4.06 PARAMETERIZATION OF DRY DEPOSITION PROCESSES IN THE SURFACE LAYER FOR ADMIXTURES WITH GRAVITY DEPOSITION

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INTRODUCTION

The dry deposition of pollutants is one of the important components of the pollution budget and so the proper description of this process is essential for successful air quality modeling. Moreover, the consequence of pollution deposition on vegetation surfaces is perceived by many to be at present one of the major environmental problems. These are the two reasons why a special attention is paid to the way dry deposition is accounted for in the pollution transport models.

THE MOST POPULAR PARAMETERIZATION SCHEME

It seems that the "big leaf" approach (*Erisman, J.W., A.J. van Pul, and G.P. Wyers,* 1994, *Jakobsen, H.A., J.E. Jonson and E. Berge,* 1996, *Seland, Ø., A. van Pul, A. Sorteberg and J.-P. Tuovinen,* 1995, *Wesley, M.L.,* 1989) to the dry deposition assessment will be the one followed by the model developers in the near future. These most popular parameterization schemes assume the following connection between the turbulent flux of gases or aerosol and their concentration at level z :

$$-F = k\frac{dc}{dz} = V_d(z)\big(c(z) - c_s\big), \tag{1}$$

where $c(z)$ is the admixture concentration, c_s is the admixture concentration at the absorbing surface (as it is unknown it is usually assumed $c_s \sim 0$), V_d is the dry deposition velocity and $k(z)$ is the coefficient of vertical turbulent exchange.

By making analogy with the Ohms law in electrical circuits the dry deposition velocity V_d is most often presented in the form:

$$V_d = \left(r_a + r_b + r_s\right)^{-1}, \tag{2}$$

where r_a is the surface layer (SL) aerodynamic resistance, r_b is the quasi-laminar or viscous sub-layer resistance, and r_s is the surface resistance.

It seems that the most general expression for the aerodynamic resistance r_a is the following:

$$r_a(z) = \int_{z_0}^{z} \frac{dz}{k(z)}, \tag{3}$$

where z_0 is the roughness length. If it is assumed, as usual, that the SL turbulent transport of admixtures is similar to these of heat and momentum, it can be written:

$$k(z) = \frac{\kappa u_* z}{\varphi(\varsigma)}, \tag{4}$$

where κ is the von Karman constant, u_* is the friction velocity, $\varphi(\varsigma)$ is the universal function of the dimensionless height $\varsigma = z/L$, L - the Monin-Obuchov length. In such a case the expression for r_a resumes the form:

$$r_a(z)=\frac{1}{\kappa u_*}\left(f(z)-f(z_0)\right),\ f(z)=\int\frac{\varphi(\varsigma)}{z}dz\,, \qquad (5)$$

From (3) it is obvious that $r_a(z_0)=0$ and thus

$$V_{d0}=V_d(z_0)=\left(r_b+r_s\right)^{-1}, \qquad (6)$$

i.e. the deposition velocity at roughness length height is subject only of the transport of the component trough the laminar layer adjacent to the surface by molecular diffusion and the various destruction or uptake processes of the component at the surface.

A MORE GENERAL APPROACH

The relation (1)-(2) between the turbulent flux and the component concentration in the SL is widely used, but is not the most general one. It does not account for factors, which may be important, like gravity deposition and pollution sources in the SL.

A more general approach based on the solution of the admixture transport equation in the SL is suggested by *Ganev, K.G. and D.L. Yordanov* (1981). As generally accepted, the vertical transport is assumed dominant in the SL, so the concentration field is assumed to be locally horizontally homogeneous and stationary. In such a case the vertical profile $c(z)$ of the concentration of an admixture with gravity deposition $-w_g$, ($w_g>0$) is described by the equation:

$$\frac{d}{dz}k\frac{dc}{dz}+w_g\frac{dc}{dz}=-q\delta(z-z_{source}), \qquad (7)$$

