Development of Alternative Methods for Estimating Dry Deposition Velocity in CMAQ

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1. INTRODUCTION

Atmospheric dry deposition plays an active role in determining the air, water, and soil quality at different spatial scales. Gaseous deposition is known to be actively responsible for various environmental problems associated with soil acidification, nitrogen-based nutrient loading in watershed regions, and agricultural productivity at a regional scale (e.g., Hampp, 1992; Erisman and Baldocchi, 1994). Hence, better representation of dry deposition is an important component in environmental modeling and assessment programs.

The issue of pollutant deposition has been addressed mainly through measurements and integrated monitoring assessments (e.g., Fowler et al., 1998). Measurements are often point based and are only snapshot representations of the prevalent environmental conditions. Further, the nonlinear interactions between the atmosphere and surface vegetation make the deposition assessment over vegetated surfaces very uncertain (Schwede and Cooter, 2000). Therefore, to obtain spatially and temporally variable environmental conditions, a modeling approach is useful in complementing the limited observations (Meyers et al., 1998). The development of realistic models is also useful for providing "what if" scenarios for designing and testing emissions control and abatement plans. Thus, it is important to have realistic, process-based gas deposition models in environmental analyses systems (Wesely and Hicks 2000).

One of the most widely used dry deposition modeling approach considers dry deposition velocity (V_d) as a resistance-in-series formulation (e.g. Wesely 1989),

$$V_d = \left(R_a + R_b + R_c\right)^{-1}$$

where R_a is the aerodynamic resistance, R_b the quasi-laminar boundary layer resistance, and R_c the canopy resistance. The total canopy resistance is estimated as the sum of various resistances offered by the soil-vegetation continuum. Over vegetated surface, resistance offered by the leaf stomates to water vapor and trace gases, also called as stomatal resistance, is the dominant component. Stomatal resistance regulates the water vapor and hence the latent heat flux exchange from the surface. Thus, it is one of the critical parameters in meteorological models, modulating the surface energy balance, which in turn impacts the kinetic energy of the turbulent eddies in the atmospheric boundary layer (ABL) and hence the structures and depths of the ABL and associated cumulus convection (Alapaty et al. 1997, Niyogi et al. 1999).

To estimate the stomatal resistance, land surface models use different formulations ranging from simple radiation use, to detailed meteorology, to photosynthesis-ecological processes (Niyogi and Raman 1997). The formulation used by Wesely (1989) is an example of a simple radiation-based formulation which uses changes in air temperature and total radiation reaching the surface to modulate a so-called minimum stomatal resistance (prescribed as a function of vegetation type). A more detailed formulation, which considers environmental feedback as a function of air temperature, water vapor pressure deficit, soil moisture, radiation, and trace gas concentrations was proposed by Jarvis (1976). This is widely used in many land surface models such as the Noilhan and Planton (1989) and other land surface models based on it (Pleim and Xiu, 1995 in MM5 and Xue et al., 2000 in ARPS), in MM5/OSU Land surface scheme (Ek and Mahrt 1991), and in the Land-Air Parameterization Scheme (e.g., Alapaty and Mihailovic, 2003). The *Noah* land surface model that is available for use in

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MM5 and the WRF mesoscale models also use the Jarvis approach to estimate stomatal resistance. Pleim et al., (1999) extended the Jarvis method for use in air quality models estimating dry deposition velocities for use in the Models-3/Community Multiscale Air Quality (CMAQ) Modeling System (Byun and Ching, 1999). A more detailed formulation of the stomatal resistance estimation involves ecological-photosynthesis based approach. In these models, the stomatal resistance/transpiration potential is considered as a by-product of plant photosynthesis. Thus, these formulations consider carbon dioxide, water vapor, and biochemical responses in estimating photosynthesis rate, transpiration rate, and then estimating stomatal resistance offered for the water vapor exchange. These models have been widely used in plant physiological studies (e.g. Farquhar et al. 1980, Collatz et al. 1994), but have not been very popular for meteorological models (which continued using Jarvis scheme). In the last decade, there has been an increased interest in using the ecological models as more detailed land surface information is becoming available from remote sensed data (e.g. gap analysis, NDVI datsets, etc). These models have been used in micrometeorological studies (e.g. Baldocchi 1994), field scale analysis (Niyogi and Raman 1997, Niyogi et al. 1998), global climate studies (Sellers et al. 1996), and in a limited manner for mesoscale modeling studies (Eastman et al. 2001).

