Ciência e Natura, Santa Maria v.38 Ed. Especial-
IX Workshop Brasileiro de Micrometeorologia, 2016, p. 560 – 565
Revista do Centro de Ciências Naturais e Exatas - UFSM
ISSN impressa: 0100-8307 ISSN on-line: 2179-460X

Influência da velocidade terminal de partículas em concentrações ao nível do solo

Influence of settling velocity of particulate matter on ground level concentrations

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Resumo

A velocidade terminal e deposição de material particulado sobre a superfície da terra tem sido introduzida em uma solução analítica da equação de difusão-advecção. A influência do diâmetro das partículas na distribuição da concentração ao nível do solo foi investigada em função de diferentes condições de estabilidade atmosférica.

Palavras-chave: *Velocidade terminal, material particulado, solução analítica..*

Abstract

The settling velocity and deposition of particulate matter on the earth's surface has been introduced in an analytical solution of advection-diffusion equation. The influence of particles diameters in ground level concentration distribution was investigated in function of different atmospheric stability conditions.

Keywords: *Settling velocity, particulate matter, analytical solution*

1 Introduction

The advection-diffusion equation is the mathematical language description of the phenomenology of atmospheric dispersion based on our knowledge of the phenomenon. Thus, the study of the behavior of its solutions allows us to know more about the phenomenon itself. Analytical solutions explicitly take into account the parameters of a problem, so that their influence can be reliably investigated. By means of numerical experiments, using the analytical solution of the advection-diffusion equation, it allows us to isolate and better understand specific behaviors.

In this paper, we introduced the settling velocity in a solution of the advection-diffusion proposed in Costa et al. (2006) and Moreira et al, (2006). This allows evaluate the influence of the diameter of the particles on their concentration distribution at the ground

2 The solution

F The atmospheric diffusion of substances released from an infinite line source taking into account particles can be described by the equation,

$$u(z)\frac{\partial c(x,z)}{\partial x}=\frac{\partial}{\partial z}\left(K(z)\frac{\partial c(x,z)}{\partial z}\right)+w_s\frac{\partial c(x,z)}{\partial z} \quad (1)$$

where c is the integrated cross-wind concentration, u is the longitudinal mean wind speed, K is the vertical eddy diffusivity and w_s is a constant gravitational settling velocity of the particles.

By considering the dependence of the u and K profiles on height z, the height of the atmospheric boundary layer (ABL) h is discretized into N sub-intervals, such that within each interval the average values in the vertical are used. Therefore, the solution to equation (1) is reduced to the solution of N equations of the following type:

$$u_n\frac{\partial c_n}{\partial x}=K_n\frac{\partial^2 c_n}{\partial z^2}+w_s\frac{\partial c_n}{\partial z} \quad (2)$$

$$z_n \le z \le z_{n+1} \;,\; n=1:N$$

for $0<z<h$ and $x>0$, where c_n denotes the concentration in the n^{th} sub-interval (in this work w_s is constant, but may be a function of z), u_n and k_n are the vertical wind speed and vertical eddy diffusivity in the n^{th} layer, respectively.

Solution of the differential advection-diffusion equation is a very fundamental approach to estimating concentrations of airborne pollutants, and the inclusion of deposition is straightforward. With gravitational settling and deposition and, e.g., the gradient-transfer assumption, the required boundary condition at the surface is (Calder, 1961):

$$K\frac{\partial c(x,z)}{\partial z}+w_s c(x,z)=V_d c(x,z)$$

$$\text{at} \quad z=z_0 \quad (3)$$

where z_0 is the roughness lenght and V_d is the total dry deposition velocity (at $z=z_0$, $K=K_1$=constant). Besides, the pollutants are also subjected to the boundary condition at the top of the ABL height:

$$K\frac{\partial c(x,z)}{\partial z}=0 \quad \text{at} \quad z=h \quad (4)$$

Indeed, it is assumed a source of constant emission rate Q:

$$c(0,z)=Q\delta(z-H_s) \quad \text{at} \quad x=0 \quad (5)$$

where $\delta(z-H_s)$ is the Dirac delta function and H_s is the source height.

