American Journal of Environmental Engineering 2018, 8(4): 112-117
DOI: 10.5923/j.ajee.20180804.05

On a Model for Pollutant Dispersion in the Atmosphere with Partially Reflective Boundary Conditions and Data Simulation Using CALPUFF

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Abstract The present work is an attempt to simulate the dispersion of pollutants in the surroundings of the thermoelectric plant located in Linhares from a new mathematical model based on partially reflective boundaries in the deterministic advection-diffusion equation. In addition to the advection-diffusion equation with partially reflective boundaries, it was used data simulated with the CALPUFF model. The exposed model was validated previously with the Hanford and Copenhagen experiments and the results indicate that effects on the boundaries are essential to model dispersion phenomenona in the atmospheric boundary layer.

Keywords Advection-diffusion equation, Reflective boundary conditions, CALPUFF

1. Introduction

The development of mathematical models is fundamental for environmental management once it can calculate the whole concentration field of pollutants based on the local micrometeorological data. Over the years there has been an improvement not only in technology, but also in mathematical techniques whether numerical or analytical, which makes the models closer to the phenomenon they are mimicking. Although the dispersion of pollutants phenomenon is not deterministic, its modelling usually is, that means there will always be a difference between simulation and measurements.

As an attempt to diminish this difference between simulation and measurements, the well-known advection-diffusion equation is solved making use of modified boundary conditions. In a previous work [11] this model was validated with reference experiments such as Hanford [8] and Copenhagen [9] and in the sense of high agreement between data and model, the results were significant. For this reason, the present work has the objective of using the presented model, together with simulated data from the model CALPUFF, to obtain the concentration field of pollutants in the surroundings of the thermoelectric plant located in Linhares – ES, Brazil.

2. A Locally Gaussian Model

The advection-diffusion equation can be obtained from the continuity equation making use of Reynolds decomposition to separate the mean components for the concentration and the velocity fields. Upon taking averages and substitution of the average fluctuations by Fick's closure, where it is assumed that the turbulent flow of concentration is proportional to the magnitude of the mean concentration gradient, the desired equation for mean concentrations is attained. Considering the source term as an instantaneous initial condition denoted by the Dirac delta functions, and the diffusive coefficients K_x, K_y and K_z (m²/s) locally constant, the initial value problem that models the dispersion of a *puff* is given by [1, 16]

$$\frac{\partial \overline{c}}{\partial t}+\overline{u}\frac{\partial \overline{c}}{\partial x}+\overline{v}\frac{\partial \overline{c}}{\partial y}+\overline{w}\frac{\partial \overline{c}}{\partial z}=K_x\frac{\partial^2 \overline{c}}{\partial x^2}+K_y\frac{\partial^2 \overline{c}}{\partial y^2}+K_z\frac{\partial^2 \overline{c}}{\partial z^2} \quad (1)$$

$$\overline{c}(x,y,z,0)=Q\delta(x-x_0)\delta(y-y_0)\delta(z-H_s), \quad (2)$$

where c is the mean concentration of the pollutant (g/m^3), u, v and w are the mean wind speeds (m/s) oriented in the x, y and z directions, respectively, x_0 and y_0 are the coordinates of the location of the source in the cartesian plane (m), Q is the intensity of the source (g/s) and H_s is the height of the source (m). This initial value problem can be solved analytically making use of the separation of variables method [13] and further applying Fourier transform [17] in each separated equation.

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Published online at http://journal.sapub.org/ajee

However, most dispersion problems are due to continuous emissions, which can be idealized by the superposition of instantaneous emissions. Considering a small time interval $d\tau$ with an instantaneous emission, then the continuous emission is approximated by a time convolution

$$\overline{C}(x,y,z,t) \propto \int_0^t \overline{c}(x,y,z,t-\tau)\,d\tau\ , \tag{3}$$

where c is the concentration for the instantaneous and C for the continuous emission. The solution of the advection-diffusion equation for continuous emission is

$$\begin{aligned}\overline{C}(x,y,z,t) &= \frac{Q}{\sqrt{64\pi^3 K_x K_y K_z}} \int_0^t \frac{1}{\sqrt{(t-\tau)^3}} \\ &\exp\left\{-\frac{[x-x_0-\overline{u}(t-\tau)]^2}{4K_x(t-\tau)} - \frac{[y-y_0-\overline{v}(t-\tau)]^2}{4K_y(t-\tau)}\right. \\ &\left.-\frac{[z-H_s-\overline{w}(t-\tau)]^2}{4K_z(t-\tau)}\right\}\,d\tau\ .\end{aligned} \tag{4}$$

