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A STUDY OF THE INFLUENCE OF SETTLING VELOCITY IN AIR POLLUTION DISTRIBUTION BY A MODEL APPLYING AN ANALYTICAL SOLUTION OF THE ADVECTION-DIFFUSION EQUATION

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Abstract: Using an analytical solution of the advection-diffusion equation we shown that the settling velocity changes the particles concentration throughout all the ABL. Moreover, the simulations showed that the phenomenon of gravitational settling can strongly influence the distribution of the air pollution concentrations and maximum concentrations near the ground. This work has also highlighted the usefulness of analytical solutions as a technical tool to study and understand the transport and diffusion in the atmosphere.

Key words: *Air pollution diffusion, settling velocity, analytical solutions*

INTRODUCTION

In physics, experimental data are essential in verifying and validating theories. Simulations and numerical experiments, though not proving, are useful in understanding physical phenomena. In fact, they have the advantage of being cheaper than experiments and easier to accomplish. Solution of the differential advection-diffusion equation is a fundamental approach to estimating concentrations of airborne pollutants. Numerical experiments using analytical solutions are useful because they allow to understand the contribution of the various physical variables to the phenomenon studied. Moreover, they help us understand the meaning of equations used.

In this paper, we will use a solution of the advection-diffusion equation to study the influence of settling velocity in the distribution of pollution emitted from point sources.

THE SOLUTION

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

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

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 the 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 (Costa et al., 2006; Moreira et al. 2006):

$$u_n\frac{\partial c_n}{\partial x} = K_n\frac{\partial^2 c_n}{\partial z^2} + w_s\frac{\partial c_n}{\partial z} \qquad z_n \le z \le z_{n+1}\ ,\ n = 1:N \qquad (2)$$

for $0 < z < h$ and x >0 , where c_n denotes the concentration in the nth 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 nth layer, respectively. Assuming the gradient-transfer approach, with gravitational settling and deposition, the required boundary condition at the surface is (Calder, 1961):

$$K\frac{\partial c(x,z)}{\partial z}+w_s c(x,z)=V_d c(x,z) \quad \text{at } z = z_0 \tag{3}$$

where z_0 is the roughness length 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:

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

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

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

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:

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

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

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 the 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 (see also Moreira et al., 2014).

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

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

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

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

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

$$R_1^n=-\frac{1}{2}\frac{w_s}{K_n}+\frac{1}{2}\left[\left(\frac{w_s}{K_n}\right)^2+\frac{4u_n s}{K_n}\right]^{1/2}, R_2^n=-\frac{1}{2}\frac{w_s}{K_n}-\frac{1}{2}\left[\left(\frac{w_s}{K_n}\right)^2+\frac{4u_n s}{K_n}\right]^{1/2}$$

and

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

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 An and Bn 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

$$s(\theta_k)=r\theta(\cot\theta+i) \quad -\pi<\theta<+\pi$$

$$\tau(\theta_k)=\theta_k+\left(\theta_k\cot\theta_k-1\right)\cot\theta_k$$

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

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

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 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):

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

where h is the atmospheric boundary layer (ABL) height and w_* is the convective velocity obtained by the $w_*=u_*\left(h/k|L|\right)^{1/3}$ expression (L is the Monin-Obukhov length and 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 stable condition is parameterized following the work of Ulke (2000):

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

THE INFLUENCE OF SETTLING VELOCITY

Particle diameter between 10 and 100 microns, different heights of emission sources were considered. In addition, two different diffusive conditions (roughly corresponding to Pasquill's stability classes B and E) were considered: unstable and stable atmosphere. The unstable one was characterized by a wind velocity u = 2.5 ms^{-1}, a friction velocity u_* = 0.17 ms^{-1}, an inverse Monin–Obukhov length 1/L = -0.09 m^{-1} and α = 0.07. While the stable atmosphere was characterized by a wind velocity u = 3.5 ms^{-1}, a friction velocity u_* = 0.16 ms^{-1}, an inverse Monin–Obukhov length 1/L = 0.03 m^{-1} and α = 0.35.

The settling velocity was calculated using the Stokes' law (Seinfeld and Pandis, 1998) and the atmospheric boundary layer height was 1000 m. We place the deposition rate equal to that of fall by gravity.

As an example of the results obtained, we show in Figures 1 and Figure 2 particles concentrations at the ground for the two ABL regimes considered.