To account for vertically inhomogeneous turbulence (dependent on z), continuity conditions are imposed for the concentration and concentration flux at the interfaces:

$$c_n=c_{n+1} \qquad n=1,2,...(N\text{-}1) \quad (6)$$

and

$$K_n\frac{\partial c_n}{\partial z}=K_{n+1}\frac{\partial c_{n+1}}{\partial z} \quad n=1,2,...(N\text{-}1) \quad (7)$$

These conditions must be considered to uniquely determine the 2N arbitrary constants appearing in the solution to the set of equations defined in (2).

At this point, it is important to mention that K_n, as well the u_n, depend only on the variable z and is assumed an averaged value. The stepwise approximation is applied in problem (1) by discretization of the height h into sub-layers in such manner that inside each sub-layer, average values for K_n and u_n are taken. This procedure transforms the domain of problem (1) into a multilayered-slab in the z direction. Concerning the issue of stepwise approximation, it is important to bear in mind that the stepwise approximation of a continuous function converges to the continuous function, when the stepwise of the approximation goes to zero. Furthermore, this approach is quite general in the sense it can be applied when these parameters are an arbitrary continuous function of the z variable. However, K_n and u_n are constant in each sub-layer, but the concentration still varies with z inside each layer.

Applying the Laplace transform to equation (2) results in the following relationship:

$$\frac{d^2}{dz^2}\hat{c}_n(s,z)+\frac{w_s}{K_n}\frac{d}{dz}\hat{c}_n(s,z)-\frac{u_n s}{K_n}\hat{c}_n(s,z)= -\frac{u_n}{K_n}c_n(0,z) \qquad (8)$$

where $\hat{c}_n(s,z)=L_p\{c_n(x,z);x\rightarrow s\}$, which has the well-known solution:

$$\hat{c}_n(s,z)=A_n e^{R_1^n z}+B_n e^{R_2^n z}+ +\frac{Q}{R_3^n}\left(e^{R_1^n(z-H_s)}-e^{R_2^n(z-H_s)}\right)H(z-H_s) \qquad (9)$$

where $H(z-H_s)$ is the Heaviside function (this last term on the right side comes from the particular solution and is included only in the region where is located the source), and

$$R_1^n=-\frac{1}{2}\frac{w_s}{K_n}+\frac{1}{2}\left[\left(\frac{w_s}{K_n}\right)^2+\frac{4u_n s}{K_n}\right]^{1/2}$$

$$R_2^n=-\frac{1}{2}\frac{w_s}{K_n}-\frac{1}{2}\left[\left(\frac{w_s}{K_n}\right)^2+\frac{4u_n s}{K_n}\right]^{1/2}$$

$$R_3^n=\left[\left(w_s\right)^2+4K_n u_n s\right]^{1/2}$$

Finally, a linear system for the integration constants is generated by applying the interface and boundary conditions. Henceforth, the concentration is obtained by numerically inverting the transformed concentration:

$$c_n(x,z)=\frac{1}{2\pi i}\int_{i-\gamma\infty}^{i+\gamma\infty} e^{sx}\left[A_n e^{R_1^n z}+B_n e^{R_2^n z}+ +\frac{Q}{R_3^n}\left(e^{R_1^n(z-H_s)}-e^{R_2^n(z-H_s)}\right)H(z-H_s)\right]ds \qquad (10)$$

