POLLUTANT DISPERSION SIMULATION IN THE ATMOSPHERE NEAR SOURCE BY THE GILTT METHOD

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Abstract. *In this work we present the GILTT method for the solution of the advection-diffusion equation using an eddy diffusivity depending of source distance. With the new approach, where no approximation is made along the solution derivation so that is an exact solution except for the round-off error and truncation of the series solution, it is possible to simulate the pollutant dispersion in the Planetary Boundary Layer. This study reinforce that the inclusion of the memory effect, characteristic of near source condition, improves the description of the turbulent transport process of atmospheric contaminants. Numerical simulations and statistical comparisons are also present.*

Keywords*: GILTT, Analytical Solution, Advection-Diffusion equation, Atmospheric Dispersion, Planetary Boundary Layer.*

1. Introduction

In the last years, special attention has been devoted to the task of searching analytical solutions for the advection-diffusion equation in order to simulate the pollutant dispersion in the Planetary Boundary Layer (PBL). Presently, analytical solutions of the advection-diffusion equation are usually obtained just for stationary conditions and by making strong assumptions about the eddy diffusivity coefficients (K) and wind speed profiles (U).

To better understand the importance of researching analytical solution of the advection-diffusion equation, in order to simulate the pollutant dispersion in the PBL, we must look for the possible sources of error either in the modeling and in the numerical simulation of the pollutant concentration. Regarding the first item, the advection-diffusion equation is a methematical description of the physical phenomena of pollutant dispersion in the PBL, assuming the K-theory model (first order closure) for the turbulence, wind velocity as well considering the eddy diffusivities. Besides these uncertainties and also the incomplete understanding of the turbulence phenomena, we have also to take into account the error inherent to the mathematical method adopted to solve the advection-diffusion equation. Here appears the relevance of an analytical solution. Indeed, bearing in mind the exactness of an analytival solution, we may state that the pollutant concentration calculation by this kind of solution is free of error except for the round-off error. Then, the error in an analytical solution is restricted to the uncertainties posed in the model.

An uncertanty posed in the advection-diffusion equation is the eddy diffusivity. Normally, to simulate the pollutant dispersion in the atmosphere is utilized an eddy diffusiviy depending only on variable z. But, to represent the near-source difusion the eddy diffusivities should be considered as functions of not only turbulence (*e.g*., large eddy length and velocity scales), but also of distance from the source (Arya, 1995). Following this idea, Degrazia et al. (2001) proposed for the Convective Boundary layer (CBL) an integral formulation for the eddy diffusivities. Therefore, the objective of this work is to applied the new GILTT method in air pollution problems considering the eddy diffusivity depending on the source distance. Besides, as no approximation is made along the solution derivation by the GILTT method so that is an exact solution except for the round-off error, to verify if the memory effect is really important as it was shown in the work of Degrazia et al. (2001).

The mean feature of the GILTT method (Wortmann et al., 2004) comprehends the steps: solution of an associate Sturn-Liouville problem, expansion of the pollutant concentration in a series in terms of the attained eigenfunction, replacement of this expansion in the advection-diffusion equation and, finally, taking moments. This procedure leads to a set of differential ordinary equations, named the transformed equation. These equations are then solved, following the idea of Wortmann (2003), by the application the Laplace Transform technique.

To reach this goal, we outline the paper as follows: in section 2, we report the derivation of the GILTT solution for the two-dimensional advection-diffusion equation. In section 3 the turbulent parameterisation assumed in this work is presented. In section 4, the numerical results attained by the new analytical method are reported as well the comparison with experimental data, and finally in section 5, the conclusions.

2. The GILTT method

The crosswind integration of advection-diffusion equation (in stationary conditions and neglecting the longitudinal diffusion) leads to:

$$U\frac{\partial \bar{c}(x,z)}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial \bar{c}(x,z)}{\partial z}\right) \tag{1}$$

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

$$\frac{\partial \bar{c}(x,z)}{\partial z} = 0 \quad \text{in } z = 0,\ z = h \tag{1a}$$

$$U\bar{c}(0,z) = Q\,\delta(z - Hs) \quad \text{in } x = 0 \tag{1b}$$

where $\bar{c}$ represents the average crosswind integrated concentration, h is the unstable boundary layer height, U is the wind speed in the x direction and K_z is the vertical eddy diffusivity. δ is the dirac delta function.

