CONTAMINANT DISPERSION SIMULATION BY SOLVING THE THREE-DIMENSIONAL ADVECTION-DIFFUSION EQUATION COMBINING THE GILTT AND ADMM METHODS

Camila Pinto da Costa
Universidade Federal do Rio Grande do Sul – Programa de Pós Graduação em Engenharia Mecânica - PROMEC
Sarmento Leite, 425, 3° andar, CEP: 90046-900, Porto Alegre, RS, Brasil
ccosta@mat.ufrgs.br

Davidson Martins Moreira
Universidade Luterana do Brasil – Departamento de Engenharia Ambiental
Miguel Tostes, 101 Prédio 11 – sala 230 Bairro São Luís, CEP: 92420-280, Canoas, RS, Brasil
davidson@ulbra.tche.br

Marco Túllio M. B. de Vilhena
Universidade Federal do Rio Grande do Sul – Programa de Pós Graduação em Engenharia Mecânica - PROMEC
Sarmento Leite, 425, 3° andar, CEP: 90046-900, Porto Alegre, RS, Brasil
vilhena@mat.ufrgs.br

Abstract. *In this work we present a model which overcomes the limits of the existing analytical ones in problems of the pollutant dispersion in atmosphere. The three-dimensional solution of the advection-diffusion equation is obtained applying the GILTT method (Generalized Integral Laplace Transform Technique) where the transformed problem is solved by the ADMM method (Advection Diffusion Multilayer Model). This is a promising result because this approach may be used for quantitative and qualitative estimations of pollutant distribution.*

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

1. Introduction

In the last years the dispersion of pollutants in the atmosphere has been study object and investigation in industrialized countries. The problems caused by the air pollution are complex and they affect natural processes, influencing in an outstanding way the ecological balance. For this reason, it is important to study and to understand the dispersion process of pollutant in the atmosphere to foresee the possible impact of the pollution on the several ecosystems. As a consequence, the computacional simulation becomes an important information source to describe the processes of pollutants dispersion in the Planetary Boundary Layer (PBL).

Technical development and growth of scientific understanding has greatly accelerated in all types of empirical, analytical and numerical models to predict the concentration variations in a plume. For this purpose, the advection-diffusion equation has been largely applied in operational atmospheric dispersion models. In principle, from this equation it is possible to obtain a theoretical model of dispersion from a source given appropriate boundary and initial conditions plus a knowledge of the mean wind velocity and concentration turbulent fluxes.

In this work, we step forward presenting a solution for the three-dimensional advection-diffusion equation in order to simulate pollutant dispersion in atmosphere. To our knowledge, the novelty of this work, relies on the semi-analytical character of the solution, not available before in the literature. To accomplish this objective we solve three-dimensional advection-diffusion equation combining the well known ADMM and GILTT methods. To more details about these approaches see the works of: Vilhena et al. (1998), Moreira et al. (1999), Costa (2003), Wortmann (2003), Costa (2004), Buske (2004), Wortmann et al. (2005) and Moreira et al. (2005).

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 and finally in section 3 we present the conclusions.

2. The solution methodology

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:

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

where c denotes the average concentration, u, v, w are the Cartesian components of the wind 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 in the longitudinal, crosswind and vertical directions.

The concentration turbulent fluxes are assumed to be proportional to the mean concentration gradient which is known as Fick-theory:

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

This assumption, combined with the continuity equation, leads to the advection-diffusion equation. For a Cartesian coordinate system in which the z is the height, we rewritten the advection-diffusion equation like (Blackadar, 1997):