Since the solution (4) was obtained by Fourier transform, it is valid for the infinite ranges $x \in (-\infty,\infty)$, $y \in (-\infty,\infty)$, $z \in (-\infty,\infty)$ although the dispersion of pollutants is limited at the vertical domain by the ground $(z=0)$ and the top of the atmospheric boundary layer $(z=z_i)$ thus the infinite range has to be mapped into a finite range.

3. Reflective Boundary Conditions

To justify the mapping of the infinite range $z \in (-\infty,\infty)$ to the finite $z \in [0, z_i]$ we first consider a cut of the distribution at $z=0$ and $z=z_i$, respectively. Formally, the reflection on the ground and in the atmospheric boundary layer may be viewed as contributions due to a virtual source in some effective heights to both sides below ground and above the boundary layer [2], those heights are the center of the gaussians formed at the ground and at the top of the atmospheric boundary layer. The sequences that represent the mirror maxima are

$$\left.\begin{array}{lcl} H_s & \to & -H_s - 2nz_i \\ H_s & \to & H_s + 2nz_i \end{array}\right\} \forall n \in Z. \tag{5}$$

Substituting those two sequences (5) in the solution for the continuous emission (4), the solution for continuous emission with complete reflection is obtained

$$\begin{aligned}\overline{C}(x,y,z,t) &= \frac{Q}{\sqrt{64\pi^3 K_x K_y K_z}} \int_0^t \left[\frac{1}{\sqrt{(t-\tau)^3}}\right. \\ &\exp\left\{-\frac{[x-x_0-\overline{u}(t-\tau)]^2}{4K_x(t-\tau)} - \frac{[y-y_0-\overline{v}(t-\tau)]^2}{4K_y(t-\tau)}\right\} \\ &\left(\sum_{n=-\infty}^{\infty} \exp\left\{-\frac{[z-H_s-2nz_i-\overline{w}(t-\tau)]^2}{4K_z(t-\tau)}\right\}\right. \\ &\left.\left.+\exp\left\{-\frac{[z+H_s+2nz_i-\overline{w}(t-\tau)]^2}{4K_z(t-\tau)}\right\}\right)\right]\,d\tau,\end{aligned} \tag{6}$$

and is now valid for $x \in (-\infty,\infty)$, $y\ (-\infty,\infty)$, $z \in [0, z_i]$.

The sequences presented in equation (5) consider that when the pollutant reaches the soil and the top of the atmospheric boundary layer, it will reflect completely, although some part may escape to the free atmosphere or infiltrate into the soil, so that a partial permeability can be considered in the problem. To consider this permeability one introduces in the sequences (5) the terms ω_b and ω_g, which are the reflection parameters for the atmospheric boundary layer and for the ground, respectively. These terms can be interpreted as a reduction factor of the quantity of pollutant between the soil and the atmospheric boundary layer. The solution for the advection-diffusion equation with partially reflective boundary conditions and continuous emission is

