J7.7

EPISODIC PARTICULATE MATTER MODELING IN A SEMI-ARID/ARID AREA OVER THE U.S./MEXICO BORDER: INCORPORATING A WIND-BLOWN DUST EMISSIONS MODEL INTO THE MODELS-3/CMAQ SYSTEM

Yu-Jin Choi and H. J. S. Fernando*
Arizona State University, Tempe, Arizona

1. INTRODUCTION

Particulate matter (PM) pollution has been of profound concern owing to its adverse effects on human health as well as its role in visibility degradation by atmospheric haze. Such quality of life issues related to PM have resulted in an increased interest in the analysis and prediction of urban PM. To this end, photochemical air quality models capable of predicting the non-linear response of pollutant concentrations to the change of precursor emissions are being used for planning and regulatory purposes. Confidence in such models is established considering their ability to satisfactorily predict the effects of emissions controls on pollutant concentrations, especially during representative air quality episodes (Held et al., 2004). One of the factors determining the violations of National Ambient Air Quality Standards (NAAQS) for PM is episodic PM events, with regard to which several modeling studies have been reported. Nevertheless, source categories representing episodic emissions such as wildfires, prescribed burns, and wind-blown dust are often poorly parameterized in these models, calling for the implementation of improved parameterizations of such sources and processes (McMurry et al., 2004). In particular, the arid/semi-arid regions in the southwestern U.S. are vulnerable to wind-blown dust, which is a major component of daily routine particle loading (Chow et al., 1992; Vasconcelos et al., 1996). Our studies on modeling episodic PM events of the U.S./Mexico border using the CMAQ/MM5/SMOKE air quality modeling system have clearly indicated the emergence of serious errors in the predictions due to lack of provisions in the system to entrain dust during (time dependent) wind events (Choi et al., 2006).

In this paper, an effort to implement time-dependent wind-blown dust emissions into the CMAQ/MM5/SMOKE air quality modeling system is described. An approach for generating a wind-blown dust emission flux for each grid cell over the study domain on an hourly basis is presented in detail. The generated dust emission flux is applied to predict episodic high PM events over the U.S./Mexico border towns, where the dust emission flux is dependent on numerous factors such as the season, soil moisture content, atmospheric stability, and wind speed. Simulation results with the newly implemented time-dependent wind-blown dust emission flux indicate an improved model performance.

* *Corresponding author address*: H. J. S. Fernando, Arizona State University, Dept. of Mechanical & Aerospace Engineering, Tempe, AZ, 85287-9809; e-mail: j.fernando@asu.edu

2. APPROACH

2.1 *Dust emission flux*

Production of soil dust aerosols depends on wind energy and soil surface properties. Dust emissions are normally defined as a continuous function of the wind, whereas many experiments clearly indicate that the dust mobilization occurs only for surface wind velocities higher than a threshold value and that the production is not linearly dependent on the wind velocity. Also, the bed erodibility depends strongly on type of soil, soil moisture content and type of vegetation cover (Gillette, 1979; Marticorena and Bergametti, 1995; Nickovic et al., 2001).

Liu and Westphal (2001) compared two general approaches used to quantify dust production; one approach relates friction velocity to the surface dust flux whereas the other to the surface wind speed. In their conclusion, the former was considered more realistic and preferable than the latter, in that the friction velocity driven dust production can account for both wind shear and thermal stability effects. Hence, in our study, the friction velocity driven dust emission flux was considered in calculating the dust production.

Westphal et al. (1987) proposed vertical mass flux formulae for dust particles less than 10 μm in radius as a function of the friction velocity (U_*). The formulae (1) and (2) below were deduced from an analysis of direct and indirect measurements in the Saharan desert, U.S. southwestern deserts and an Israeli desert.

$$F_a = 10^{-14} \times U_*^4 \quad \text{when } U_* \geq U_{*t}, \qquad (1)$$
$$F_a = 2 \times 10^{-13} \times U_*^3 \quad \text{when } U_* \geq U_{*t}, \qquad (2)$$

where F_a is dust emission flux in grams per square centimeter per second, U_* in centimeters per second, and U_{*t} represents threshold friction velocity, which is the minimal friction velocity required to mobilize a soil grain. Equation (1) was supposed to be appropriate for soils with less sand and more silt or clay sizes with (2) for more sandy type of soils. Park and In (2003) introduced reduction factors to their emission flux equation for 24 U.S. Geological Survey (USGS) Vegetation categories, considering that dust emission occurs in arid desert and/or barren areas with no vegetation while the presence of vegetation in source regions would reduce the dust flux. In addition, Liu and Westphal (2001) estimated that on the average, only 13% of the erodible lands are capable of emitting dust. Considering all, we changed the equations of dust emission flux for a grid cell as below.

