A new analytical solution of the advection-diffusion equation for a ground-level finite area source

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1. Introduction

Despite wide use due to the simplicity of its formulation, the Gaussian plume model for turbulent atmospheric dispersion of a contaminant is not adequate for ground-level pollution sources because the mean wind velocity is assumed to be uniform and the vertical eddy diffusivity constant. For a more realistic description of turbulent dispersion near the surface of the earth it is essential to account for the variation of the mean wind velocity and the vertical eddy diffusivity with height above the ground. In this work, we take a step forward regarding the Gaussian concepts to simulate pollutant dispersion in the atmosphere, presenting a new three-dimensional solution of the steady-state advection-diffusion equation considering a vertically heterogeneous atmospheric boundary layer (ABL) for a ground-level finite area source. The model incorporates realistic profiles for the variation of wind speed, lateral and vertical eddy diffusivity with height. The model is well suited for accurate prediction of emission concentration levels in the vicinity of an area source, as well as farther downwind, under all stability atmospheric conditions. We reach this goal by using two methods: the generalized integral transform technique (GITT), a hybrid method that has solved a wide class of direct and inverse problems mainly in the area of heat transfer and fluid mechanics, and the transformed problem is solved by the advection-diffusion multilayer method (ADMM), a semi-analytical solution based on a discretization of the ABL in sub-layers where the advection-diffusion equation is solved by the Laplace transform technique.

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 section 3 the turbulent parameterisation assumed in this work is presented; in section 4, the numerical results given by the method are announced as well as the comparison with experimental data; finally, in section 5 we present the conclusions.

2. The mathematical model

The advection-diffusion equation of air pollution in the atmosphere is essentially a statement of conservation of suspended material. The concentration turbulent fluxes are assumed to be proportional to the mean concentration gradient, which is known as Fick-theory. This assumption, combined with the continuity equation, leads to the advection-diffusion equation (Blackadar, 1997):

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

where c denotes the average concentration, K_x, K_y, K_z and u, v, w are the Cartesian components of eddy diffusivity and wind, respectively, and S is the source term. The x-axis of the Cartesian coordinate system is aligned in the direction of the actual wind near the surface, the y-axis is oriented in the horizontal crosswind direction, and the z-axis is chosen vertically upwards.

In order to solve the Eq. (1) we include the following assumptions: the pollutants are inert and have no additional sinks or sources downwind from the source. The vertical and lateral components of the mean flow are assumed to be zero. The mean horizontal flow is incompressible, horizontally homogeneous and stationary. Then, we have:

$$u\frac{\partial c}{\partial x}=\frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right) \quad (2)$$

for $0<z<h$, $0<y<L$ and $x>0$. The mathematical description of the dispersion problem (2) is completed by boundary conditions. In the *z*-direction, the pollutants are subjected to the boundary conditions of zero flux at ground and ABL top:

$$K_z\frac{\partial c}{\partial z}=0 \quad \text{at} \quad z=0,h \quad (3a)$$

where and *h* is the height of the ABL. In the *y*-direction, we have the conditions:

$$\frac{\partial c}{\partial y}=0 \quad \text{at} \quad y=0,L \quad (3b)$$

and, for the source condition, a continuous point source of constant emission rate Q is assumed, with a fixed frame of reference with the *x*-axis coinciding with the plume (Arya, 2003):

$$uc(0,y,z)=Q\delta(z-H_s)\delta(y-y_o) \quad \text{at} \quad x=0 \quad (3c)$$

where δ is the Dirac delta function and H_s is the height source.

To solve the advection-diffusion equation for inhomogeneous turbulence by the ADMM method (Moreira and Vilhena, 2009), we must take into account the dependence of the eddy diffusivities and wind speed profiles on the height variable (variable *z*). Therefore, we perform a stepwise approximation of these coefficients. To reach this goal, we discretize the height *h* of the ABL into *N* sub-intervals in such manner that inside each sub-region the eddy diffusivities and wind velocities assume average values. For the eddy diffusivity depending on *x* and *z*, we take the average of the *x* and *z* variables. Indeed, it is now possible to recast problem (2) as a set of advective-diffusive problems with constant parameters, which for a generic sub-layer reads like:

$$u_n\frac{\partial c_n}{\partial x}=K_{x\,n}\frac{\partial^2 c_n}{\partial x^2}+K_{y\,n}\frac{\partial^2 c_n}{\partial y^2}+K_{z\,n}\frac{\partial^2 c_n}{\partial z^2} \qquad z_n\le z\le z_{n+1} \quad (4)$$

for n = 1:*N*, where *N* denotes the number of sub-layers and c_n denotes the concentration at the n^{th} sub-interval. Besides which, two boundary conditions are imposed at $z=0$ and *h* given by equation (3a) together with the continuity conditions for the concentration and flux of concentration at the interfaces. Namely:

$$c_n=c_{n+1} \qquad n = 1, 2,...(N-1) \quad (5a)$$

$$K_n\frac{\partial c_n}{\partial z}=K_{n+1}\frac{\partial c_{n+1}}{\partial z} \qquad n = 1, 2,...(N-1) \quad (5b)$$

must be considered in order to uniquely determine the 2*N* arbitrary constants appearing in the solution of the set of problems (4).