The difusive term in the equation (1) is rewritten using the chain rule. This procedure was used by Wortmann (2003) and allow a simplification of the auxiliary problem, whose choice is made as custom procedure in the use of GITT according to Cotta and Mikhaylov (1997). Then, we can write:

$$U\frac{\partial \bar{c}}{\partial x} = K_z\frac{\partial^2 \bar{c}}{\partial z^2} + \left(\frac{\partial K_z}{\partial z}\right)\frac{\partial \bar{c}}{\partial z} \tag{2}$$

The formal application of GITT begins with the choice of the problem of associated eigenvalue (also known in the literature as the auxiliary problem) and their respective boundary conditions:

$$\psi_i''(z) + \lambda_i^2 \psi_i(z) \quad \text{in} \quad 0 < z < h \tag{3a}$$

$$\psi_i'(z) \quad \text{in} \quad z = 0,\ h \tag{3b}$$

The solution is $\psi_i(z) = cos(\lambda_i z)$, where λ_i are the positive roots of the expression $sen\ (\lambda_i h)=0$. It is observed that the functions $\psi_i(z)$ and λ_i, known respectively, as the eigenfunctions and eigenvalues associated with the problem of Sturm-Liouville, satisfy the following orthonormality condition:

$$\frac{1}{N_m^{1/2} N_n^{1/2}} \int_v \psi_m \psi_n dv = \begin{Bmatrix} 0\ ,\ m \neq n \\ 1,\ m = n \end{Bmatrix}, \tag{4}$$

where N_m is given by $\int_v \psi_m^2 dv$.

Following the formalism of GITT, the first step is to expand the variable $\bar{c}(x,z)$ into the following form:

$$\bar{c}(x,z) = \sum_{i=0}^{\infty} \frac{\overline{c_i(x)}\ \psi_i(z)}{N_i^{\frac{1}{2}}} \tag{5}$$

Substituting Eq. (5) into Eq. (2) we obtain:

$$U\sum_{i=0}^{\infty}\frac{\overline{c_i'(x)}\ \psi_i(z)}{N_i^{1/2}} = K_z\sum_{i=0}^{\infty}\frac{\overline{c_i(x)}\ \psi_i''(z)}{N_i^{1/2}} + K_z'\sum_{i=0}^{\infty}\frac{\overline{c_i(x)}\ \psi_i'(z)}{N_i^{1/2}} \tag{6}$$

where ' and " are used to indicate derivatives of first and second order, respectively.

The next step is to apply the operator $\int_0^h \frac{\psi_j(z)}{N_j^{1/2}}dz$ in the Eq. (6) and use the Eq. (3a) to observe that $\psi_i''(z) = -\lambda_i^2 \psi_i(z)$. Recall that $\psi_i = \psi_i(z)$, $U = U(z)$ and $K_z = K_z(x,z)$. Then,

$$\sum_{i=0}^{\infty}\left[-\frac{\overline{\overline{c_i'(x)}}}{N_i^{1/2}N_j^{1/2}}\int_0^h U\,\psi_i\,\psi_j\,dz-\frac{\overline{\overline{c_i(x)}}\lambda_i^2}{N_i^{1/2}N_j^{1/2}}\int_0^h K_z\psi_i\psi_j dz+\frac{\overline{\overline{c_i(x)}}}{N_i^{1/2}N_j^{1/2}}\int_0^h K_z'\,\psi_i'\,\psi_j dz\right]=0 \qquad (7)$$

Now, taking

$$Y(x)=\left\{\overline{\overline{c_i(x)}}\right\}\;;\;B=\{b_{i,j}\};\;E=\{e_{i,j}\};\;F=-B^{-1}.E \qquad (8)$$

where $b_{i,j}=\int_0^h U\,\psi_i\,\psi_j\,dz$ and $e_{i,j}=\int_0^h K_z'\,\psi_i'\,\psi_j\,dz-\lambda_i^2\int_0^h K_z\,\psi_i\,\psi_j\,dz\cdot$

The integrals in B and E are numerically solved by Gauss Quadrature.

