Considering Ecological Formulations for Estimating Deposition Velocity in Air Quality Models

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Abstract: A dry deposition modeling approach that includes vegetation-atmosphere interactions through photosynthesis/carbon assimilation relationships was recently developed. In this approach, gas deposition velocity (Vd) is calculated using an electrical resistance-analog approach in a coupled soil-vegetation-atmosphere transfer (SVAT) model. For this, a photosynthesis-based model is dynamically coupled to an atmospheric model with prognostic soil hydrology and surface energy balance. The effective surface resistance (composed of aerodynamic, boundary layer, and canopy-based resistances) is calculated for a realistic and fully interactive estimation of gaseous deposition velocity over natural surfaces. Results from the coupled model studies to estimate observed deposition velocity estimates for ozone over agricultural fields showed good agreement. The same model was tested for its ability to simulate ammonia Vd near an animal agricultural facility. The scheme did not reproduce the bidirectional exchange and had a much smaller range as compared to observations. The ecological scheme was modified to include a simple ammonia compensation point formulation and the model results were much closer to the observations. Study results indicate that ecological approaches with default parameterization and biophysical are convenient and effective approaches for developing Vd estimates in air quality models.

Keywords: Biosphere – Atmosphere Interaction, Photosynthesis Model, Deposition Velocity, Ammonia, Compensation Point, Bi-directional Exchange.

1 Introduction

Assessing the deposition of gaseous compounds to the earth's surface continues to be an important component of the air quality studies. In coastal communities the air emissions can deposit near water bodies causing water quality concerns. Examples of these have been reported in ecologically sensitive regions of eastern North Carolina (e.g. Walker et al. 2001) as well as the Great Lakes region (US EPA, 2005). Traditionally, efforts have been directed in studying ozone and sulfate deposition to understand the impacts due to industrial emissions. In recent years, atmospheric deposition studies have broadened in scope by considering the role of non-industrial, agricultural sources for emissions of nitrogen compounds such as ammonia.

Dry deposition of gaseous compounds, including ammonia, is most efficient on vegetated land surfaces. Some of the depositing gases, particularly nitrogenous species, can have significant ecological impacts on the natural system. For example, as increased ozone deposition could lead to decrease in agricultural productivity, while an increased nitrogen deposition could lead to fertilization of the landscape leading to higher net ecosystem productivity. Efforts are underway to understand and represent the coupled role of the biosphere - atmosphere interactions leading to enhanced deposition potential and the impacts of atmospheric deposition on the land surface health and vulnerability.

Even though monitoring of atmospheric deposition continues to be a critical component of understanding the environmental loading, such measurements are limited (Erisman et al. 1994). The limitations are even more significant for assessing the deposition from ammonia and other nitrogenous compounds, where the sources could be localized and the range of values obtained could vary significantly spatially. Therefore, models are often used in conjunction with field monitoring data to understand the spatial and temporal variations. The deposition models are also used to help determine what fraction of the total deposition can be attributable to the dry versus wet deposition.

The dry deposition models estimate the deposition flux based on the atmospheric concentration of the deposition gas, and a value of the deposition velocity (Vd). The accuracy of the deposition models thus largely depends on accurate estimation of the Vd values that are representative of the depositing surface and the dynamic environment.

In simpler models, Vd is prescribed as a constant typically on the basis of field observations and look-up tables. A degree of realism can be added to the Vd calculations by providing variations as a function of environmental changes (e.g. wind speed or temperature) through empirical equations. In more comprehensive air quality models however, Vd is routinely estimated following a electrical resistance –based analogy (Figure 1, Baldocchi et al. 1987) as:

$$Vd = (Ra + Rb + Rc)^{-1}$$

In the above, Ra is the aerodynamic component (relating to the wind speed, surface friction velocity, roughness, etc.); Rb is the surface boundary layer resistance (function of shape of the vegetation, surface temperature, etc.), and Rc is the canopy or the surface resistance (which is the resistance offered by the surface to the depositing material). As shown in Figure 2, of the three resistances the canopy or surface resistance is the dominant term (often about 90% of the total resistance). Therefore, in order to bring improvements in the Vd estimates, efforts are directed towards improving the Rc term. Accordingly, in this paper, we will discuss the potential of applying ecological approaches in developing realistic canopy resistance and deposition velocity estimates.

2 Current Paradigm

The surface canopy resistance term is the aggregate representation of the resistance offered by the stoma (a conduit within the leaf from where carbon dioxide and water vapor exchange take place). The stomatal resistance can be scaled to a leaf, which is further scaled to a canopy and the landscape.