Now we are in position of applying the GITT method in the *y*-direction. The formal application of the GITT method (Cotta, 1993, Cotta and Mikhaylov, 1997) begins with the choice of the problem of associated eigenvalues (also known in the literature as the auxiliary problem) and their respective boundary conditions:

$$\psi_i^{''}(y)+\lambda_i^2\psi_i(y)=0 \qquad \text{at} \quad 0<y<L \quad (6a)$$

$$\psi_i^{'}(y)=0 \qquad \text{at} \quad y=0,L \quad (6b)$$

The solution is $\psi_i(y)=\cos(\lambda_i y)$, where λ_i are the positive roots of the expression $\sin(\lambda_i L)=0$. Then, $\lambda_0=0$ and $\lambda_i=i\pi/L$. 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, satisfy the following orthonormality condition:

$$\frac{1}{\mathrm{N}_m^{1/2}\mathrm{N}_n^{1/2}}\int_{\mathrm{v}}\psi_m(z)\psi_n(z)dv=\left\{\begin{matrix}0,\mathrm{m}\neq\mathrm{n}\\1,\mathrm{m}=\mathrm{n}\end{matrix}\right\}$$

where N_m is given by:

$$\mathrm{N}_m=\int_{\mathrm{v}}\psi_m^2(z)dv \tag{7}$$

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

$$c_n(x,y,z)=\sum_{i=0}^{\infty}\frac{\bar{c}_{ni}(x,z)\psi_i(y)}{\mathrm{N}_i^{1/2}} \tag{8}$$

In the traditional GITT method the transformed problem is solved numerically. In this work the transformed problem is solved applying the Laplace Transform technique (ADMM method). After some steps, we obtain (for more details see the work of Costa et al., 2006):

$$c_n(x,y,z)=\sum_{i=0}^{\infty}\frac{\psi_i(y)}{N_i^{1/2}}\left\{\sum_{k=1}^{M}\frac{p_k}{x}a_k\left[C_{1n}e^{G_nz}+C_{2n}e^{-G_nz}+\frac{Q}{2F_a}\left(e^{G_n(z-H_s)}-e^{-G_n(z-H_s)}\right)H(z-H_s)\right]\right\} \tag{9}$$

where

$$G_n=\sqrt{\frac{1}{K_z}\left(\frac{p_k}{x}u_n\beta^*+K_y\lambda_j^2\right)}\ ;\ F_a=\frac{N_i^{1/2}}{\psi_i(y_0)}\frac{\sqrt{K_z\left(\frac{p_k}{x}u_n\beta^*+K_y\lambda_i^2\right)}}{\beta^*}\ \text{ and }\ \beta^*=\left(1-\frac{p_k}{P_e}\right)$$

and $H(z-H_s)$ is the Heaviside function and $P_e=\frac{u_nx}{K_x}$ is the well known Peclet number, essentially representing the ratio between the advective transport to diffusive transport. The constants a_k and p_k are the weights and roots of the Gaussian quadrature scheme and are tabulated in the book by Stroud and Secrest (1966) while k is the quadrature points.

To get an accurate estimate of the concentrations from an isolated area source, integrations should be done over both the along-wind (x-axis) and crosswind (y-axis) dimensions of the source. To obtain an analytical solution for a ground-level finite area source, the solution for a ground-level point source (Eq. 9) is used (Park and Baik, 2008), resulting:

$$c_n(x,y,z)=\int_{x_1}^{x_2}\int_{y_1}^{y_2}\sum_{i=0}^{\infty}\frac{\psi_i(y)}{N_i^{1/2}}\left\{\sum_{k=1}^{M}\frac{p_k}{x}a_k\left[C_{1n}e^{G_nz}+C_{2n}e^{-G_nz}+\frac{Q}{2F_a}\left(e^{G_n(z-H_s)}-e^{-G_n(z-H_s)}\right)H(z-H_s)\right]\right\}.$$
$$.dydx \tag{10}$$

3. Turbulence Parameterization

This work considers the results obtained by Degrazia et al. (2001), which follows:

$$\frac{K_\alpha}{w_*h}=\frac{0.09c_i^{1/2}\psi^{1/3}(z/h)^{4/3}}{(f_m^*)_i^{4/3}}\int_0^{\infty}\frac{sin\left(\frac{7.84c_i^{1/2}\psi^{1/3}(f_m^*)_i^{2/3}Xn'}{(z/h)^{2/3}}\right)}{(1+n')^{5/3}}\frac{dn'}{n'} \tag{11}$$

where w_* is the convective velocity scale (α = x, y, z), φ is the non-dimensional molecular dissipation rate functions associated to buoyancy productions, $(f^*_m)_i$ is the reduced frequency of the convective spectral peak and $c_i=\alpha_i\alpha_u(2\pi k)^{-2/3}$ with α_u = 0.5± 0.05 and α_i = 1, 4/3, 4/3 for u, v and w components, respectively, and X is a non-dimensional time since is the ratio of travel time x/u and the convective timescale h/w_*.