where q is the capacity of a flat (locally) homogeneous admixture source, δ is the Dirac function. The boundary condition at $z=z_0$ is, according to (1), (2), (6), the following:

$$k\frac{dc}{dz}=V_{d0}c_0, \qquad (8)$$

c_0 - the concentration at $z=z_0$. The integration of (7), having in mind also (8) leads to:

$$kdc/dz+w_gc=\left(w_g+V_{d0}\right)c_0-qH_{source}(z), \qquad (9)$$

where $H_{source}(z)$ is the Heavyside function ($H_{source}(z)=0$ for $z<z_{source}$; $H_{source}(z)=1$ for $z>z_{source}$). By the transformation

$$c=xe^{-w_gr_a}, \qquad (10)$$

where r_a is the aerodynamic resistance (see (3)), equation (9) can be simplified to the form (from (10) it is obvious that $x(z_0)=c_0$):

$$kdx/dz=\left(w_g+V_{d0}\right)c_0e^{w_gr_a}-qH_{source}(z)e^{w_gr_a}, \qquad (11)$$

and after some trivial manipulations an expression for $c(z)$ to be obtained:

$$c(z)=\left[1+\frac{V_{d0}}{w_g}\left(1-e^{-w_gr_a(z)}\right)\right]c_0-H_{source}(z)\frac{q}{w_g}\left(1-e^{w_gr_a(z_{source})-w_gr_a(z)}\right), \qquad (12)$$

By calculating c_0 from (12) and then inserting it in (9) the SL flux/concentration relation for the case of admixtures with gravity deposition and possible sources in the SL can be obtained:

$$k\frac{dc}{dz}=V_d(z)c(z)-H_{source}(z)\frac{V_d(z)}{V_d(z_{source})}q, \qquad (13)$$

where

$$V_d(z) = \left[\frac{1}{w_g} \left(e^{w_g r_a(z)} - 1 \right) + e^{w_g r_a(z)} \frac{1}{V_{d0}} \right]^{-1}, \tag{14}$$

It is easy to calculate that in case of admixture with no gravity deposition ($w_g \to 0$) the expression (14) takes the form (2). Further, if there are no sources in the SL the flux/concentration relation transforms into the form (1).

The particular cases when $V_{d0} \to \infty$ (total absorption at $z = z_0$) and $V_{d0} \to 0$ (total reflection at $z = z_0$) can also be considered. Obviously in the first case

$$V_d(z) \to \left[\frac{1}{w_g} \left(e^{w_g r_a(z)} - 1 \right) \right]^{-1} \text{, when } V_{d0} \to \infty, \tag{15}$$

and, as it can be easily seen from (13), there will be zero concentration at $z = z_0$. In the second case $V_d \to 0$ when $V_{d0} \to 0$, but the ratio $V_d(z) / V_d(z_{source})$ remains limited, so the relation (13) obtains the form:

$$k \frac{dc}{dz} = -H_{source}(z) \frac{e^{w_g r_a(z_{source})}}{e^{w_g r_a(z)}} q \ , \tag{16}$$

or in the case with no gravity deposition ($w_g \to 0$):

$$k \frac{dc}{dz} = -H_{source}(z) q \, , \tag{17}$$

SOME EXAMPLES

If the deposition velocity, calculated according to (1) is denoted by V_{d1}, then having in mind (6) the aerodynamic resistance r_a may be expressed in the form:

$$r_a = V_{d1}^{-1} - V_{d0}^{-1} \ , \tag{19}$$

Inserting (19) in (15), leads, after some simple transformations to the dimensionless relation:

$$\widetilde{V}_d = \left[\frac{1}{\widetilde{w}_g} \left(e^{\widetilde{w}_g \left(\widetilde{V}_{d1}^{-1} - 1 \right)} - 1 \right) + e^{\widetilde{w}_g \left(\widetilde{V}_{d1}^{-1} - 1 \right)} \right]^{-1}, \tag{19}$$

where $\widetilde{V}_d = V_d / V_{d0}$, $\widetilde{V}_{d1} = V_{d1} / V_{d0}$, $\widetilde{w}_g = w_g / V_{d0}$.