$$\begin{aligned}\overline{C}(x,y,z,t) = \frac{Q}{\sqrt{64\pi^3 K_x K_y K_z}} \int_0^t \frac{1}{\sqrt{(t-\tau)^3}} \exp\left(-\frac{[x-x_0-\overline{u}(t-\tau)]^2}{4K_x(t-\tau)}\right. \\ \left.-\frac{[y-y_0-\overline{v}(t-\tau)]^2}{4K_y(t-\tau)}\right)\left\{\exp\left(-\frac{[z-H_s-\overline{w}(t-\tau)]^2}{4K_z(t-\tau)}\right) + \exp\left(-\frac{[z+\omega_g H_s-\overline{w}(t-\tau)]^2}{4K_z(t-\tau)}\right)\right. \\ +\sum_{n=1}^{\infty}\sum_{m=0}^{1}\left[\exp\left(-\frac{[z-\omega_b((-1)^m H_s+2nz_i)-\overline{w}(t-\tau)]^2}{4K_z(t-\tau)}\right)\right. \\ \left.\left.+\exp\left(-\frac{[z+\omega_g((-1)^m H_s+2nz_i)-\overline{w}(t-\tau)]^2}{4K_z(t-\tau)}\right)\right]\right\}\,d\tau\end{aligned} \tag{7}$$

4. Turbulent Diffusivity Parametrisation

The parametrisation for the eddy diffusion coefficient for convective conditions is based on the turbulent diffusion theory [18] and on the turbulent kinetic energy spectrum [14] and is given by [6]

$$K_\alpha = \frac{0.09 w_* z_i c_i^{1/2} \psi^{1/3} (z/z_i)^{4/3}}{(f_m^*)_i^{4/3}} \times \int_0^\infty \frac{\sin\left[\frac{7.84 c_i^{1/2}\psi^{1/3}(f_m^*)_i^{2/3} X n'}{(z/z_i)^{2/3}}\right]}{(1+n')^{5/3}} \frac{dn'}{n'}. \tag{8}$$

where $\alpha = x, y, z$ and $i = u, v, w$. w_* is the convective velocity scale, z is the observation height, z_i is the inversion height, X is the dimensionless distance, n' is the dimensionless frequency of the turbulent kinetic energy spectrum, $c_i = \alpha_i(0.5 \pm 0.05)(2\pi k)^{-2/3}$ is a constant [6], $(fm_*)_i$ is the normalized frequency of the spectral peak regardless of stratification and ψ is the dissipation function and has the form [10, 7]

$$\psi^{1/3} = \left[\left(1 - \frac{z}{z_i}\right)^2 \left(\frac{z}{-L}\right)^{-2/3} + 0.75\right]^{1/2}, \tag{9}$$

where L is the Obukhov length in the surface layer. The values for the normalized frequency of the spectral peak are $(f_m^*)_u = 0.67$, $(f_m^*)_v = 0.67$ [12] and $(f_m^*)_w = z/(\lambda_m)_w$ with $(\lambda_m)_w = 1.8 z_i [1 - \exp(-4z/z_i) - 0.0003 \exp(8z/z_i)]$ [4].

4.1. Wind Speed Profile

The wind speed profile was parametrised according to the Monin-Obukhov's similarity theory and the OML-model [3], where close to the surface and because of its roughness, there is a raising profile, whereas sufficiently far from the surface the wind speed remains approximately constant. If $z_b = \min(|L|, 0.1 z_i)$, then

$$\begin{aligned} U &= \frac{u_*}{k}\left[\ln\left(\frac{z}{z_0}\right) - \Psi_m\left(\frac{z}{L}\right) + \Psi_m\left(\frac{z_0}{L}\right)\right], z \le z_b, \\ U &= \overline{u}(z)\ ,\ z > z_b, \end{aligned} \tag{10}$$

where z_0 is the roughness length and Ψ_m is the stability function. For convective conditions the stability function is [15]

$$\Psi_m = 2\ln\left(\frac{1+A}{2}\right) + \ln\left(\frac{1+A^2}{2}\right) - 2\tan^{-1}(A) + \frac{\pi}{2}, \tag{11}$$

with $A = [1 - (16z/L)]^{1/4}$.

5. Methodology

The thermoelectric plant that was simulated consists of 24 continuous emission chimneys, and for this purpose each of the chimneys was simulated by the solution (7). Subsequently, the solution for each of the chimneys was superimposed.

In addition to the source data, it was used the CALPUFF model in the version of the system officially approved by the USEPA (United States Environmental Protection Agency) [19]. CALPUFF is a Gaussian non-stationary state puff type model that simulates pollutant packages that are transported and dispersed in a tridimensional field. The simulation makes use of the preprocessors TERREL, CTGPROC, MAKEGEO, SMERGE and READ62 for later use in the CALMET meteorological model.