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

where K_x, K_y, K_z are the Cartesian components of eddy diffusivity. In this work we are considering stationary conditions and $v = w = 0$. Besides, its considered that the axis x is oriented in the direction of the mean wind. So, the Eq. (3) is rewritten as:

$$U\frac{\partial c}{\partial x} = \frac{\partial}{\partial x}\left(K_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right) \tag{4}$$

for $0 < z < z_i$, $0 < y < L$ and $x > 0$, subject to the boundary conditions:

$$K_z \frac{\partial c}{\partial z} = 0 \qquad \text{at } z = 0, z_i \tag{4a}$$

$$K_y \frac{\partial c}{\partial y} = 0 \qquad \text{at } y = 0, L \tag{4b}$$

and

$$Uc(0,y,z) = Q\delta(z - H_s)\delta(y - yo) \qquad \text{at } x = 0 \tag{4c}$$

where H_s is the height source, z_i is the height of the PBL and Q is the contaminant continuous emission rate.

To solve the advection-diffusion equation for non-homogeneous turbulence we must take into account the dependence of the eddy diffusivity K and wind speed profile U on the height variable (variable z). Therefore, to solve this kind of problem by the Laplace Transform technique, we perform a stepwise approximation of these coefficients (Vilhena, 1998, Moreira, 1999, Costa, 2003, Costa, 2004).

To reach this goal we discretize the height z_i of the PBL into N sub-intervals in such manner that inside each sub-region, $K(z)$ and $U(z)$ assume respectively the following average values:

$$K_n = \frac{1}{z_{n+1} - z_n}\int_{z_n}^{z_{n+1}} K_z(z)dz \tag{5}$$

$$U_n = \frac{1}{z_{n+1} - z_n}\int_{z_n}^{z_{n+1}} U(z)dz \tag{6}$$

for $n = 1 : N$.

Now we are in position to solve the advection-diffusion equation by the GILTT and ADMM methods for each sub-interval.

Assuming that the non-homogeneous turbulence is modeled by an eddy diffusivity depending on the z-variable, we have to consider the stepwise approximation discussed above. Therefore, after this procedure the Eq. (4) has the form for every sub-interval $z_n < z < z_{n+1}$:

$$U_n \frac{\partial c_n}{\partial x} = K_{xn} \frac{\partial^2 c_n}{\partial x^2} + K_{y_n} \frac{\partial^2 c_n}{\partial y^2} + K_{zn} \frac{\partial^2 c_n}{\partial z^2} \tag{7}$$

for $n = 1,\ldots,N\text{-}1$, where c_n denotes the concentration at the n^{th} sub-interval. To determine the *2N* integration constants the additional (*2N-2*) conditions namely continuity of concentration and flux at interface are considered:

$$c_n = c_{n+1} \qquad n = 1, 2,...(N-1) \tag{8a}$$

$$K_n \frac{\partial c_n}{\partial z} = K_{n+1} \frac{\partial c_{n+1}}{\partial z} \qquad n = 1, 2,...(N-1) \tag{8b}$$

The formal application of the GITT method (Cotta, 1993, Cotta and Mikhaylov, 1997) begins with the choice of the problema of associated eigenvalues (also known in the literature as the auxiliary problem) and their respective boundary conditions. Applying then the method in Eq. (7) we have that the auxiliary problem and the boundary conditions are:

$$\psi_i''(y) + \lambda_i^2 \psi_i(y) \quad \text{em } 0 < y < L \tag{9a}$$

$$\psi_i'(y) \quad \text{em } y = 0, L \tag{9b}$$

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

$$\frac{1}{N_m^{1/2} N_n^{1/2}} \int_v \psi_m \psi_n dv = \begin{Bmatrix} 0\,,\ m \neq n \\ 1,\ m = n \end{Bmatrix}, \tag{10}$$

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

Following the formalism of the GITT method, the first step is to expand the variable $c_n(x,y,z)$ into the following form:

$$c_n(x,y,z) = \sum_{i=0}^{\infty} \frac{c_{in}(x,z)\ \psi_i(y)}{N_i^{\frac{1}{2}}} \tag{11}$$