The difference between $\widetilde{V}_d$ and $\widetilde{V}_{d1}$ is well demonstrated by Figure 1. It is clear that even in the cases when w_g is of the order of magnitude of V_{d0} the effect of gravity deposition on the turbulent (aerodynamic) deposition is significant. The gravity deposition modifies the admixture profiles and thus the admixture turbulent fluxes in the SL, which results in a decrease of the dry deposition velocity.

The application of the dry deposition parameterization suggested above can be demonstrated by the following example: Let a two-layer model for k is assumed - $k = k(z)$, calculated according to (4) in the SL ($z_0 \le z \le h_{SL}$), h_{SL} - the SL height; $k = k_h = k(h_{SL})$ for $h_{SL} \le z < \infty$. Then, in the horizontally homogeneous case, the vertical profile above SL of the concentration $c(z,t)$ from an instantaneous flat source with height $h > h_{SL}$ can be obtained from the equation:

$$\frac{\partial c}{\partial t} - w_g \frac{\partial c}{\partial z} - k_h \frac{\partial^2 c}{\partial z^2} = 0 \, , \; h_{SL} \le z < \infty \, , \qquad (20)$$

under the following initial and boundary conditions:

$$c(z,0) = \delta(z-h) \, ; \; k_h \frac{\partial c}{\partial z} = \beta c(h_{SL}, t) \, , \qquad (21)$$

Here β is the dry deposition velocity at $z = h_{SL}$. Depending on the chosen parameterization β is equal to $V_d(z = h_{SL})$ or to $V_{d1}(z = h_{SL})$ - respectively the cases when the gravity deposition effects on the aerodynamic resistance are accounted, or not accounted for.

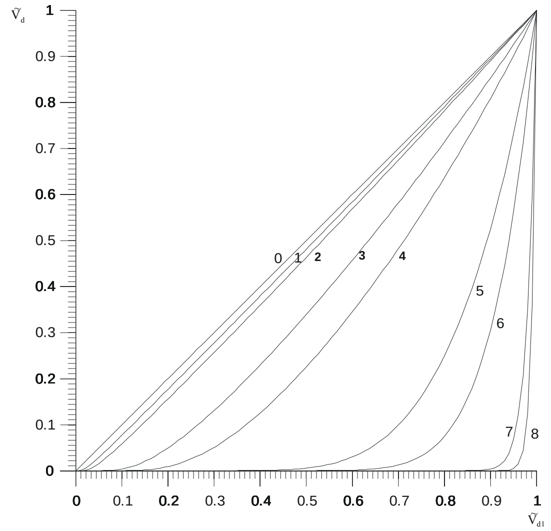

Figure 1. The difference between $\widetilde{V}_d$ and $\widetilde{V}_{d1}$ for different $\widetilde{w}_g$ values: $\widetilde{w}_g$ =0 (0). 0.05 (1), 0.1 (2), 0.5 (3), 1 (4), 3 (5), 10 (6), 50 (7) and 100 (8)

As it can be easily shown (*Galperin M., D.L. Yordanov and K.G. Ganev*, 2000), the solution of (20-21) is:

$$c(z,t) = e^{-\frac{w_g(z'-h')}{2k_h} - \frac{w_g^2 t}{4k_h}} \left\{ \frac{1}{2\sqrt{\pi k_h t}} \left[e^{-\frac{(z'-h')^2}{4k_h t}} + e^{-\frac{(z+h)^2}{4k_h t}} \right] - \frac{\widetilde{\beta}}{k_h} e^{\frac{\widetilde{\beta}(z'+h'+\widetilde{\beta}\, t)}{k_h}} erfc\left(\frac{z'+h'+2\widetilde{\beta}\, t}{2\sqrt{k_h t}} \right) \right\} \, , \qquad (23)$$

where $\widetilde{\beta} = \beta + w_g / 2$, $z' = z - h_{SL}$ and $h' = h - h_{SL}$.