The formulae used for evaluating mean wind are those of similarity (Panofsky and Dutton, 1988):

$$u = \frac{u_*}{k_a}\left[\ln\frac{z}{z_0} - \Psi_m\left(\frac{z}{L}\right)\right] \tag{12}$$

where, u_* is the scale velocity relative to mechanical turbulence, k_a the von Karman constant, L is the Monin-Obukhov length, z_o roughness length and Ψ_m the stability function expressed in Businger relations:

$$\Psi_m\left(\frac{z}{L}\right) = \ln\left(\frac{1+A^2}{2}\right) + \ln\left(\frac{1+A}{2}\right)^2 - 2\arctan x + \frac{\pi}{2} \qquad \text{for} \qquad 1/L < 0$$

with $A = (1 - 15\,z/L)^{1/4}$.

4. Numerical results

Realistic experimental datasets for area sources are difficult to find in the literature. To verify the physical consistency of the model and the connection between theory and reality, the model performance was evaluated using 3D experimental data of Copenhagen (Gryning and Lick, 1984., Gryning et al. 1987). These experiments were carried out north of the city of Copenhagen, where a pollutant SF6 was released without buoyancy from a tower at a height of 115m and collected at the surface positions by samplers. The site of the experiment was mainly residential with a roughness length of 0.6 m. Weather conditions during the experiment varied between moderately unstable and convective.

Figure 1 shows the scattering diagram between the observed and model-predicted concentrations. According to the figures, the concentrations satisfactorily reproduce the experimental results.

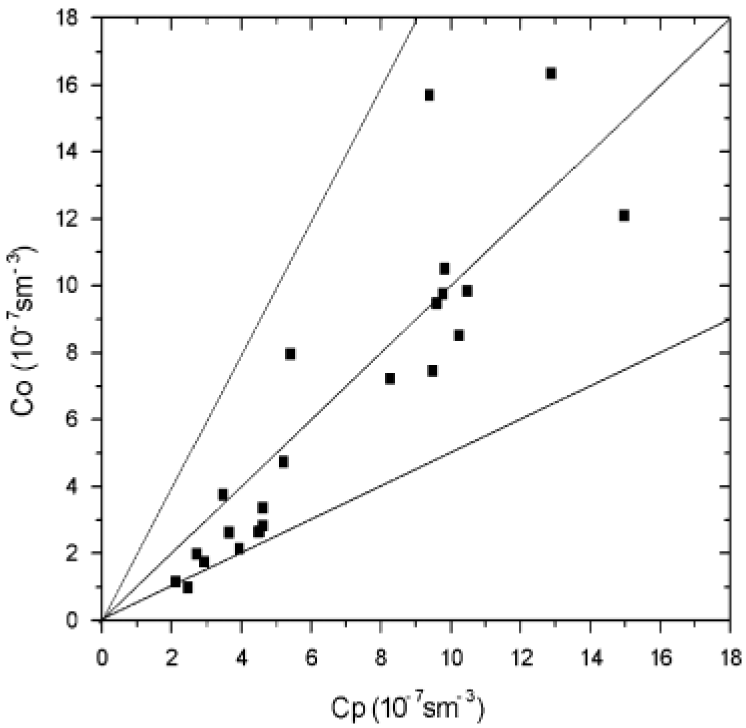

Figure 1: Scatter diagram for the solution (9): Observed (Co) and predicted (Cp) centerline ground-level concentration normalized with emission rate (c/Q). Data between lines correspond to ratio Co/Cp ∈ [0.5, 2].

Table 1 shows the statistical indexes defined by Hanna (1989), experimental data obtained from Copenhagen. The indices indicate that the model simulates satisfactorily the observed concentrations, with values *nmse*, *fb* and *fs* relatively close to zero, and *r* and fa2 relatively close to 1.

Table 1: Statistical evaluation of the model results with Copenhagen data set.

Model	nmse	R	Fa2	fb	Fs
c(x,0,0)/Q	0.15	0.87	0.96	0.01	0.09

5. Conclusions

We present in this work a new steady-state, three-dimensional, semi-analytical solution of the advection-diffusion equation considering a vertically inhomogeneous ABL for a ground-level finite area source (Eq. 10). It is relevant to underline that in this approach no approximation is made in the solution derivation, except for the stepwise approximation of the parameters and the Laplace numerical inversion. Also it is important to mention that the semi-analytical method is quite general in the sense that it solves one, two and three-dimensional diffusion problems. It Is a promising technique for simulating contaminant dispersion in the atmosphere for more realistic problems.

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