Substituting Eq. (11) into Eq. (7) we obtain:

$$U_n \sum_{i=0}^{\infty} \frac{\partial c_{in}(x,z)}{\partial x} \frac{\psi_i(y)}{N_i^{\frac{1}{2}}} = K_{xn} \sum_{i=0}^{\infty} \frac{\partial^2 c_{in}(x,z)}{\partial x^2} \frac{\psi_i(y)}{N_i^{\frac{1}{2}}} + K_{y_n} \sum_{i=0}^{\infty} c_{in}(x,z) \frac{\psi_i''(y)}{N_i^{\frac{1}{2}}} + K_{zn} \sum_{i=0}^{\infty} \frac{\partial^2 c_{in}(x,z)}{\partial z^2} \frac{\psi_i(y)}{N_i^{\frac{1}{2}}} \tag{12}$$

where " is used to indicate the derivative of second order.

The next step is to apply the operator $\int_0^L \frac{\psi_i(y)}{N_i^{1/2}} dy$ in the Eq. (12) and use the Eq. (9a) to observe that $\psi_j''(y) = -\lambda_j^2 \psi_j(y)$. Recall that $\psi_j = \psi_j(y)$. Then,

$$\sum_{j=0}^{\infty} \left[-U_n \frac{\partial c_{jn}(x,z)}{\partial x} \int_0^L \frac{\psi_i\, \psi_j}{N_i^{\frac{1}{2}} N_{ji}^{\frac{1}{2}}} dy + K_{xn} \frac{\partial^2 c_{jn}(x,z)}{\partial x^2} \int_0^L \frac{\psi_i\, \psi_j}{N_i^{\frac{1}{2}} N_{ji}^{\frac{1}{2}}} dy - K_{y_n} \lambda_j^2 c_{jn}(x,z) \int_0^L \frac{\psi_i\, \psi_j}{N_i^{\frac{1}{2}} N_{ji}^{\frac{1}{2}}} dy + + K_{zn} \frac{\partial^2 c_{jn}(x,z)}{\partial z^2} \int_0^L \frac{\psi_i\, \psi_j}{N_i^{\frac{1}{2}} N_{ji}^{\frac{1}{2}}} dy \right] = 0 \tag{13}$$

Using the property of orthonormality given in Eq. (10) , Eq. (13) can be rewritten as

$$-U_n \frac{\partial c_{jn}(x,z)}{\partial x} + K_{xn} \frac{\partial^2 c_{jn}(x,z)}{\partial x^2} - K_{yn} \lambda_j^2 c_{jn}(x,z) + K_{zn} \frac{\partial^2 c_{jn}(x,z)}{\partial z^2} = 0 \tag{14}$$

Dividing the above equation by K_{x_n} :

$$\frac{\partial^2 c_{jn}(x,z)}{\partial x^2} - \frac{U_n}{K_{xn}} \frac{\partial c_{jn}(x,z)}{\partial x} - \frac{K_{yn}\lambda_j^2}{K_{xn}} c_{jn}(x,z) + \frac{K_{zn}}{K_{xn}} \frac{\partial^2 c_{jn}(x,z)}{\partial z^2} = 0 \tag{15}$$

For the boundary condition of Eq. (4c), using the same arguments, we have that:

$$\sum_{j=0}^{\infty} U_n c_{jn}(0,z) \int_0^L \frac{\psi_i \, \psi_j}{N_i^{1/2} N_j^{1/2}} dy = \int_0^L \frac{Q\,\delta(z\text{-}Hs)\,\delta(y\text{-}yo)\psi_i}{N_i^{1/2}} dy \tag{16}$$

Then, performing the due substitutions and integrations, the boundary condition is:

$$c_{jn}(0,z) = \frac{Q\;\delta(z\text{-}Hs)\;\psi_j(yo)}{U_n\;N_i^{1/2}} \tag{17}$$