From the simulation it was obtained the data which its mean values are presented at Table 1, it was simulated for 1 hour of emission in three different hours, 8, 13 and 18 o'clock, with the intention to observe the variation of results throughout the day. In a first approach it was used averages of the data in the whole terrain, and then different values were used at each point of the terrain. The total distance simulated was 14 km in each direction.

Table 1. Mean values of the data simulated by the model CALPUFF

Hour	w_* (m/s) (ms^{-1})	u (m/s)	v (m/s)	z_i (m)	u_* (m/s)	z_0 (m)	L (m)
8h	0.475	-0.797	-2.832	291.85	0.237	0.143	-119.1
13h	1.313	-2.387	-5.522	1007.7	0.482	0.143	-204.5
18h	0.759	-4.438	-4.68	757.58	0.5	0.143	-699.9

6. Results

In this section are presented the results of the simulations, it will be exposed the concentration contour lines (g/m^3) for the 8, 13 and 18 o'clock simulations, respectively. Figures 1, 2 and 3 refer to the simulations using mean values of the data, exposed in Table 1. In Figures 4, 5 and 6 it was used different values of the data at each point of the terrain. All simulations presented make use of the reflection parameters $\omega_b=\omega_g=0.3$. Each asterisk ($*$) refers to a group of 6 sources.

Comparing Figures 1, 2, 3 with Figures 4, 5, 6, one observes that the use of mean values of the data does not produce the same concentration field in comparison to when their values are used at each point in the domain. In addition, the same conditions were simulated with different values for the reflection parameters and it was obtained similar final concentrations, although the number of reflections is not the same. For $\omega_b=\omega_g=0.3$ it was obtained 4 reflections, and for $\omega_b=\omega_g=0.5$ it was obtained 2 reflections. In these cases, the values of the reflection parameters simulated have no direct influence on the final result.

One can also observe that the concentration contour lines structures are similar, however according to the hour simulated the values for the concentrations change, which is expected because the convectivity changes during the day. Furthermore, the highest concentrations are near the location of the sources. It should be noted that in some points of the domain CALPUFF was not able to simulate coherent values for the length of Obukhov (L) and the convective velocity scale (w_*), it was necessary to use repeated values to work around the CALPUFF problem.

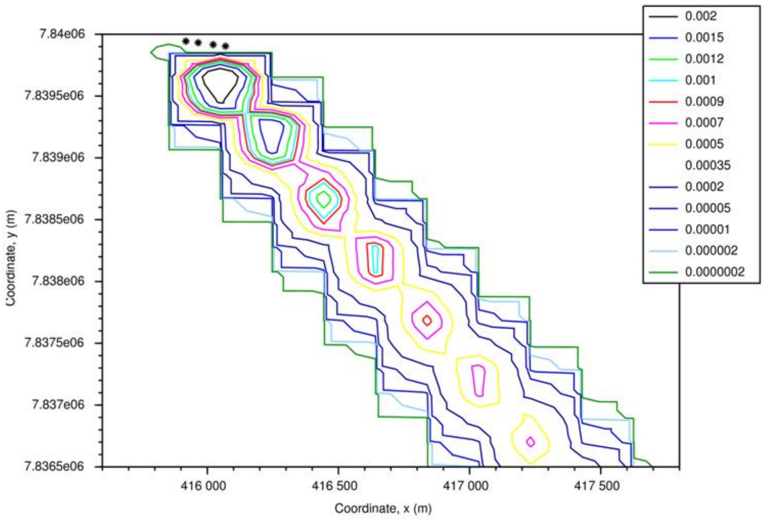

Figure 1. Concentration contour lines (g/m³) for the simulation at 8 o'clock, using averages of the CALPUFF simulated data

