Why Road Dust Concentrations Are Over-Estimated in Eulerian Grid Models

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1. Introduction

Air quality modelers involved in airshed and regional PM_{10} simulations know that Eulerian grid dispersion models generally overestimate road dust concentrations (Watson, et al. 2000), with coarse particles being removed near the source by gravitational settling and impaction in a relatively short time (Pace, 2003; Countess, 2001; Watson, et. al., 2000). Compared to monitoring data and receptor modeling analyses, grid modeling overestimates road dust contributions to the ambient PM_{10} concentration (Countess, 2003; Pace, 2003), leading to a "divide by four" approach to reconciling estimates with measurements. Research regarding this problem has focused on emission inventory, with some recent studies revealing that the rapid near-source deposition and the resulting overestimation of emissions may be responsible for the discrepancy between observations and modeling results in regional air quality modeling (Etyemezian, 2002; Countess, 2001).

2. Method

This study focuses on two factors that appear to account for the four-fold overestimation of road dust concentration seen with current Eulerian grid dispersion models:

Models typically remix coarse particles throughout the first layer at the start of each time step. Measurements and modeling indicate that road dust only reaches an elevation of a few meters above the ground, so this practice underestimates the rate at which coarse (2.5-10 micrometer) particles are removed. Deposition processes fail to account for wind speed—particularly low wind speed conditions. For coarse particles in particular, the dependence of deposition rate on wind speed is much greater than is the case for other pollutants. The under-estimated deposition velocity of coarse particles causes overestimating the pollutant concentrations under stagnation conditions.

The combined effect of these factors, under stagnation conditions for variable low wind speeds, is estimated to be about a factor of four.

2.1 Particle Overestimation Due to Particle Mixing at Each Time Step

It has been shown that the initial thickness of the road dust layer is about 2 to 3 meters (Cowherd et al., 1998), whereas in most grid models the lowest layer, due to the limitations of meteorological data, is assumed to be about 20 meters or higher. Because the models automatically re-mix the particles into the whole layer for every time step, the assumption of a 20-meter modeling layer significantly reduces the deposition rate. Even if the deposition velocity is correct, the model underestimates the actual deposition rate by assuming a uniform distribution of particles.

Continuous Emission, With Mixing

Consider the scenario in which emitted particles continuously enter the cell, with mixing again occurring at each time step. (In this scenario, the effect of mixing at each time step is demonstrated assuming a mono-dispersed aerosol with constant deposition velocity, but the same equations apply for each particle size and deposition velocity independently.)

A general form for the mass at time step t_n can be written:

$$M_n=M_0(1- R_{d0})^n+E_{k=0}\Sigma^{n-1}(1- R_{d0})^k \quad (1)$$

R_{do} is the removal rate (percentage of total mass deposited in the time step), because $(1-R_d) < 1$, the first term of Equation 6 vanishes as $n \to \infty$, while the second term converges to the total mass in the cell at an equilibrium state:

$$M_{n \to \infty} = E / R_{d0} \quad (2)$$

Continuous Emission, Without Mixing

In contrast, for the continuous emissions scenario without mixing, the total mass in the cell at each time step n is given by the following:

$$M_0(1-nR_{d0})+E(1-(n-1)R_{d0})+E(1-(n-2)R_{d0}) +...+ E(1-R_{d0})+ E \quad (3)$$

When $n = 1/R_{d0}$, then $M_0(1-nR_{d0}) = 0$, and the equilibrium state is reached. The total mass in the cell for all subsequent time steps will then be given by the following:

$$M_n\ (n \geq 1/R_{d0}) = E\ (1/R_{d0} +1)/2 \quad (4)$$

For $n \geq 1/R_{d0}$, M_n will remain constant as long as the emission and deposition rate remain constant. The ratio of total mass in the cell after the equilibrium is reached is the ratio of Equations (7) and Equation (9):

Mass ratio = $2/(R_{d0}+1) \approx 2$

(if $R_{d0} << 1$) (5)

Figure 2 shows M_n for these two processes, assuming an initial deposition rate of 5%. Mass continues to accumulate in the cell until time step number 100 in the mixing scenario, while an equilibrium state is reached much earlier for the non-mixing scenario. The total mass in the cell with mixing is about two times greater than in the cell without mixing,

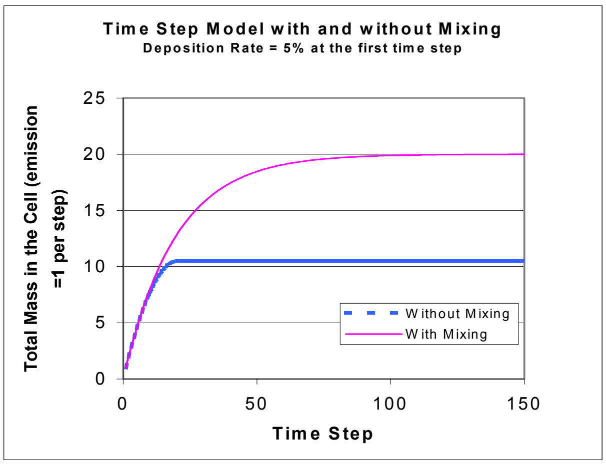

Figure 1. Mass continues to accumulate in the cell in the scenario with mixing, while mass reaches an equilibrium state much earlier in the scenario without mixing. The total mass at the equilibrium in the cell with mixing is about two times greater than in the cell without mixing. The factor is insensitive to the deposition rate when deposition rates are small