$F_a = 0.13 \times (1\text{-}R) \times 10^{-14} \times U_*^4$
when $U_* \geq U_{*t}$, (3)
$F_a = 0.13 \times (1\text{-}R) \times 2 \times 10^{-13} \times U_*^3$
when $U_* \geq U_{*t}$, and (4)
$F_a = 0$ when $U_* < U_{*t}$ (5)

where R is a reduction factor. In our work, USGS satellite data with horizontal grid resolution of 1 km was used to assign land use categories to each 1-km computational grid, based on 24 vegetation categories.

Nickovic et al. (2001) divided particles into four classes, resulting from the structure of desert soils based on the content of clay, small silt, large silt, and sand. Table 1 shows the four categories with properties of typical dust particles. The focus in this study is on PM_{10} so that the first two types, clay and small silt, were considered as $PM_{2.5}$ and coarse PM (PM_{10}-$PM_{2.5}$) respectively. Hence, the dust production flux could be obtained by correctly apportioning $PM_{2.5}$ and coarse PM dust fluxes; clay and small silt soil contents of each grid in the modeling domain were used.

Table 1. Features of typical dust particles.

Type	Typical particle radius(μm)	Particle density, ρ_p (g cm^{-3})
Clay	0.73	2.5
Small silt	6.10	2.65
Large silt	18.00	2.65
Sand	38.00	2.65

In so doing, we have used Food and Agricultural Organization (FAO) and US State Soil Geographic (STATSGO) soils data in 1 km grid resolution to assign a representative soil category to each grid cell. The data have 16 categories of soils. Each soil category has different relative proportions of sand, silt, and clay, and the relative fractions were obtained from the USDA soil texture triangle, which gives the ranges of sand, silt and clay percentages of each soil category. We assumed that 50% of silt belongs to small silt and 50% to large silt. In this way, we could obtain approximate percentages of $PM_{2.5}$ and coarse PM soils in a grid cell. The fractions of clay and small silt were multiplied by F_a to obtain $F_{a,fine}$ and $F_{a,coarse}$.

$F_{a,\,fine} = f_{clay} \times F_a$, (6)
$F_{a,\,corse} = f_{small\ silt} \times F_a$, (7)

where f_{clay} and $f_{small\ silt}$ are the fractions of clay and small silt.

2.2 *Threshold friction velocity*

With regard to dust production in arid/semiarid areas, the mobilization of particles from rest are dependent on the forces such as the weight, interparticle cohesion forces and wind shear stress gradients, which depends on the transfer of wind energy to the erodible surface, the latter being controlled by the presence of roughness elements on the surface. All of these factors determine the U_{*t} required to initiate particle motion (Marticorena and Bergametti, 1995). A semi-empirical expression for particles < 10 μm in diameter proposed by Marticorena et al., (1995, 1997) was used here, viz.,

$$U_{*t,1} = U_{*ts}\left(1 - \frac{\ln\left(Z_0 / Z_{0s}\right)}{\ln\left(0.35\left(10 / Z_{0s}\right)^{0.8}\right)}\right) \qquad (8)$$

where $U_{*ts} = \dfrac{0.129K}{(1.928B^{0.092} - 1)^{0.5}}$,

$$K = \left(\frac{\rho_p g D_p}{\rho_a}\right)^{0.5}\left(1 + \frac{0.006}{\rho_p g D_p^{2.5}}\right)^{0.5} ,$$

$B = 1331 D_p^{1.56} + 0.38$, D_p is the particle diameter, ρ_p the particle density, ρ_a the air density, 0.00123 g cm^{-3}, Z_0 the surface roughness length, and Z_{0s} a smooth surface roughness length, 10^{-3} cm. Accordingly, $U_{*t,1}$ for $PM_{2.5}$ and coarse PM were obtained using the properties of clay and small silt shown in Table 1.

Furthermore, the threshold friction velocity is a function of the soil moisture content, which was parameterized as follows (Fecan et al., 1999; Gong et al., 2003).

$U_{*t} = U_{*t,1}$ when $w < w'$, and (9)

$U_{*t} = U_{*t,1}\left[1 + 1.21(w - w')0.68\right]^{0.5}$
when $w > w'$, (10)

where w and w' are the ambient and threshold volumetric soil moisture with $w' = 0.0014(\%clay)^2 + 0.17(\%clay)$. The %clay is the fraction of clay in each soil category.