In the traditional GITT (Cotta, 1993, Cotta and Mikhaylov, 1997) method the transformed problem, represented by the Eq. (17), is solved numerically. In the work of Wortmann (2000) this problem was analitically solved for the first time. Therefore, the GITT method with analitically solution of the transformed problem is called GILTT method (Wortmann, 2003, Buske, 2004, Wortmann et al., 2005, Moreira et al., 2005). So, following this idea, in this work the transformed problem is also solved applying the Laplace Transform technique:

$$L\{c_{jn}(x,z)\} = F_{jn}(s,z) \tag{18}$$

After the application of the Laplace transform procedure the Eq. (15) is:

$$\left[s^2 F_{jn}(s,z) - s c_{jn}(0,z) - \frac{\partial c_{jn}(0,z)}{\partial x}\right] - \frac{U_n}{K_{x_n}}\left[sF_{jn}(s,z) - c_{jn}(0,z)\right] - \frac{K_{y_n}}{K_{x_n}} \lambda_j^2 F_{jn}(s,z) + \frac{K_{z_n}}{K_{x_n}} \frac{\partial^2 F_{jn}(s,z)}{\partial z^2} = 0 \tag{19}$$

Replacing Eq. (17) in Eq. (19) we have:

$$s^2 F_{jn}(s,z) - s\left(\frac{Q\,\delta(z\text{-}Hs)\,\psi_j(yo)}{U_n\,N_i^{1/2}}\right) - \frac{U_n s}{K_{x_n}} F_{jn}(s,z) + \frac{U_n s}{K_{x_n}}\left(\frac{Q\,\delta(z\text{-}Hs)\,\psi_j(yo)}{U_n\,N_i^{1/2}}\right) - \frac{K_{y_n}}{K_{x_n}} \lambda_j^2 F_{jn}(s,z) + \frac{K_{z_n}}{K_{x_n}} \frac{\partial^2 F_{jn}(s,z)}{\partial z^2} = 0 \tag{20}$$

$$F_{jn}(s,z)\left(s^2 - \frac{U_n s}{K_{x_n}} - \frac{K_{y_n}}{K_{x_n}} \lambda_j^2\right) + \frac{K_{z_n}}{K_{x_n}} \frac{\partial^2 F_{jn}(s,z)}{\partial z^2} = -\left(\frac{Q\,\delta(z\text{-}Hs)\;\psi_j(yo)}{U_n\,N_i^{1/2}}\right)\left(\frac{U_n}{K_{x_n}} - s\right) \tag{21}$$

Now, taking in Eq. (21)

$$A_n = \frac{K_{zn}}{K_{xn}}\;,\quad B_{jn}(s) = -\left(s^2 - \frac{U_n s}{K_{xn}} - \frac{K_{yn}\lambda_j^2}{K_{xn}}\right) \text{ and } h_{jn}(s) = -\frac{Q}{U_n} \frac{\psi_j(yo)}{N_j^{1/2}}\left(\frac{U_n}{K_{xn}} - s\right) \tag{22}$$

we have that

$$-B_{jn}(s) F_{jn}(s,z) + A_n \frac{\partial^2 F_{jn}(s,z)}{\partial z^2} = h_{jn}(s)\;\delta(z - H_s) \tag{23}$$

Dividing the Eq. (23) by A_n, the equation is rewriten as:

$$\frac{\partial^2 F_{jn}(s,z)}{\partial z^2} - \frac{B_{jn}(s)}{A_n} F_{jn}(s,z) = \frac{h_{jn}(s)}{A_n} \ \delta(z - H_s) \tag{24}$$

The general solution of the above equation can be writen in the following form:

$$F_j = F_{jp} + F_{jh} \tag{25}$$

where F_{jp} is the particular solution and F_{jh} is the homogeneous solution of the homogeneous equation associated.