Eq. (7) in matrix notation becomes:

$$Y'(x) + F.Y(x) = 0 \qquad (9)$$

For the boundary condition of Eq. (1b), using the same arguments, we have that:

$$\int_0^h\sum_{i=0}^{\infty}\frac{\overline{\overline{c_i(0)}}\;U\,\psi_i\,\psi_j}{N_i^{1/2}N_j^{1/2}}dz=\int_0^h\frac{Q\,\delta(z\text{-}Hs)\psi_j}{N_j^{1/2}}dz \qquad (10)$$

Then, performing the due substitutions and integrations, the boundary conditions for U constant are:

$$c_0(0)=\frac{Q}{U\sqrt{z_i}}\quad\text{for}\quad i=0\quad\text{and}\quad c_i(0)=\frac{Q\,\psi_i(Hs)}{U\sqrt{z_i/2}}\quad\text{for}\quad i\neq 0 \qquad (11)$$

The transformed problem represented by the Eq. (9) can be solved by the Laplace Transform technique and diagonalization (Segatto et al., 1999; Wortmann, 2003). First, transforming x into s and Y into $\overline{Y}$ the equation becomes:

$$s\overline{Y}(s)-Y(0)+F.\overline{Y}(s) \qquad (12)$$

where the overbar represents the transformed potential.

The matrix F is decomposed into eigenvectors and eigenvalues as $F = X.D.X^{-1}$, where X is the matrix of the eigenvectors and D is the diagonal matrix of eigenvalues from F. This procedure is valid when the eigenvalues of matrix F are different and not null. Then, Eq. (12) becomes:

$$(sI+X.D.X^{-1}).\overline{Y}(s)=Y(0) \qquad (13)$$

where I is the matrix identity. Given that $X.X^{-1} = I$, we can write:

$$X(sI+D)X^{-1}.\overline{Y}(s)=Y(0) \qquad (14)$$

Multiply both sides of the Eq. (14) by X^{-1}, $(sI + D)^{-1}$ and finaly by X we obtain:

$$\overline{Y}(s) = X.(sI + D)^{-1}.X^{-1}.Y(0) \qquad (15)$$

An alternative procedure for the inversion of the matrix X is suggested by Segatto et al. (1999). Firstly, one determines the vector ξ ($\xi = X^{-1}.\ Y(0)$). Substituting in the Eq. (11) the result is:

$$\overline{Y}(s) = X(sI + D)^{-1}\xi \tag{16}$$

where ξ is found solving the equation $X.\xi = Y(0)$, and calculated using the *LU* decomposition, whose cost computacional is smaller than an inversion of matrix. The elements of the matrix $(sI + D)$ have the form $\{s + d_i\}$ where d_i are the eigenvalues of the matrix F given in Eq. (12). It is known that the inverse of a diagonal matrix is the inverse of their elements, in other words, the elements of $(sI + D)^{-1}$ are $\frac{1}{s + d_i}$ whose transformed inverse of Laplace is $e^{-d_i x}$. G(x) being the diagonal matrix with elements $e^{-d_i x}$ the final solution is given by:

$$Y(x) = X.G(x).\xi \tag{17}$$

Using the form of the inverse,

$$\overline{c}(x,z) = \sum_{i=0}^{\infty} \frac{\overline{\overline{c_i(x)}}\ \psi_i(z)}{N_i^{\frac{1}{2}}} \tag{18}$$

the final solution of the proposed problem is obtained. $\psi_i(z)$ comes from the problem of Sturm-Liouville and $\overline{\overline{c_i}}(x)$ from the solution of the transformed problem.