3. APPLYING THE EMISSIONS FLUX IN CMAQ PM_{10} SIMULATIONS

As a case study, we applied the formulae described above to the U.S./Mexico border area, in particular to a semi-arid rural land with small twin cities (Douglas/Agua Prieta) across the border. This area has experienced frequent PM events. Fig. 1 shows the modeling domains and the location of observation sites. More details about this area can be found in Choi et al. (2006).

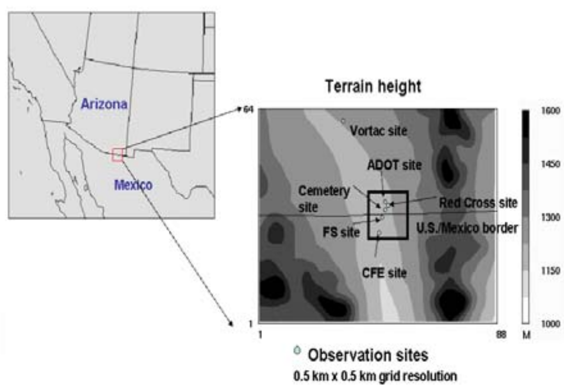

Fig .1 Modeling domains.

Four high PM days were selected to investigate the suitability of proposed windblown dust flux formulae: 3/07, 4/24, and 12/02 for high wind days and 2/23 for a low wind day.

U_* and *w* for each grid cell for each modeling hour, which are required to calculate windblown dust flux, were calculated using MM5, version 3.7.3, with a new nocturnal parameterization within the Medium Range Forest (MRF) Planetary Boundary Layer (PBL) scheme (Lee at al., 2006). In general, this area is assigned to shrub land and grass land, except for the urban center of the domain. Loam type of soil is predominant over the modeling area.

Both formulae (3) and (4) of windblown dust flux in Section 2.1 were investigated. Generally, the formula (3) for higher clay and silt soil content produced dust emissions twice as high as formula (4), which is applicable for more sandy type soils. In addition, except for a few hours of the 4/24 case, no dust $PM_{2.5}$ were produced by wind. The hourly wind-blown emissions flux so generated was combined with model-ready emissions from other emissions sources such as area, point, on-road, non-road and biogenic sources for PM_{10} in conducting CMAQ runs.

4. RESULT AND CONCLUSIONS

Fig. 2 compares the observed 24-h averaged PM_{10} with that of several predictions, with windblown dust emissions calculated using formulae (3) and (4). Note that the calculations without a dust formula have been made using a pollution inventory (supplied by the Arizona Department of Environmental Quality) where wind blown dust is parameterized using seasonal averaged weather conditions in the area; as such, it does not take into account the in situ winds that are responsible for episodes.

The results show that on the low wind day, 2/23, there are no differences between the predictions. In contrast, for high wind days in the spring (3/07 and 4/24), the formula (3) appears to overestimate PM substantially while (4) shows better or similar estimations to the case with seasonal-averaged dust emissions inventory. However, as far as the diurnal variation is concerned, the predicted PM_{10} with (4) and with the seasonal averaged inventory showed significant differences (Fig. 3). As expected, predictions with the formula (4) show a change of PM_{10} in response to high winds.

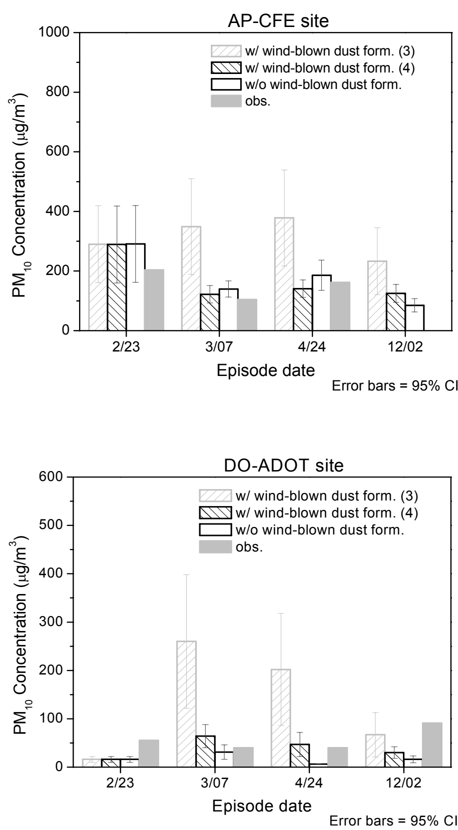

Fig. 2 Comparison of observed versus predicted 24h averaged PM_{10} at a Douglas (DO), U.S. site and an Agua Prieta (AP), Mexico site.

The preliminary results suggest that the approach used here can lead to improved PM predictions using the CMAQ/MM5/SMOKE system for semiarid or arid regions, and hence can serve to better characterize high PM events and severe visibility impairments. It will also help implement better control strategies for air quality improvement.

