{\partial y}\right) - \dfrac{\partial}{\partial z}\left(\bar{K}_z \dfrac{\partial c_0}{\partial z}\right) = 0 \\ \dfrac{\partial c_1}{\partial t} + \bar{U}\dfrac{\partial c_1}{\partial x} - \dfrac{\partial}{\partial x}\left(\bar{K}_x \dfrac{\partial c_1}{\partial x}\right) - \dfrac{\partial}{\partial y}\left(\bar{K}_y \dfrac{\partial c_1}{\partial y}\right) - \dfrac{\partial}{\partial z}\left(\bar{K}_z \dfrac{\partial c_1}{\partial z}\right) = S_0 \\ \vdots \\ \dfrac{\partial c_l}{\partial t} + \bar{U}\dfrac{\partial c_l}{\partial x} - \dfrac{\partial}{\partial x}\left(\bar{K}_x \dfrac{\partial c_l}{\partial x}\right) - \dfrac{\partial}{\partial y}\left(\bar{K}_y \dfrac{\partial c_l}{\partial y}\right) - \dfrac{\partial}{\partial z}\left(\bar{K}_z \dfrac{\partial c_l}{\partial z}\right) = S_{l-1} \end{cases}$$

Note, that the decomposition procedure is not unique. Our choice for reshuffling term with the specific form of source terms is justified because it allows to solve the resulting recursive system analytically by the GILTT method. Further, the time dependence of the eddy diffusivity and wind field in the proposed solution is entirely accounted for in the source term, which is constructed from the solutions of previous recursion steps and thus are known. Moreover, the recursion initialisation satisfies the boundary conditions

of the original problem, whereas all the subsequent recursion steps satisfy homogeneous boundary conditions. Once the set of problems is solved, the solution of equation (5) is well determined.
A remark on the truncation is in order here, the accuracy of the results may be controlled by the proper choice of the number of terms in the solution series.

DATA SET USED FOR PRELIMINARY VALIDATION

For a preliminary validation, we used the OLAD experiment (Biltoft et al., 1999). In particular, we used the dataset of the 12th September 1997, where sulfur-hexafluoride (SF6) was released by a truck mounted disseminator at 3 m above ground level and following the Bravo route for 10 km. The beginning of the emission was at 6 hours and 58 minutes with duration of 10 minutes. According to Chang et al. (2001) this experiment has the characteristic of low wind speed (less or equal 3.5 m/s). Further, the planetary boundary layer showed a stable condition during the sampling period. The pollution concentrations where measured by fifteen analysers (LC101-LC115) located along the route Foxtrot at a distance of 2 km "parallel" to the Bravo Route. The whole-air samplers produced time-averaged (15-min) tracer gas concentrations.

While the real experiment used a continuous line source to dissemination the tracer, we used in the simulations a finite number of point source to represent the line source. We used ten points source and in each source the release duration was Δt. Thus the concentration in each sampler is defined by:

$$C_l(x,y,z,t) = \sum_{a=0}^{9} c_l(x,y,z,t - a\Delta t - \frac{\Delta t}{2})$$

where a denotes the displacement centred line segment source.

PLANETARY BOUNDARY LAYER PARAMETERIZATION

The dataset utilized presents stable condition only. For a stable PBL we used eddy diffusion parameterization proposed by Degrazia et al. (2000):

$$\mathrm{K_z} = \frac{0.3(1 - \mathrm{z/z_i})\mathrm{u_*z}}{1 + 3.7(\mathrm{z}/\Lambda)}$$

where $\Lambda = \mathrm{L}(1 - \mathrm{z/z_i})^{5/4}$. Whereas Degrazia et al. (1996) proposed for a stable boundary layer an algebraic formulation for the eddy diffusivity in the x and y direction according to:

$$\frac{\mathrm{K_\eta}}{\mathrm{u_*z_i}} = \frac{2\sqrt{\pi}0.64\mathrm{a}_\nu^2\left(1 - \frac{\mathrm{z}}{\mathrm{z_i}}\right)^{\alpha_1}\left(\frac{\mathrm{z}}{\mathrm{z_i}}\right)\mathrm{X'}\left[2\sqrt{\pi}0.64\mathrm{a}_\nu^2\left(\frac{\mathrm{z}}{\mathrm{z_i}}\right) + 8\mathrm{a}_\nu(\mathrm{f_m})_\nu\left(1 - \frac{\mathrm{z}}{\mathrm{z_i}}\right)^{\frac{\alpha_1}{2}}\mathrm{X'}\right]}{\left[2\sqrt{\pi}0.64\left(\frac{\mathrm{z}}{\mathrm{z_i}}\right) + 16\mathrm{a}_\nu(\mathrm{f_m})_\nu\left(1 - \frac{\mathrm{z}}{\mathrm{z_i}}\right)^{\frac{\alpha_1}{2}}\mathrm{X'}\right]^2}$$

where $(\mathrm{f_m})_\nu = (\mathrm{f_m})_{\mathrm{n},\nu}(1 + 3.7(\mathrm{z}/\Lambda))$ is the frequency of the spectral peak, $(\mathrm{f_m})_{\mathrm{n},\nu} = 0.33$ is the frequency of the spectral peak in the neutral stratification (Sorbjan, 1989), $\Lambda = \mathrm{L}(1 - \mathrm{z/z_i})^{(1.5\alpha_1 - \alpha_2)}$ $\alpha_1 = 1.5, \alpha_2 = 1$) is the local Monin-Obukhov length, $\mathrm{a}_\nu = (2.7\mathrm{c}_\nu)^{1/2}/(\mathrm{f_m})_{\mathrm{n},\nu}^{1/3}$, where $\mathrm{c}_\nu = 0.4$, u_* is the friction velocity and $\mathrm{X}' = \mathrm{xu_*}/\bar{\mathrm{u}}\mathrm{z}$ represents the non-dimensional distance.

The wind speed profile can be described by the power law (Irwin, 1979)

$$\frac{\bar{\mathrm{u}}}{\overline{\mathrm{u_1}}} = \left(\frac{\mathrm{z}}{\mathrm{z_1}}\right)^{\mathrm{n}}$$

where $\bar{\mathrm{u}}$ and $\overline{\mathrm{u_1}}$ are the horizontal wind velocity at height z and $\mathrm{z_1}$. The power parameter n is related to the intensity of turbulence.

NUMERICAL RESULTS

We used the experiment five of OLAD dataset. The meteorological data are presented in Table 1 and were calculated in Degrazia (2005). The data u, u∗, L and z_i represent the wind speed in 10 meters, the friction velocity, Monin-Obukhov length and the height of the planetary boundary layer, respectively.

Table 1. Meteorological conditions of OLAD 5 (Degrazia, 2005)

OLAD 5	$\mathbf{u\ (10m)}$ $(\mathbf{m/s^{-1}})$	$\mathbf{u_*}$ $(\mathbf{m/s^{-1}})$	$\mathbf{L}$ $(\mathbf{m})$	$\mathbf{z_i}$ $(\mathbf{m})$
6:45 – 7:00	1,71	0,10	43,48	171,60
7:00 – 7:15	1,95	0,12	64,81	223,80
7:15 – 7:30	1,82	0,11	127,27	303,03
7:30 – 7:45	1,90	0,11	221,12	407,32

In Table 2 concentration results observed in the experiment (CO) and concentrations predicted by model proposed (CP) are shown. The results are referred to the concentrations observed in the first sampling line of the experiment (samplers denoted LC101 to LC115).

Table 2. Tracer concentration for the fifteen samplers of experiment five of OLAD and model prediction

LC	**CO (pptv)**	**CP (pptv)**
101	470,10	5533,69
102	5,24	5744,58
103	76,04	5719,13
104	7951,42	7841,28
105	6433,66	6809,26
106	5697,37	6648,48
107	5930,83	6603,05
108	5974,47	6631,44
109	7565,40	7010,36
110	8498,44	8473,20
111	7878,68	7505,47
112	7329,51	7487,19
113	8294,43	8345,55
114	10190,91	11396,06
115	9198,10	10658,07

In Figure 1 it is shown the scatter plotter of observed and computed data.