The objective of this paper is to test the different stomatal resistance formulations for their ability to estimate deposition velocities for use in the CMAQ model simulations. Unfortunately, lack of dry deposition velocity measurements at a sufficiently high spatial and temporal resolution precludes a detailed regional assessment. Most of the observations for deposition velocity are from dedicated field campaigns for a short duration (and are at a field scale). These observations are sufficient for testing the models in a 1-D mode and we have already undertaken such an evaluation. In our study, there was a good agreement between the photosynthesis scheme based deposition velocity and field observations particularly when there was no water–stress or wilting of the vegetation. These results are summarized in Niyogi et al. (2003). To test the models in a 3-D mode, which is the objective here, the limited, field scale observations are not sufficient. Therefore, we will take an alternate approach in which first we evaluate the different stomatal resistance formulations in a mesoscale meteorological model and compare the results obtained from these models with special and routine meteorological observations (e.g., temperature). Since the underlying pathways associated with correct estimation of surface temperature and humidity and the stomatal resistance/deposition velocity are similar, this evaluation will in a way help evaluate how the models would perform in estimating the regional deposition velocities. Additionally, a large of number of surface meteorological measurements are available for use in arriving at a statistically significant summary. We will then use the different stomatal resistance models in a mesoscale air quality model, CMAQ.

Thus, introducing additional options to users of community atmospheric models such as MM5, WRF, and CMAQ, to choose different stomatal resistance formulations helps to facilitate usage of the same formulation across meteorological and air quality models contributing to and supporting the "*one-atmosphere*" paradigm. To achieve our objective, we have performed research to (1) develop and implement a photosynthesis based Gas-exchange Evapotranspiration Model (GEM) (Niyogi 2000, Niyogi et al., 2003) that includes a carbon assimilation-based stomatal resistance (R_s) estimation, and (2) implement Wesely and GEM formulations, into the *Noah* land surface model used in the MM5 and WRF models in addition to the existing Jarvis formulation, and (3) intercompare Wesely-, Jarvis-, GEM-type of formulations using the MM5 and CMAQ models. Similar inter-comparison studies using the WRF and CMAQ modeling systems are under progress and these results will be presented in the near future.

2. DESCRIPTION OF METHODOLOGY

We implemented Wesely and GEM formulations into the *Noah* land surface model (Chen and Dudhia, 2001a; 2001b) used in the MM5 (and the WRF) model. The Noah LSM already contained the Jarvis formulation. Here, we briefly describe the three methods for estimating stomatal resistance. In the Wesely (1989) formulation, stomatal resistance R_s is estimated as:

$$R_s = R_i \left\{ 1 + \left(\frac{200}{0.1 + G_{sw}} \right)^2 \right\} \left\{ \frac{400}{T_c(40 - T_c)} \right\}$$

where, R_i is minimum stomatal resistance, G_{sw} is solar radiation reaching the canopy, and T_c air temperature in the canopy (in Celsius). The Jarvis formulation as used in the *Noah* land surface model to estimate the R_s is:

$$R_s = \frac{R_i}{LAI(F_1[R]F_2[W2]F_3[T]F_4[RH])}$$

where *LAI* is leaf area index, and F_1, F_2, F_3, and F_4 are function of solar radiation, root-level moisture, air temperature, and air humidity deficit, respectively. Details can be found in the Chen and Dudhia (2001a). In the GEM formulation, the Ball – Berry approach is used and is given as:

$$R_s = \frac{C_S}{m\,A_n\,H + bC_S}$$

where A_n is the net CO_2 assimilation or photosynthesis rate, H the relative humidity at the canopy level, C_S is the CO_2 concentration at the leaf surface, and '*m'* and '*b'* are linear coefficients based on gas-exchange considerations and are functions of land use and photosynthesis pathways. Unlike, the Wesely or Jarvis approach, each of the term in the photosynthesis-based R_s estimation have detailed sub-models associated in their calculations (with the exception of the '*m*' and '*b*' vegetation constants, which are specified). For instance, the photosynthesis rate is estimated as an iterative solution of CO_2 concentrations within the leaf cell, air humidity, and photosynthesis rate estimated as a minimum of light use, carbon use, and leaf biochemical response.