Vertical Distribution and Comparison With Measured Data

When the vertical distribution predicted by the non-mixing model is compared with observed data, as shown in Figure 2 from Watson et al. (2000), a good match with the lowest curve is obtained. The dashed line indicates the mass contribution with linear model (mixing at every time step), which has much lower concentration near the surface, therefore much lower deposition flux.

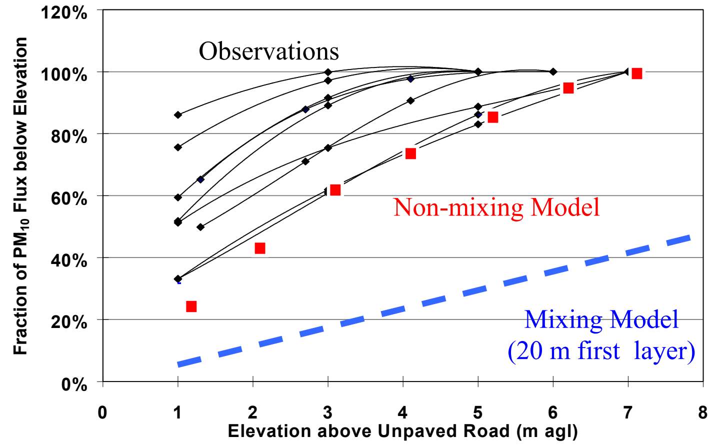

Figure 2. Comparison of mixing and non-mixing model with observation. The mass distribution with height predicted by non-mixing model matches observations well.

Correction Factor for Mixing as a Function of Wind Speed

Because the mixing process is directly related to wind speed, we can define a correction factor accordingly. Assuming no mixing at zero wind speed and complete mixing at a wind speed of 10 m s^{-1} and above, the correction factor due to mixing, F_m, can be conceptualized as follows:

$F_m = 2 - Vw/10$ ($V_w \leq$ 10m s-1)

and

$F_m = 1$ ($V_w >$ 10m s-1) (6)

The function can also be defined based on physics parameters, such as τ_z, the vertical turbulent flux (Countess, 2001). We use the simple linear form here because only the low wind situation is a concern, and the function is nearly linear over such a small range.

2.2 Dry Deposition Velocity Under-estimation

Dry deposition rates are estimated using the concept of *deposition velocity*, which is based on the well-known *resistance* model. However, most deposition models only consider deposition in the *vertical* direction, and while this may be a good approach for pollutants in a layer much higher than the canopy, it is not proper for coarse particles that are generated within—and mainly transport and deposit within—the canopy.

Studies have been conducted to measure and model deposition velocities of particulate matter (Sehmel G.A., 1980; EPA, 1993), but few studies account for the relationship between deposition velocity and wind speed. Limited data are used in the following analisis.

Comparison of Models With Measured Data

Doran and Horst (1985) measured the deposition velocity of particles (4.8 to 8.0 µm diameter) with good information for wind speeds. Figure 4 shows Doran's measurements compared against the predictions of Slinn's model and ISC3. (The roughness, the ratio of frictional wind speed and reference wind speed were determined using Slinn's estimations.) Both Slinn's model and the ISC3 algorithm under-estimate deposition velocity, especially for low wind speed.

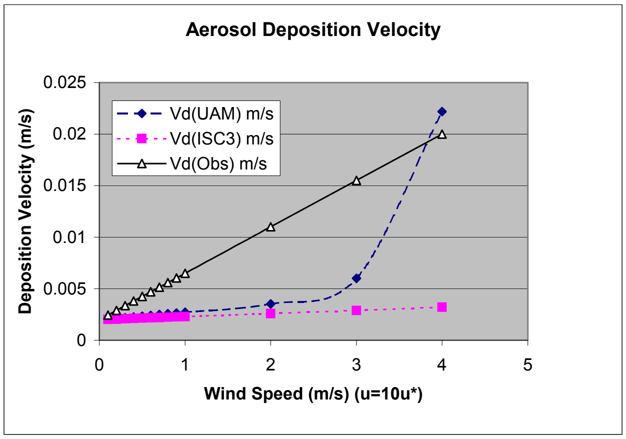

Figure 3. Measured and modeled deposition velocity as a function of wind speed. The measured data show that the deposition velocity is linearly proportional to wind speed. Models under-estimate the deposition velocity.