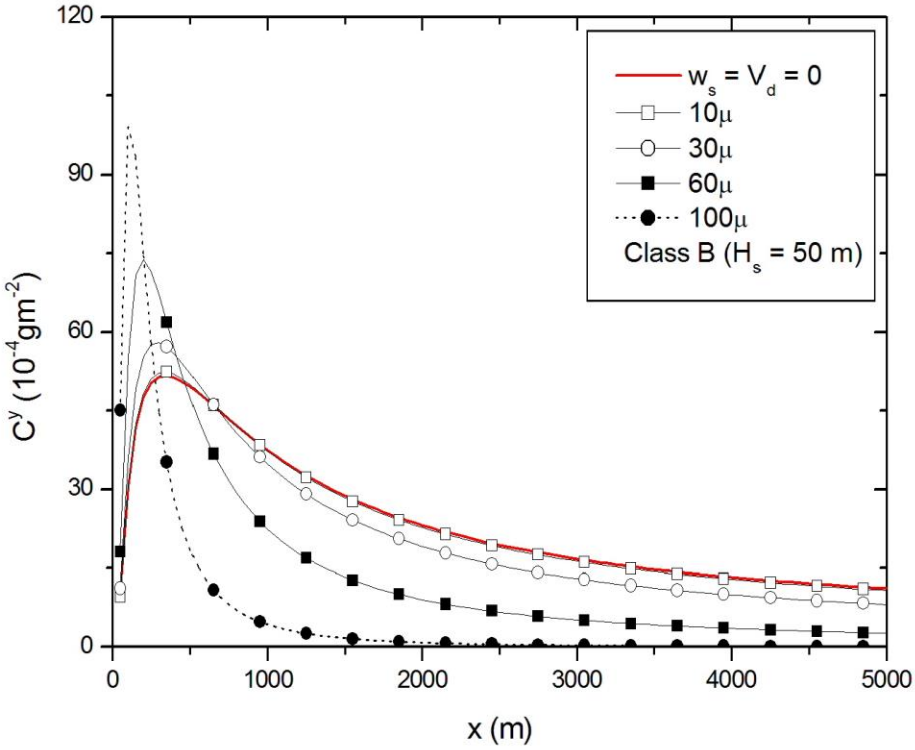

Figure 1. Ground level concentrations for an ABL convective regime.

We can see that particle settling velocity can be neglected for particles with diameter less than 10 microns, but not in the case of ABL stable regimes, where the distributions on the ground are very different if we consider the settling velocity different from zero. 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.

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. The first results show that settling velocity significantly changes the concentration distribution at the ground. In future studies, we will also investigate the concentration vertical profiles.

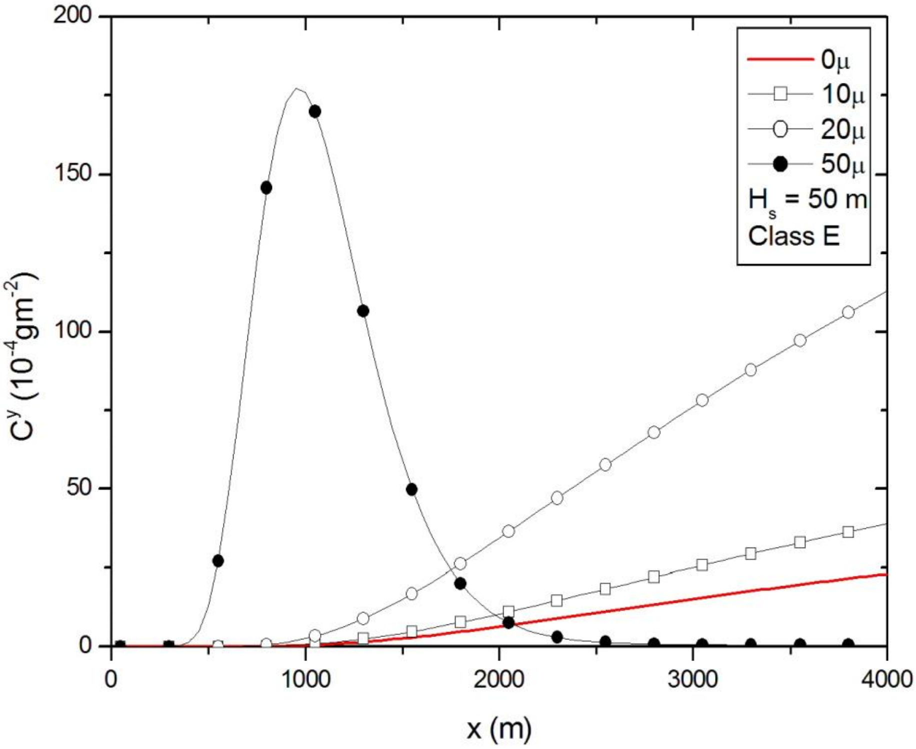

Figure 2. Ground level concentrations for an ABL stable regime**.**

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