The current paradigm, based on Jarvis' (1972) plant physiological studies, involves scaling a so-called minimum canopy resistance (Rc*min*) term to the actual canopy resistance value as a function of ambient air temperature, radiation, humidity, and soil moisture status. One example of the Jarvis-approach is illustrated in the Noilhan and Planton (1989) scheme. This Noilhan – Planton scheme is used in various meteorological models, including the Penn State – NCAR Mesoscale Model ver 5 (MM5), for estimating the canopy resistance. The Jarvis' formulation can be summarized as:

$Rc = Rcmin. LAI (F1. F2. F3. F4)^{-1}$

Where, LAI is the leaf area index (an indicator of vegetation leaf density), and F1 through F4 are environmental terms typically ranging from 0.2 to 0.95. The Rc*min* term is user-specified and is generally a function of landuse category and vegetation type. Typical Rc*min* values range from around 30 s/m for actively growing grass and crops to about 300 s/m for aged shrubs and trees.

One of the advantages of the Rc*min* approach for estimating Rc (and hence Vd) is that, the concept has evolved over time and has been tested in several different biogeographical settings, and at various grid spacings. The formulations have been modified and tested to be generalized enough for a wide range of environmental applications. Further, these formulations are used in weather forecast models and thus provide a convenient way for the meteorological and the air quality modeling results to be interpreted and communicated.

There are several disadvantages with the Rc*min* based approach for estimating deposition velocity. First, at a regional scale, the concept has a poor scientific basis particularly since Rc*min* cannot be measured or determined independently in the laboratory. Additionally, even though Rc*min* is treated as a constant, it shows large seasonal and intra-specie variability and its prescription has significant uncertainty. Furthermore, the results are nearly linearly dependent on the Rc*min* value and can be tuned with relative ease. As an example, Figure 3 shows the possible variations in the surface latent heat fluxes over a grassland simulated using the MM5 modeling system using USGS land use categorization. In the model, the grassland landscape could be represented by three possible Rc*min* values: 40, 150 and 300 s/m. Corresponding to these Rc*min* values, the modeled latent heat flux varies inversely by about 375 W/m^2 to about 150 W/m^2. As shown in the figure, the observed fluxes could be best simulated by tuning the Rc*min* value to 60 s/m. Note that, the example discussed variation in the latent heat fluxes since the results are easier to visualize, and similar results are seen for deposition velocity. Further, as demonstrated in Niyogi and Raman (1997), the effect of Rc*min* on surface fluxes can propagate all through the boundary layer and can further impact the surface – atmosphere exchanges as a feedback.

3 Ecological perspective

An alternative to the Rc*min* based approach is the photosynthesis based ecological approach. In this approach, canopy conductance (inverse of Rc) is assumed to correlate with photosynthesis (Wong et al. 1979). Carbon assimilation (A*n*) or photosynthesis is the net primary productivity (gross minus loss due to respiration) estimated as a complex, interactive function of plant biochemical response, environmental temperature and moisture, and the carbon dioxide availability for photosynthesis. The canopy conductance is strongly coupled to the surface characteristics as well as the regional hydrology and the atmospheric boundary layer, and is considered more interactive than the Jarvis-type approach (Niyogi et al. 1998).

The use of ecological approach for estimating deposition velocity would also be consistent with the developments occurring in the modeling and monitoring (remote sensing) of the land surface. The Jarvis-type approach can be considered of the modeling systems with relatively coarse grid spacing (order of 50 to 100km) and limited interaction between the vegetation – land surface and the atmosphere. For finer grid spacing, and more realistic analysis, more interactive coupling between the biosphere and the atmosphere is required as seen for instance with the ecological schemes.

One photosynthesis / ecological approach that can be adopted in the deposition velocity parameterizations is based on the Ball –Woodrow - Berry model (Ball et al. 1987; Niyogi et al. 1998). In this model, the canopy resistance can be estimated as:

$1/Rc = (m.An / Cs.\ hs) + b$,

where, *m, b* are specie specific 'constants', *An* is net assimilation or photosynthesis, *Cs* is the CO_2 at leaf surface, and *hs* is the humidity at leaf surface.

In the air quality modeling perspective the following framework can be followed. Information on the structural (e.g. leaf and stem area index, leaf angles), physical characteristics (e.g. optical absorptance, transmittance, heat capacity) of the land surface, as well as the environmental / meteorological conditions over the surface (radiation, temperature, humidity, winds, etc) are integrated into the photosynthesis model to solve the Rc equation at the leaf scale. The leaf level results are then integrated over the canopy adopting geometrical and physical considerations for radiation penetration and specie specific information (such as leaf photosynthetic capacity). At every model time-integration and scale-up calculation the model considers explicit feedback between the atmosphere and the vegetated surface (Collatz et al. 1991, 1992).