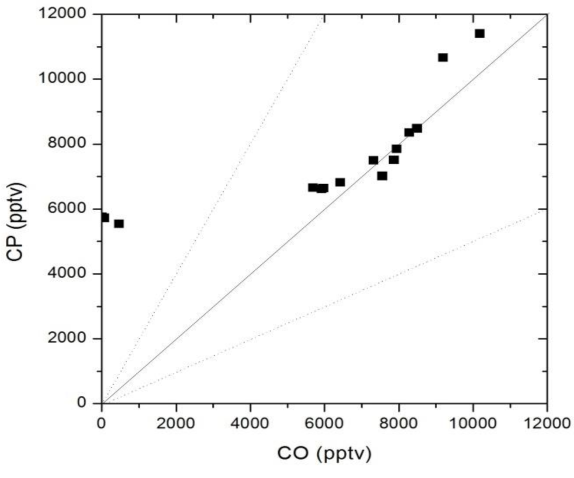

Figure 1. Observed (CO) and predict (CP) scatter plot

The statistical indices normalized mean square error (NMSE), correlation coefficient (COR) and fractional standard deviations (FS) are shown in Table 3.

Table 3. Statistical comparison between observed and predict concentration

NMSE	COR	FB	FS
0,14	0,80	-0,20	0.64

CONCLUSIONS

A progressive and continuous effort to obtain analytical solutions of the advection-diffusion equation has been made in the last years. In fact, analytical solutions of equations are of fundamental importance in understanding and describing physical phenomena. Analytical solutions explicitly take into account all the parameters of a problem, so that their influence can be reliably investigated and it is easy to obtain the asymptotic behaviour of the solution, which is usually very much more tedious to generate through numerical calculations. A general solution of the of the steady-state advection–diffusion equation, that is with any restriction on wind and eddy diffusivity vertical profiles, is known in the literature as the GILTT approach (Tirabassi et al., 2008; Moreira et al., 2009). In this paper we extend these last results and we present a time-dependent solution.

The advection-diffusion equation was solved by a combination of a decomposition method, and the GILTT approach. While the first part of the solution method produces a recursive set of equations, where each of the equations have a known solution by GILTT. We also analysed stability of the procedure (not included here) which showed that only a small recursion depth is necessary in order attain an acceptable accuracy.

The model had a first partial validation using data from OLAD experiment with a moving source. In this experiment a tracer substance was emitted from a facility mounted on a truck that run on the route along 10 km and thus represents a time dependent line source, while air pollution concentration and meteorological data have a resolution of 15 minutes.

REFERENCES

Adomian G., 1988: A Review of the Decomposition Method in Applied Mathematic, *J. Math. Anal. Appl.*, **135**, 501-544.

Biltoft C.A., S.D. Turley, T.B. Watson, G.H. Crescenti, R.G. Carter, 1999: Over-Land Atmospheric Dispersion (OLAD) Test Summary and Analysis. Customer report, U.S. Army Dugway Proving Ground, USA.

Chang J.C., K. Chayantrakom, S. R. Hanna, 2001: Evaluation of CALPUFF, HPAC and SLSTRACK with the Over-Land Alongwind Dispersion (OLAD) Field Data. Scholl of Computation Sciences, George Manson University.

Degrazia F.C. 2005: Evolução da camada limite planetária para dispersão de poluentes pelo método da GILTT, UFRGS, Porto Alegre, Brazil.

Degrazia G.A., M.T. Vilhena, O.L.L., Moraes, 1996: An algebraic expression for the eddy diffusivities in the stable boundary layer: A description of near-source diffusion. *Il Nuevo Cimento*, 19C, 399–403.

Degrazia, G.A. D. Anfossi, J. C. Carvalho, C. Mangia, T. Tirabassi, H. F. C. Velho, 2000: Turbulence parameterisation for PBL dispersion models in all stability conditions. *Atmospheric Environment*, **34**, 3575–3583.

Moreira, M. T. Vilhena, D. Buske, T. Tirabassi, T 2009: The state-of-art of the GILTT method to simulate pollutant dispersion in the atmosphere. *Atmospheric Research*, **92**, 1–17.

Sorbjan Z, 1989: Structure of the atmospheric boundary layer, Prentice Hall, New Jersey, USA.

Tirabassi T., D Buske, DM Moreira, MT Vilhena, 2008: A two-dimensional solution of the advection–diffusion equation with dry deposition to the ground- *Journal of Applied Meteorology and Climatology* **47** (8), 2096-2104