3. Turbulent parameterisation

The vertical eddy diffusivity described in terms of energy-containing eddies and function of the downwind distance X and the height z can be written as (Degrazia et al., 2001):

$$\frac{K_z}{w_* z_i} = 0.12\psi^{1/3}\left[1 - \exp\left(-\frac{4z}{z_i}\right) - 0.0003\exp\left(\frac{8z}{z_i}\right)\right]^{4/3} \int_0^{\infty} \frac{\sin\left\{3.17\left[1 - \exp\left(-\frac{4z}{z_i}\right) - 0.0003\exp\left(\frac{8z}{z_i}\right)\right]^{-2/3} \psi^{1/3} X n'\right\}}{(1+n')^{5/3}} \frac{dn'}{n'} \tag{19}$$

where X is a nondimensional distance ($X = xw_*/uz_i$), w_* is the convective velocity scale and z_i is the top of the CBL.

The dissipation function ψ according (Hφjstrup, 1982), has the form:

$$\psi^{1/3} = \left[\left(1 - \frac{z}{z_i}\right)^2 \left(\frac{z}{-L}\right)^{-2/3} + 0.75\right]^{1/2} \tag{20}$$

where L is the Monin-Obukhov length in the surface layer.

The formula, appropriate for far source distance, reads as (Degrazia et al., 2001):

$$\frac{K_z}{w_* z_i} = 0.19\psi^{1/3}\left[1 - \exp\left(-\frac{4z}{z_i}\right) - 0.0003\exp\left(\frac{8z}{z_i}\right)\right]^{4/3} \tag{21}$$

For a given height, the $K_z/w_* z_i$ as given by (19) is initially zero, increases with X at first linearly and then more slowly, and finally tends to a constant value that can be obtained from Eq. (21). Thus, in this study we introduce the vertical eddy diffusivities (19) and (21) in the new air pollution model to simulate the ground-level crosswind-integrated concentrations of contaminants released from an elevated continuous source in an unstable PBL.

4. Experimental data and evaluation of the model

The performance of the present model have been evaluated against experimental crosswind ground-level concentrations using tracer SF_6 data from dispersion experiments carried out in the northern part of Copenhagen, which is described in Gryning et al. (1987). The tracer was released without buoyancy from a tower at a height of 115 m, and collected at ground-level positions at a maximum of three crosswind arcs of tracer sampling units. The site was mainly residential with a roughness length of the 0.6 m. The wind speed profile used in the air pollution model has been parameterized following the similarity theory of Monin-Obukhov and OML model (Berkowicz et al., 1986) where the stability function is given by (Paulson, 1970).

Figure 1 shows the observed and predicted scatter diagram of ground-level crosswind concentrations using the approach (Eq.(18)) with vertical eddy diffusivity given by Eqs. (19) and (21). In this respect, it is important to note that the model reproduced fairly well the observed concentration.

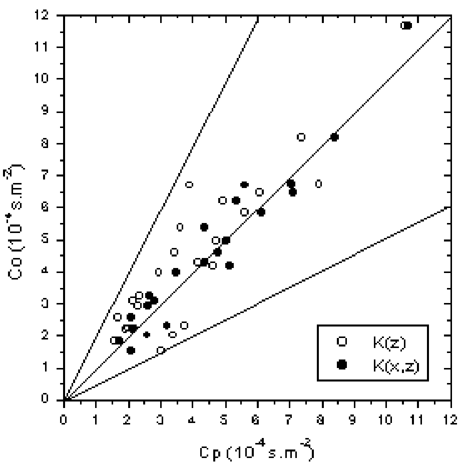

Figure 1: Observed (Co) and predicted (Cp) crosswind ground-level integrated concentration, normalised with emission ($\bar{c}/Q$), scatter diagram for the new model with eddy diffusivities given by $K(z)$ and $K(x,z)$. Lines indicate a factor of two.