This formula was applied for calculating the concentrations $c'(h_{SL}, t)$ and $c''(h_{SL}, t)$ at SL height for the cases when gravity deposition is accounted ($\beta = V_d(z = h_{SL})$) and not accounted ($\beta = V_{d1}(z = h_{SL})$) for. The calculations were made for a wide range of V_{d0} and w_g values for the cases of stable ($u_* = 0.5\, m/s$, $L = 10$), neutral ($u_* = 0.2\, m/s$) and unstable ($u_* = 0.2\, m/s$, $L = -10$) stratification for source height $h = 200 m$. The corresponding maximal concentration values $c'_{\max}(V_{d0}, w_g)$, $c''_{\max}(V_{d0}, w_g)$ and their relative difference $D(V_{d0}, w_g) = (c'_{maz} - c''_{maz}) / c'_{maz}$ are determined for all the stability cases. The results can be seen in Figure 2. The following conclusions can be maid by the comparison: 1) taking into account the gravity deposition may have a significant effect on the calculated concentrations, especially in stable and neutral cases; 2) the effect is maximal for gravity deposition velocities between 0.01 and 0.1 *ms*$^{-1}$; 3) the effect increases with the increasing of V_{d0} up to values of 0.1 *ms*$^{-1}$, after which the value of the relative difference D does not change much.

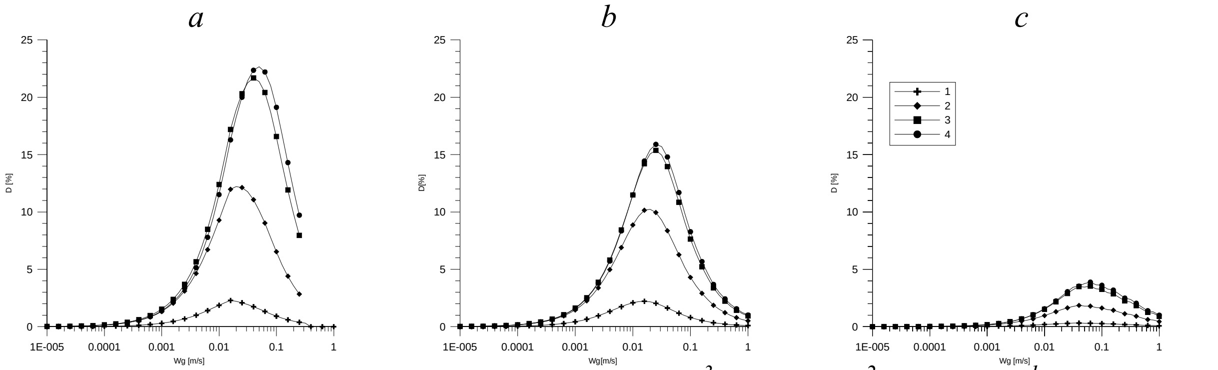

Figure 2. Dependence of D on w_g and V_{d0} - V_{d0} =10^{-3}m/s (1); 10^{-2}m/s (2); 10^{-1}m/s (3); 1m/s (4) for the cases of stable (a), neutral (b) and unstable (c) stratification

CONCLUSIONS

The most popular parameterization schemes treat the aerodynamic resistance and the gravity deposition independently, most often by simply adding the gravity deposition velocity. As the gravity deposition modifies the admixture profiles and thus the admixture turbulent fluxes in the SL, this approach is obviously incorrect. The present paper suggests a more general approach, based on the exact solution of the pollution transport (turbulent and gravity deposition) equation in the SL, which provides a correct expression for the aerodynamic resistance, accounting also for the gravity deposition effects. The demonstrated examples show the importance of a joint treatment of turbulent transport and gravity deposition in calculating the aerodynamic resistance.

ACKNOWLEDGEMENT

The present work is partially funded by the Bulgarian National Science Council (Contract No. ES-1002/00).

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