Further case studies with this approach should be performed to evaluate the robustness of this approach.

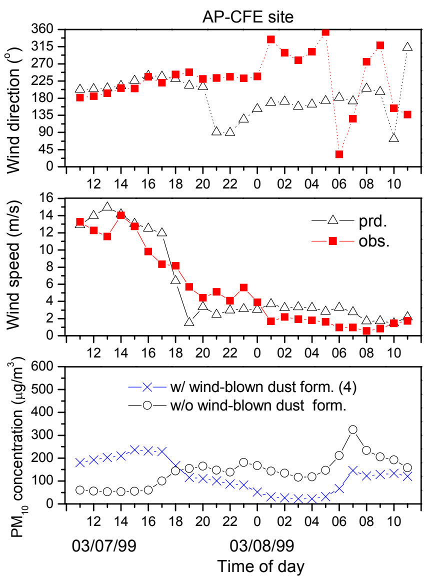

Fig. 3 Comparison of the diurnal variation of predicted wind and observations, and PM_{10} with the windblown dust formula (4) and without the formula but a typical day windblown dust emissions.

5. REFERENCES

Choi, Y. -J., Hyde, P., Fernando, H. J. S., 2006. Modeling of episodic particulate matter events using a 3D air quality model with fine grid: Applications to a pair of cities in the U.S./Mexico border. Atmospheric Environment 40, 5181-5201.

Chow, J. C., Watson, D. H., Lowenthal, P.A., Solomon, P. A., Magliano, K .L., Ziman, S. D., Richards, L. W., 1992. PM_{10} source apportionment in California's San Joaquin Valley. Atmospheric Environment 26, 3335-3354.

Fecan, F., Marticorena, B., Bergametti, G., 1999. Parameterization of the increase of the aeolian erosion threshold wind friction velocity due to soil moisture for arid and semi-arid areas. Ann. Geophy. 17, 149-157.

Gong, S. L., Zhang, T. L., McKendry, I. G., Jaffe, D. A., Lu, N. M., 2003. Characterization of soil dust aerosol in China and its transport and distribution during 2001 ACE-Asia: 2. Model simulation and validation. Journal of Geophysical Research 108, doi:10.1029/2002JD002633.

Gillette, D. A., 1979. Environmental factors affecting dust emissions by wind erosion in Saharan Dust, pp 71-94, John Wiley, New York.

Held, T., Ying, Q., Kaduwela, A., Kleeman, M., 2004. Modeling particulate matter in the San Joaquin Valley with a source-oriented externally mixed three-dimensional photochemical grid model. Atmospheric Environment 38, 3689-3711.

Lee, S. -M., Fernando, H. J. S., Grossman-Clarke, S., 2006. MM5-SMOKE-CMAQ a s a modeling tool for 8-h ozone regulatory enforcement: application to the stat of Arizona. Environ. Model. Assess. DOI 10.1007/s10666-006-9053-7.

Liu, M., Westphal, D. L., 2001. A study of the sensitivity of simulated mineral dust production to model resolution. Journal of Geophysical Research 106, 18099-18112.

Marticorena, B., Bergametti, G., 1995. Modeling the atmospheric dust cycle: 1. Design of a soil-derived dust emission scheme. Journal of Geophysical Research 100, 16415-16430.

Marticorena, B., Bergametti, G., Aumont, B., Callot, Y., N'Doume', C., Legrand, M., 1997. Modeling the atmospheric dust cycle: 2. Simulation of Saharan dust sources. Journal of Geophysical Research 102, 4387-4404.

McMurry, P. H., Shepherd, M. F., Vickery, J. S., 2004. Particulate matter science for policy makers: A NARSTO assessment. Cambridge University Press.

Nickovic, S., Kallos, G., Papadopoulos, A., Kakaliagou, O., 2001. A model for prediction of desert dust cycle in the atmosphere. Journal of Geophysical Research 106, 18113-18129.

Park, S., In, H., 2003. Parameterization of dust emission for the simulation of the yellow sand (Asian dust) event observed in March 2002 in Korea. Journal of Geophysical Research 108(D19), 4618, doi:10.1029/2003JD003484.

Vasconcelos, L. A., Kahl, J. D. W., Liu, D., Macias, E. S., White, W. H., 2006. Patterns of dust transport to the Grand Canyon. Geophysical Research Letters 23, 3187-3190.

Westphal, D. L., Toon, O. B., Carlson, T. N., 1987. A two-dimensional numerical investigation of the dynamics and microphysical of Saharan dust storms. Journal of Geophysical Research 92, 3027-3049.