Table 1 shows the statistical analysis (Hanna, 1989) of the new model compared with the ADMM model considering the moderately unstable experiments of Copenhagen. The ADMM model (Vilhena et al., 1998; Moreira et al., 1999; Degrazia et al., 2001; Mangia et al., 2002) was obtained by a Laplace Transform technique with numerical inversion considering the PBL as a multilayer system where in each layer the eddy diffusivity and wind are constants. The statistical indices point out that a good agreement is obtained between experimental data and the new model. Analysing the statistical indices in Table 1 it is possible to notice that the new model simulate very well the observed concentrations, with *NMSE*, *FB* and *FS* values relatively near to zero, *R* relatively near to 1 and *FA2* equal to 1. It is observed quickly that the simulations that use the eddy diffusivity depending of the source distance present the best results, mainly for the GILTT method.

In Table 2, the measured and computed ground level crosswind concentrations ($\bar{c}\,(x,0)/Q$) of the current approach and the ADMM model are presented. Various distances from the source of the Copenhagen experiment are considered.

Figure 2 shows the ground-level crosswind integrated concentration as a function of source distance for two different source heights (*Hs* = 104 and *Hs* = 209m) using Eq. (19) and Eq. (21). For the height *Hs* = 104m an accentuated peak is verified in an area close to the source. With the increase of the source height there is observed a decrease of the peak and a different location of the same. Figure 3 shows the vertical profile of concentration at various downstream distances (x = 2000m, x = 4000m and x = 6000m) considering experiment 9 of Copenhagen. The traditional behavior is verified presenting larger values of concentration for short distances, which become smaller with an increase in the downstream distance. Furthermore, with the increase of the distance the tendency is to obtain a homogeneous profile concentration.

Table 1: Results of statistical indices used to evaluate the model performance, where subscripts *o* and *p* refer to observed and predicted quantities.

			GILTT $K(z)$	GILTT $K(x,z)$	ADMM $K(z)$	ADMM $K(x,z)$
NMSE	Normalised Mean Square Error	$\overline{(C_o - C_p)^2} \big/ \overline{C_o}\,\overline{C_P}$	0.07	0.02	0.16	0.06
FA2	Fraction of data (%)for	$0.5 \le (C_p / C_o) \le 2$	1.00	1.00	1.00	1.00
R	Correlation Coefficient	$\overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} \big/ \sigma_o \sigma_p$	0.90	0.97	0.89	0.89
FB	Fractional Bias	$\overline{C_o} - \overline{C_p} \big/ 0.5(\overline{C_o} + \overline{C_p})$	0.09	0.01	0.28	0.03
FS	Fractional Standard deviations	$(\sigma_o - \sigma_p) \big/ 0.5(\sigma_o + \sigma_p)$	0.09	0.05	0.27	0.10

Table 2: Observed and modeled ground-level crosswind integrated concentration ($\overline{c}$ (x,0)/Q) at different distances from the source.

Exp.	Distance (m)	Data ($.10^{-4}$ sm^{-2})	GILTT K(z) ($.10^{-4}$ sm^{-2})	ADMM K(z) ($.10^{-4}$ sm^{-2})	GILTT K(x,z) ($.10^{-4}$ sm^{-2})	ADMM K(x,z) ($.10^{-4}$ sm^{-2})
1	1900	6.48	6.07	5.37	7.11	8.33
	3700	2.31	3.74	3.12	3.21	4.53
2	2100	5.38	3.62	3.16	4.37	4.28
	4200	2.95	2.28	1.84	2.63	2.56
3	1900	8.20	7.36	6.53	8.43	8.67
	3700	6.22	4.95	3.99	5.35	5.32
	5400	4.30	4.19	3.31	4.38	3.99
4	4000	11.66	10.56	7.96	10.67	8.97
5	2100	6.72	7.92	7.12	7.06	7.55
	4200	5.84	5.60	4.58	6.14	5.64
	6100	4.97	4.74	3.74	5.03	4.43
6	2000	3.96	2.95	2.58	3.48	3.22
	4200	2.22	1.91	1.53	2.15	2.02
	5900	1.83	1.57	1.24	1.72	1.58
7	2000	6.70	3.88	3.39	5.62	4.91
	4100	3.25	2.36	1.89	2.66	2.73
	5300	2.23	1.99	1.59	2.20	2.21
8	1900	4.16	4.62	4.11	5.15	5.30
	3600	2.02	3.39	2.70	2.58	3.35
	5300	1.25	3.06	2.37	2.11	2.60
9	2100	4.58	3.44	2.96	4.78	4.19
	4200	3.11	2.15	1.73	2.80	2.48
	6000	2.59	1.69	1.34	2.11	1.80