The homogeneous equation associated to Eq. (24) is:

$$\frac{\partial^2 F_{jn}(s,z)}{\partial z^2} - \frac{B_{jn}(s)}{A_n} F_{jn}(s,z) = 0 \tag{26}$$

So the solution of the homogeneous equation is given by:

$$F_{jh} = C_{1n} e^{R_{jn} z} + C_{2n} e^{-R_{jn} z} \tag{27}$$

where $R_{jn} = R_{jn}(s) = \sqrt{\frac{B_{jn}(s)}{A_n}}$.

The particular solution is:

$$F_{jp} = \frac{e^{R_{jn} z}}{2R_{jn}} \int \frac{h_{jn}(s)}{A_n} e^{-R_{jn} z} \ \delta(z - H_s) dz + \frac{e^{-R_{jn} z}}{-2R_{jn}} \int \frac{h_{jn}(s)}{A_n} e^{R_{jn} z} \ \delta(z - H_s) dz \tag{28}$$

$$F_{jp} = \frac{h_{jn}(s)}{2R_{jn} A_n} \left(e^{R_{jn}(z - H_s)} - e^{-R_{jn}(z - H_s)} \right) \tag{29}$$

Returning to Eq. (25) and adding Eq. (27) and Eq. (29):

$$F_{jn}(s,z) = C_{1n} e^{R_{jn} z} + C_{2n} e^{-R_{jn} z} + \frac{h_{jn}(s)}{2R_{jn} A_n} \left(e^{R_{jn}(z - H_s)} - e^{-R_{jn}(z - H_s)} \right) \tag{30}$$

The constants C_{1n} and C_{2n} are determined solving a linear system apllying the ($2N$-2) interface conditions given in Eq. (8a) and Eq. (8b).

In this moment its necessary to take the Laplace inversion of Eq. (30), so that:

$$c_{jn}(x,z) = L^{-1}\{F_{jn}(s,z)\} = \sum_{k=1}^{\infty} \frac{P_k}{x} w_k F_{jn}\left(\frac{P_k}{x}\right) \tag{31}$$

this inversion is numericaly using the Gaussian Quadrature scheme.

Applying Eq. (31) in Eq. (30) we finally found the solution of the transformed problem:

$$c_{jn}(x,z) = \sum_{k=1}^{Ni} \frac{P_k}{x} w_k \left[C_{1n} e^{R^*_{jn} z} + C_{2n} e^{-R^*_{jn} z} + \frac{h^*_{jn}(s)}{2R^*_{jn} A_n} \left(e^{R^*_{jn}(z - H_s)} - e^{-R^*_{jn}(z - H_s)} \right) \right] \tag{32}$$

where w$_k$ and P$_k$ are the Gaussian Quadrature parameters tabulated in the book of Stroud and Secrest (1966), Ni is the number of inversions,

$R^*_{jn} = \sqrt{\frac{R^*_{jn} z(s)}{A_n}}$; $A_n = \frac{K_{zn}}{K_{xn}}$; $B^*_{jn}(s) = -\left(\left(\frac{P_k}{x} \right)^2 - \frac{U_n}{K_{xn}} \frac{P_k}{x} - \frac{K_{yn} \lambda_j^2}{K_{xn}} \right)$ and $h^*_{jn}(s) = -\frac{Q}{U_n} \frac{\psi_j(yo)}{N_j^{1/2}} \left(\frac{U_n}{K_{xn}} - \frac{P_k}{x} \right)$.

Using the form of the inverse,

$$c_n(x,y,z) = \sum_{i=0}^{\infty} \frac{c_{in}(x,z)\,\psi_i(y)}{N_i^{\frac{1}{2}}} \tag{33}$$

the final solution of the proposed problem is obtained. $\psi_i(y)$ comes from the problem of Sturm-Liouville and $c_{in}(x,z)$ from the solution of the transformed problem:

$$c_n(x,y,z) = \sum_{i=0}^{\infty} \frac{\psi_i(y)}{N_i^{\frac{1}{2}}} \left\{ \sum_{k=1}^{Ni} \frac{P_k}{x} w_k \left[C_{1n} e^{R^*_{jn} z} + C_{2n} e^{-R^*_{jn} z} + \frac{h^*_{jn}(s)}{2R^*_{jn} A_n} \left(e^{R^*_{jn}(z-H_s)} - e^{-R^*_{jn}(z-H_s)} \right) \right] \right\} \tag{34}$$