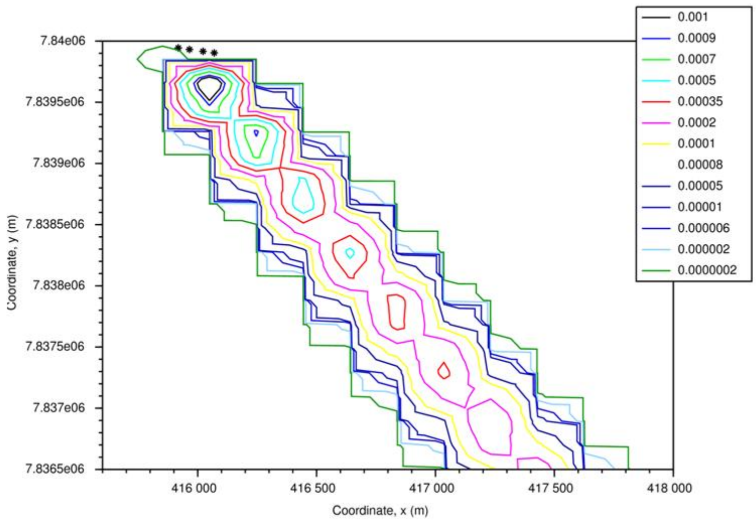

Figure 2. Concentration contour lines (g/m³) for the simulation at 13 o'clock, using averages of the CALPUFF simulated data

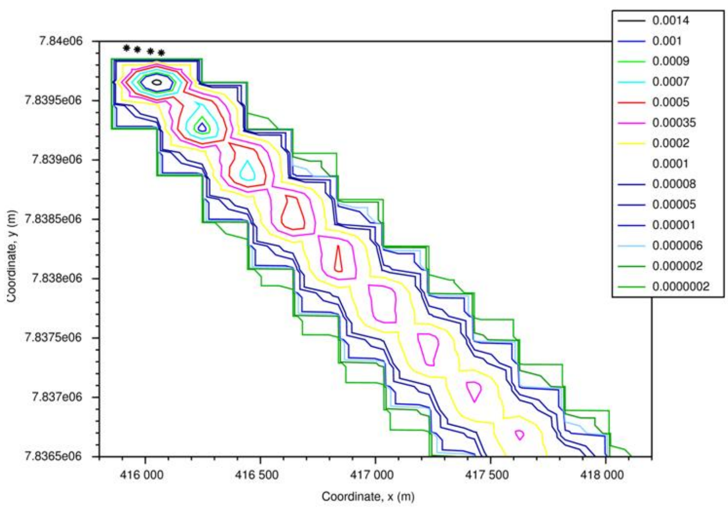

Figure 3. Concentration contour lines (g/m³) for the simulation at 18 o'clock, using averages of the CALPUFF simulated data

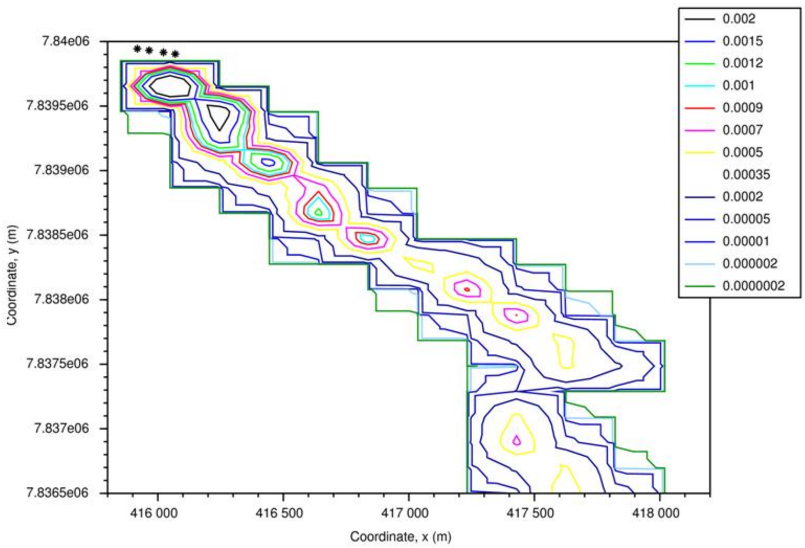

Figure 4. Concentration contour lines (g/m³) for the simulation at 8 o'clock, using the CALPUFF simulated data