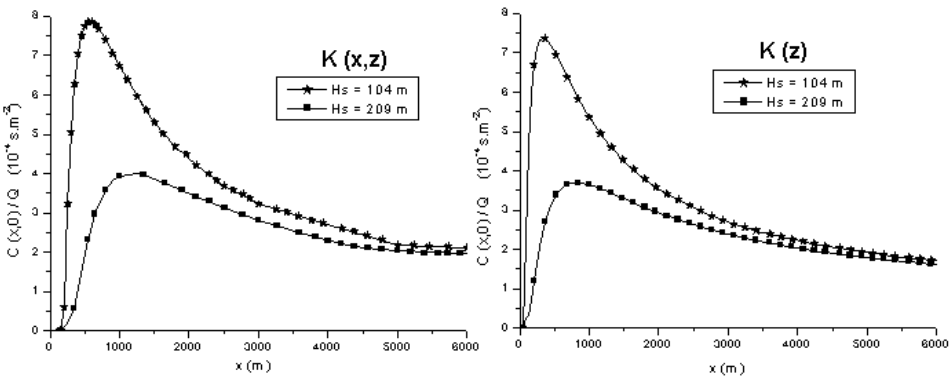

Figure 2: Crosswind integrated concentration as a function of source distance for two differents source height.

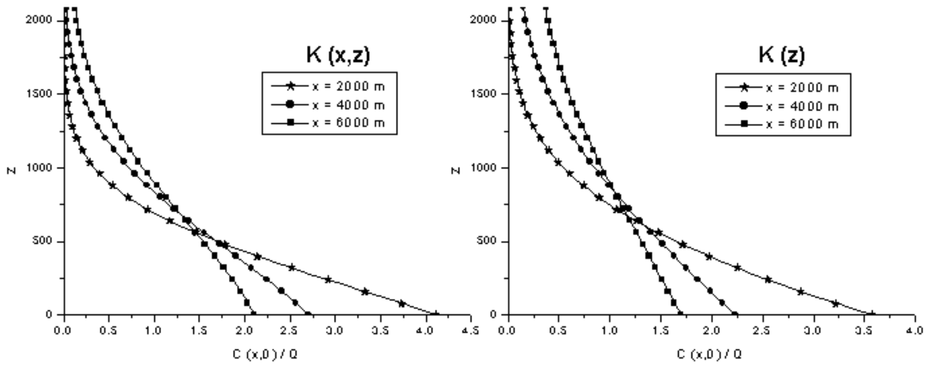

Figure 3: Vertical profile of concentration for various downstream distances considering the experiment 9 of Copenhagen.

We can observe from this figures and tables that Eq. (18) represents a formula appropriate to describe dispersion in the near and intermediate fields of an elevated source.

5. Conclusions

The statistical analysis of the results shows a good agreement between the results of the proposed approach with the experimental ones and ADMM results. Furthermore it is important to emphasize that the results obtained with the eddy diffusivity depending on the source distance (Eq. (19)) are better than the ones reached with asymptotic eddy diffusivity (Eq. (21)), valid only for the far field of an elevated source. The present analysis reinforce the work previous of the authors 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 an elevated continuous point source.

Bearing in mind the exactness of the analytival solution, we may state that the pollutant concentration calculation by this kind of solution is free of error except for the round-off error and series truncation. Therefore we believe that the error in the GILTT numerical results is due to the uncertainties of the K-theory model. Given a closer look to the results reported in Table 1 we promptly realize a very good agreement, under statistical point of view, for both the semi-analytical ADMM model and GILTT results with the experimental datas. From these arguments we are confident to mention that the GILTT method with the eddy diffusivity coefficient considered is a quite suitable method to handle contaminant dispersion in atmosphere for the near source case.

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