3. NUMERICAL SIMULATIONS

After implementing Wesley and GEM formulations into the *Noah* land surface model available in the MM5, we have performed MM5 model simulations using each of the three methods. In order to develop meteorological inputs to CMAQ, we modified the Models-3/Meteorological-Chemistry Interface Processor (MCIP) such that it can accept all required meteorological variables for use in its *m3dep* module. Using the modified MCIP, we produced three different meteorological inputs to CMAQ. Since the three meteorological inputs differed in terms of dynamics and thermodynamics, to effectively study the influence of the different stomatal resistance formulations on air quality simulations, we chose the meteorological inputs obtained by using the Jarvis method, i.e., MM5 simulations obtained using the standard *Noah* land surface model as *base-case*. Using these *base-case* meteorological inputs we prepared emissions inputs using the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System (Houyoux and Vukovich, 1999). Finally, we performed three CMAQ model simulations using identical emission sources inputs. However, in each of the CMAQ model simulations we used dry deposition velocity fields obtained from the three methods described above. All other meteorological inputs used in the CMAQ model simulations are exactly same otherwise. Thus, any differences in the simulated concentrations of the trace gas species are entirely attributed to differences in the estimated dry deposition velocities using the three schemes, and the nonlinearity that arises due to these differences.

The MM5 and CMAQ simulations are performed for 5 days starting from 1200 UTC 23 August 2000. The simulation domain included about 70-75% area of the continental US (Figure 1) using a 36 km grid resolution in the horizontal. We have used 28 layers in the vertical.

4. RESULTS

The hourly surface data (about 800 stations for the simulation domain showed in Figure 1) available from the Techniques Development Laboratory (see http://dss.ucar.edu/datasets/ds472.0) were used to generate various statistical indices to evaluate model results obtained by using the Wesely, Jarvis, and GEM formulations in MM5. Each of the observational sites is paired with the corresponding grid cell in the modeled domain for preparing statistics.

Table 1 shows the mean statistical results for the three cases. In a global sense, the RMS errors for temperature for each of the cases are comparable while some differences exist for water vapor mixing ratio. However, our local and regional analysis indicated mixed results for each of the cases when compared to observations. Figure 2 shows the area averaged (over land) dry deposition velocities for ozone obtained from the three schemes. Analysis of local and regional values showed pronounced differences among the three cases. Additional analyses of the MM5 outputs and results from the CMAQ simulations will be presented at the workshop.

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REFERENCES

Alapaty, K., N. Seaman, D. Niyogi, and A. Hanna, 2001: Assimilating Surface Data to Improve the Accuracy of Atmospheric Boundary Layer Simulations, *J. Appl. Meteorol*., 40, 2068-2082.

Alapaty, K, and D.T. Mihailovic, 2003: An Intercomparison Study of Two Land Surface Models using a 1-D Model and FIFE Measurements. *Environmental Fluid Mechanics*. (submitted).

Byun, D.W. and J.K.S. Ching, ed., Science Algorithms of the EPA Models-3 Community

Multiscale Air Quality (CMAQ) Modeling System, 1999, EPA/600/R-99/030(peer reviewed). [Available from National Exposure Research Laboratory, Research Triangle Park, NC

Chen, F., and J. Dudhia, 2001a: Coupling an advanced land-surface/hydrology model with the Penn State/NCAR MM5 modeling system. Part I: Model implementation and Sensitivity. *Mon. Wea. Rev.*, 129, 569-585.