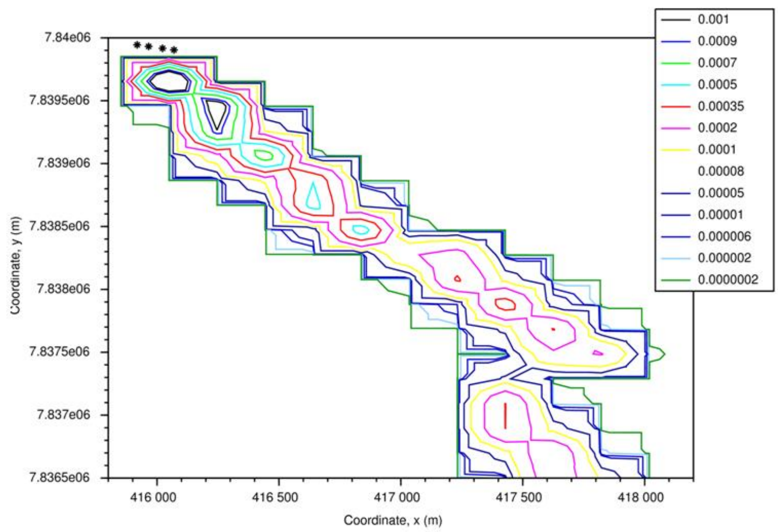

Figure 5. Concentration contour lines (g/m³) for the simulation at 13 o'clock, using the CALPUFF simulated data

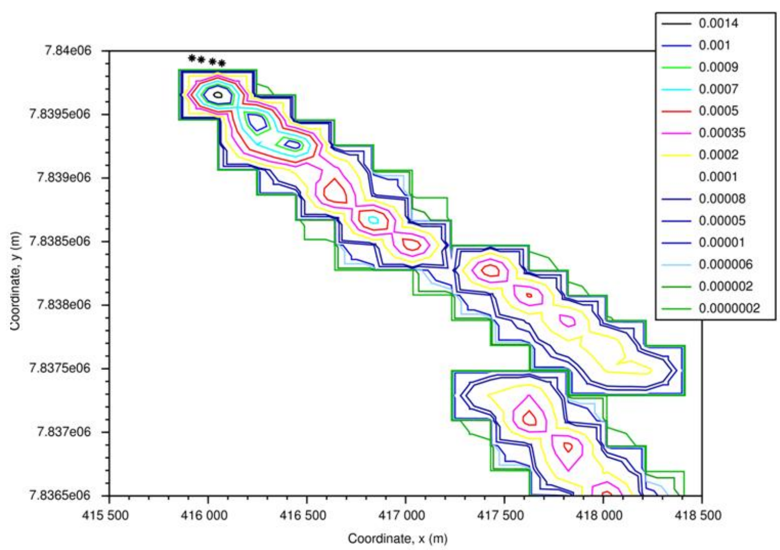

Figure 6. Concentration contour lines (g/m³) for the simulation at 18 o'clock, using the CALPUFF simulated data

7. Conclusions

The purpose of this work was to make use of data from CALPUFF together with a new mathematical model for pollutant dispersion and simulate the surroundings of a thermoelectric power located in Linhares - ES, Brazil. At first, only mean values of the data simulated by the CALPUFF model were used. Besides these data are not the best approximation, since the model is outdated, the use of averages also hinders proper simulation. When it was used different data for each point of the terrain, the concentration of pollutants has become more precise, despite the difficulty found in the simulated data, which contained errors.

As future work, it is expected to obtain data from the meteorological tower settled on the site of the thermoelectric plant and then simulate the model without needing the data provided by CALPUFF, due to the problems found in them.

ACKNOWLEDGEMENTS

This work was supported by Linhares Geração SA, Coordination for the Improvement of the Higher Level Personnel (CAPES - Brazil) and National Council for Scientific and Technological Development (CNPq - Brazil).

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