Factor of Over-prediction Due to Deposition Velocity Error

Under calm conditions, the main removal mechanism is dry deposition, whereas for high wind speed horizontal air motion (transport and dispersion) dominates. Since the deposition velocity is expected to be a linear function of wind speed, and removal by dispersion is a function of wind speed with higher power, it is expected that the net effect of deposition velocity on estimated concentration decreases for higher wind speeds. CMAQ was used to test the effect of deposition velocity on the prediction of coarse particle concentration. Figure 4 shows the results.

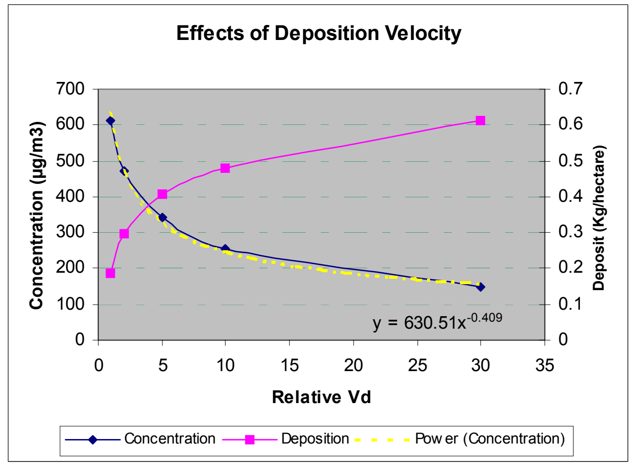

Figure 4. The predicted concentration as a function of deposition velocity (CMAQ results). Data from Dec.22, 1999, Boise, ID.

Explaining the "Factor of Four"

Now we are able to estimate the net effect due to errors in deposition velocity and artificial mixing processes. The total correction factor, F_{total}, is the product of the correction factor due to mixing (F_m, Equation 6) and the correction factor due to deposition velocity bias:

$$F_{total} = F_{Vd} F_m$$

F_{Vd} is calculated using CMAQ results (Figure 4). The results are shown in Fugure 5.

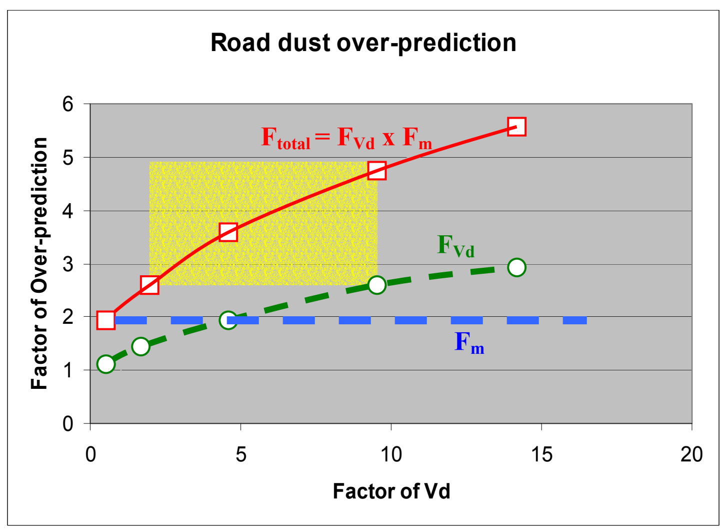

Figure 5. The total factor of over-estimation is product of the factor due to mixing and the factor due to deposition velocity under-estimation. While the deposition error could vary over a large range, the error of final predicted concentration falls within a narrower range near 4.

This analysis suggests that the over-prediction is a combined result of the errors in the mixing and dry deposition processes. Although the factor cannot be a unique value, as some authors have pointed out (Etyemezian, Countess), the values lie within a relatively narrow range, representing different environments.

5. Correction in the modeling practice

The simplest way to correct the road dust over-estimating error in current modeling is to apply the correction factors of Figure 5, assuming the data of deposition velocity is available. Because the value of the factor is fairly consistent for different environments, much of the error can be removed without knowing the details of each local situation.

Applying the proper deposition velocity corrects not only the levels of concentration prediction, but also the spatial distribution and makes the transportable fraction smaller. The effects were demonstrated by CMAQ modeling, the results from reducing the deposition velocity showed smaller mass spreading compared to the results from the default deposition velocity.

6. Conclusion

Traditional grid models systematically overestimate road dust concentrations due to artificial mixing in the bottom layer and underestimating deposition due to horizontal winds within canopies. Similar problems may also exist in plume and puff models.

This analysis provides support to recent studies that suggest near field deposition and transportable fraction is in the right direction to solve the problem.

In view of these results, it may be appropriate to reconcile model-predicted road dust concentrations using other data, such as receptor modeling and rollback modeling results until the proper corrections are made for the models. Since these errors are related to the deposition rate, it is recommended that if it is desired to modify the model results, deposition velocity in the modeling should be modified instead of modifying the emission rates, because in this way the mass horizontal distribution will be simulated more accurately. The factor of about two due to mixing under stagnation conditions cannot be corrected easily in modeling; however it can be treated post-modeling since the error is understood and can now be explicitly estimated.

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