Cooter, E., and Schwede D.: 2000, 'Sensitivity of the National Oceanic and Atmospheric Administration multiplayer model to instrument error and parameterization uncertainty', *J. Geophys. Res.*, **105**, 6695 – 6704.

Houyoux, M., R. and J. M. Vukovich, 1999: Updates to the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System and Integration with Models-3. Presented at The Emission Inventory: Regional Strategies for the Future, 26-28 October, Raleigh, NC, Air & Waste Management Association.

Noilhan, J., and S. Planton, 1989: A simple parameterization of land surface processes for Meteorological Models', *Mon. Wea. Rev.* **117**, 536--549.

Niyogi, D., and Raman, S.: 1997, 'Comparison of Four Different Stomatal Resistance Schemes Using FIFE Observations', *J. Appl. Meteor.* **36**, 903--917.

Pleim, J., and A. Xiu, 1995: Development and Testing of a Surface Flux Planetary Boundary Layer Model with Explicit Soil Moisture Parameterization for Applications in Mesoscale Models', *J. Appl. Meteor.* 34, 16-32.

Pleim, J., P. Finkelstein, and T. Ellestad, 1999: A Technique for Estimating Dry Deposition Velocities Based on Similarity with Latent Heat Flux', *Atmos. Environ*. **33**, 2257--2265.

Wesely, M.: 1989, 'Parameterization of Surface Resistance to Gaseous Dry Deposition in Regional scale Numerical Models', *Atmos. Environ.* **23**, 1293--1304.

Wesely, M., and Hicks, B.: 2000, 'A review of the current status of knowledge on dry deposition, *Atmos. Environ.*, **34**, 2261-2282.

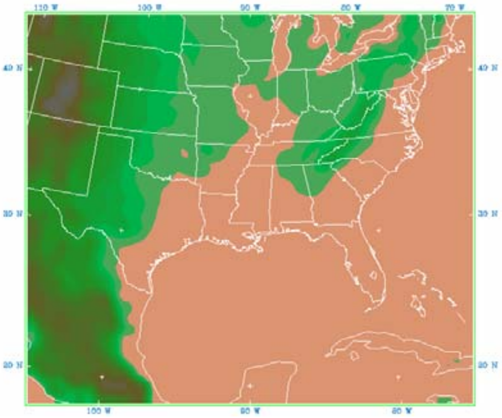

Figure 1. Simulation domain and terrain used in the MM5 simulations using the 36 km grids.

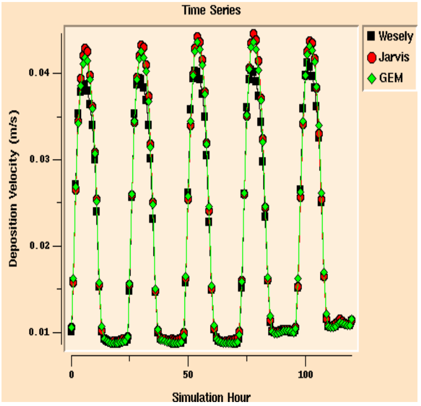

Figure 2. Area averaged dry deposition velocity from the three cases for ozone.

Table 1. Global average statistics for surface air temperature (K), and water vapor mixing ratio (g/kg) for the three cases. Total number of measurements used in 121 hours of simulation is 98,262.

Case	Parameter	Modeled Mean	Observed Mean	Bias	Mean Abs. Error	RMS Error	Coeff. of Determination	Index of Agreement
WESELY	Temperature	296.94	297.16	-0.22	2.15	2.80	0.843	0.949
JARVIS	Temperature	296.07	297.16	-1.09	2.07	2.68	0.838	0.947
GEM	Temperature	296.68	297.16	-0.48	2.08	2.71	0.837	0.950
WESELY	Mixing Ratio	11.76	13.79	-2.03	2.32	2.95	0.560	0.782
JARVIS	Mixing Ratio	12.90	13.79	-0.88	1.54	1.97	0.690	0.890
GEM	Mixing Ratio	12.16	13.79	-1.63	2.03	2.58	0.618	0.827