The integration constants A_n and B_n are previously determined by solving the linear system resulting from the application of the boundary and interfaces conditions. Due to the complexity of the integrand, the line integral in Eq. (10) is numerically solved using the Fixed Talbot (FT) algorithm (Abate and Valkó, 2004). This procedure yields the following:

$$c_n(x,z)=\frac{r}{M^*}\left[\frac{1}{2}\hat{c}_n(r,z)e^{rx}+ +\sum_{k=1}^{M^*-1}\mathrm{Re}\left[e^{xS(\theta_k)}\,\hat{c}_n\left(s(\theta_k),z\right)\left(1+i\tau(\theta_k)\right)\right]\right] \qquad (11)$$

where

$$s(\theta_k)=r\theta(\cot\theta+i), \qquad -\pi<\theta<+\pi$$
$$\tau(\theta_k)=\theta_k+\left(\theta_k\cot\theta_k-1\right)\cot\theta_k$$

and

$$\theta_k=\frac{k\pi}{M^*}$$

Moreover, r is a parameter based on numerical experiments and M* is the number of terms in the summation.

The stepwise approximation of a continuous function converges to the continuous function when the individual steps in the approximation approach zero (see the work of Moreira et al., 2014). For this study, it is necessary to choose an appropriate number of sub-layers by considering the smoothness of the functions for K and u. This obtained solution is semi-analytical in the sense the only approximations considered along its derivation are the stepwise approximation of the parameters and the numerical Laplace inversion of the transformed concentration. Therefore, this model preserves the beauty of an analytical solution without compromising the accuracy of the wind speeds and the eddy diffusivity to compute the concentration.

3 The atmospheric boundary layer parameterization

In this study, the wind u is parameterized as a function of height z in the manner suggested by Panofsky and Dutton (1984):

$$u = u(z) = u_r\left(\frac{z}{z_r}\right)^{\alpha} \qquad (12)$$

where u_r is the measured wind speed at a reference height z_r and α is a constant that depends on the atmospheric stability.

The unstable vertical eddy diffusivity K is parameterized as a function of height z following the work of Degrazia et al. (1997):

$$K(z) = 0.22 w_* h\left(\frac{z}{h}\right)^{1/3}\left(1-\frac{z}{h}\right)^{1/3}\cdot \left[1-\exp\left(-\frac{4z}{h}\right)-0.0003\exp\left(\frac{8z}{h}\right)\right] \qquad (13)$$

where h is the atmospheric boundary layer (ABL) height and w_* is the convective velocity obtained by the expression:

$$w_* = u_*\left(h/k|L|\right)^{1/3}$$

(k is the von Karman constant ~ 0.4). The eddy diffusivity parameterization is based on turbulent kinetic energy spectra and Taylor's diffusion theory.

The neutral and stable conditions are parameterized following the work of Ulke (2000):

$$K(z) = k u_* h\left(\frac{z}{h}\right)\left(1-\frac{z}{h}\right)\left(1+6.9\frac{h}{L}\frac{z}{h}\right)^{-1} \qquad (14)$$

This proposed eddy diffusivity profile (14) coincide in neutral conditions (h/L=0) and agree with surface layer similarity close to the surface

4 Results and discussion

Particle diameter between 10 and 100 microns, different heights of emission sources were considered. In addition, three different diffusive conditions were considered: atmosphere unstable, neutral and stable.

The parameters that identify the three stability conditions are presented in Table 1.

Table 1: Parameterizations of the three ABL regimes.

	Convective ABL	Neutral ABL	Stable ABL
u (ms^{-1})	2.5	4.5	3.5
u_* (ms^{-1})	0.17	0.26	0.16
1/L (m^{-1})	-0.09	0	0.03
α	0.07	0.015	0.35

The settling velocity was calculated using the Stokes' low (Seinfeld and Pandis, 1998) and the atmospheric boundary layer height was 1000 m.

In this study, we place the deposition rate equal to that of fall by gravity, to obtain scenarios more understandable, not masked by any particle materials resuspension. As an example of the results obtained, we are shown in Figures 1, 2, 3 particles concentrations at the ground for the three ABL regimes considered.