This equation is then truncated in a suficiently large number os terms to obtain the final solution of the problem. Therefore the solution of problem (4) is expressed by equation (34). To this point it is relevant to underline that this solution is semi-analytical in the sense that the only approximations considered along its derivation are the stepwise approximation of the parameters, the numerical Laplace inversion of the transformed concentration and the series truncation in the inverse of the GITT (Eq. (33)).

3. Conclusions

Recalling the good computational performance of both GILTT and ADMM methods to simulate pollutant dispersion in atmosphere by solving the two-dimensional advection-diffusion equation, we are confident to point out that the proposed methodology, besides the novelty of the semi-analytical character of the solution, this approach is a promising technique to simulate contaminant dispersion in atmosphere for more realistic problems. We focus our future attention in the task of using this solution to solve the time-dependent problem and compare with results in the literature.

4. Acknowledgements

The authors thank to CNPq and FAPERGS for the financial support of this work.

5. References

Blackadar, A.K., 1997. “Turbulence and diffusion in the atmosphere: lectures in environmental sciences”. Springer-Verlag. 185 pp.

Buske, D., 2004. “Analytical solution of the advection-diffusion equation by the GILTT method aplicated to atmospheric pollutant dispersion”. MSc Degree dissertation, Federal University of Rio Grande do Sul, in portuguese.

Costa, C.P, 2003. “Influence of non-local effects in the pollutants dispersion in the Planetary Boundary Layer”. MSc Degree dissertation, Federal University of Rio Grande do Sul, in portuguese.

Costa, C.P., Moreira, D.M. and Vilhena, M.T., 2004. “Influence of the non-local effects in pollutant dispersion in the Convective Boundary Layer”. XIII CBMET, in portuguese.

Cotta, R.M., 1993. “Integral transforms in computational heat and fluid flow”, CRC Press, Boca Raton, Florida.

Cotta, R. and Mikhaylov, M., 1997. “Heat Conduction Lumped Analysis, Integral Transforms, Symbolic Computation”, John Wiley Sons, Baffins Lane, Chinchester, England.

Moreira, D.M., Degrazia, G.A. and Vilhena, M.T., 1999. “Dispersion from low sources in a convective boundary layer: An analytical model”. Nuovo Cimento 22C, 685-691.

Moreira, D.M., Vilhena, M.T., Tirabassi, T., Carvalho, J., Buske, D., Cotta, R.M., 2005. “Near source atmospheric pollutant dispersion using the new GILTT method”. Atmospheric Environment . Submitted.

Stroud, A.H. and Secrest, D., 1966. “Gaussian quadrature formulas”. Englewood Cliffs, N.J., Prentice Hall Inc.

Vilhena, M.T., Rizza, U., Degrazia, G.A., Mangia, C., Moreira, D.M. and Tirabassi, T., 1998. “An analytical air pollution model: Development and evaluation”. Contrib. Atmos. Phys. 71, 315-320.

Wortmann, S., Moura, A. and Vilhena, M.T., 2000. “solution of the one dimensional transient polutant problem with variable eddy diffusivity coefficient”. Anais ENCIT , in portuguese.

Wortmann, S., 2003. “Generalized integral transform with Laplace transform in solution of applied problems”. Ph.D. thesis. Federal University of Rio Grande do Sul, in portuguese.

Wortmann, S., Vilhena, M.T., Moreira, D.M. and Buske, D., 2005. “A New Analytical Approach to Simulate The Pollutant Dispersion in the PBL”. Atmospheric Environment 39, 2187-2194.

6. Responsibility notice

The authors are the only responsible for the printed material included in this paper.