Analyzing the figures, the first consideration that we can make is that it is true that particle settling velocity can be neglected for particles with diameter less than 10 microns, but not in the case of ABL stable regimes.

Looking at the figures, we can see how the distributions on the ground are very different if we consider the settling velocity. The differences increase toward more stable ABL regimes.

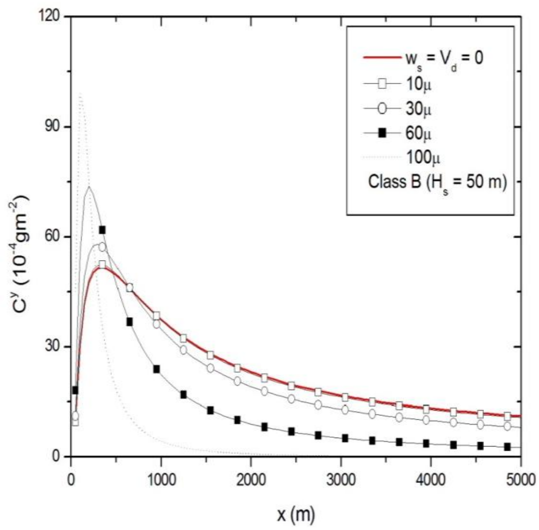

Figure1: Ground level concentrations for ABL convective regime.

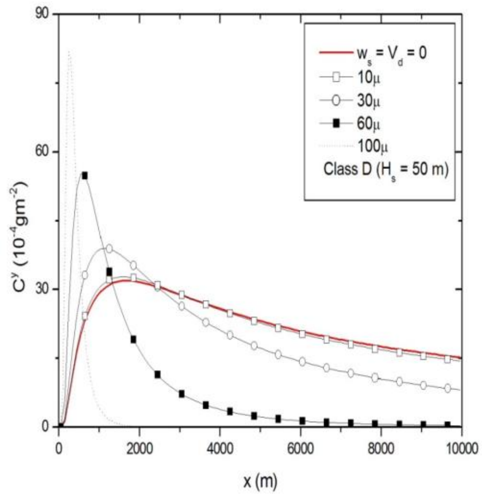

Figure 2: Ground level concentrations for ABL neutral regime-

Looking at the figures, we can see how the distributions on the ground are very different if we consider the settling velocity. The differences increase toward more stable ABL regimes.

From the point of view of environmental management, it is important to outline that, with the increase of the particle diameter, increases the maximum concentration at the ground.

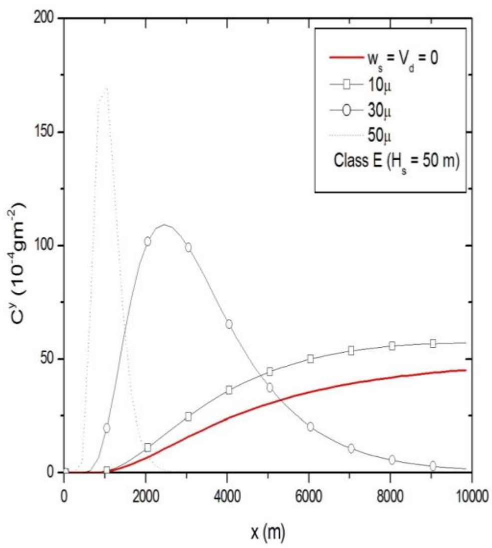

Figure 3: Ground level concentrations for ABL stable regime

5 Conclusions

The fall velocity and deposition of particulate matter on the earth's surface has been introduced in an analytical solution of advection-diffusion equation. The influence of particles diameters in ground level concentration distribution was showed in function of different ABL regimes (from convective to stable ABL). The first results show that settling velocity significantly changes dramatically the concentration distribution at the ground. In future studies, we will also investigate the concentration vertical profiles and we will try to relate the concentration maxima to meteorological parameters and source characteristics.

Acknowledgements

The authors thank CNPq for the partial financial support of this work.

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