The advantages of the ecological approach include: (i) the parameters (e.g. *m* and *b* in Ball-Berry model) can be measured in laboratory as well as in the field (unlike the Rc*min* parameter); (ii) the photosynthesis parameters have fairly universal values across species as a function of vegetation type; (iii) unlike the Jarvis-type approach, different plant species (C3 and C4 grass, mixed landuse) can be represented with the differences in the photosynthesis pathways; and (iv) the coupling between the vegetation and the atmosphere is more explicit leading to more interactive feedbacks evident in the model results. Additionally, the developments in the satellite remote sensing of the biophysical properties of the land surface appear to be better suited for the ecological modeling approaches (e.g. Sellers et al. 1996).

Some of the disadvantages of the photosynthesis approach for estimating deposition velocity can be identified. First, the photosynthesis- based equations such as the Ball-Berry model are "deceptively simple" (Niyogi et al. 1998). The variables required to solve the Ball – Berry model, for instance, are not routinely available and iterative solutions are often needed. The iterative solutions, if not mathematically constrained, can yield unrealistic results. Second, unlike the Rc*min* based approach, the interactive nature of the ecological models makes the response highly nonlinear and hence difficult to interpret (or tune).

In the following section, we demonstrate the applicability of the photosynthesis / ecological approach for the deposition velocity assessments.

4 Testing the Photosynthesis based Vd estimation for Ammonia deposition:

Niyogi et al. (2003) applied the photosynthesis based approach for Vd estimation for ozone deposition. In their study, the models results were compared with observed ozone Vd observations (Meyers et al. 1998) and a good performance was seen. For example, Figure 4, adapted from their study, shows the ability of the photosynthesis model to reproduce the observed variability of the deposition velocity estimates. The model was run without any 'tuning' (with default biophysical parameters) and hence the good performance was considered noteworthy.

We will further test the same photosynthesis-based deposition model for its ability to simulate ammonia Vd values. The ammonia deposition problem is challenging because of several factors. First, there are very few direct measurements of ammonia Vd. This provides a relatively small dataset to understand the variability possible. Second, ammonia, unlike ozone, can show bidirectional exchange. In that, the vegetated surface can show both deposition as well as emission of ammonia from the land surface within a relative short-time interval (few minutes to hours). Third, ammonia undergoes transformation when it is emitted and can lead to large variability in the ammonia versus its transformed ammonium or other chemical constituent and can affect the deposition potential (Asman 1998).

Ammonia Vd Observational Data: The ammonia deposition velocity observations used for testing the model were reported in Phillips et al. (2004). Their measurements were made over an experimental agricultural air quality study site in Raleigh, NC (USDA-ARS, 3908 Inwood Rd., Raleigh, NC 35°44'N, 78°41'W). The study surface was natural vegetation, short grass with seasonal growth. Soil texture was sand,clay, loam mixture. For estimating the Vd values, atmospheric ammonia concentrations were measured at two heights (2 and 6 m) by two Thermo Environmental Instruments, Inc. Model 17C chemiluminescent nitrogen oxides (NO_X)–ammonia (NH_3) analyzers along with a solenoid for each analyzer to alternate measurements between the two elevations. Simultaneously, mean winds and temperatures were also measured at the same two heights. The micrometeorological flux gradient method was used in conjunction with the Monin–Obukhov similarity theory, to estimate the vertical flux and dry deposition velocity of ammonia under different meteorological conditions (Arya 2001). The experimental site is located near a swine production facility, which employs an anaerobic lagoon for disposal of swine waste. The farm consisted of seven production barns to house the swine, from the time of breeding to finishing. During each measurement period, the swine production facility averaged a total volume inventory of approximately 1200 swine. Thus field measurements routinely showed bi-directional exchange of ammonia i.e. deposition to and emissions from the surface.

Model Simulations: The deposition velocity model was coupled to an atmospheric boundary layer model similar to that described in Alapaty et al. (1997) and Alapaty et al.

(2001).

In the coupled atmospheric system, net radiation at the surface was the sum of incoming solar radiation (function of solar zenith angle, surface albedo, and atmospheric turbidity), atmospheric longwave back-scattering radiation, and outgoing longwave surface radiation (Anthes et al. 1987). Upward and downward longwave radiation was calculated as functions of soil emissivity, ground temperature, atmospheric longwave emissivity, and atmospheric temperatures. The model used surface layer similarity with turbulent kinetic energy (TKE) approach for the mixed layer parameterization.

The photosynthesis scheme based surface resistance module was embedded in the soil-vegetation scheme. Five prognostic equations for top soil (0.1m) and deep soil (1 m) temperature, moisture, and rainfall interception were solved. The model calculated the evaporation at the soil surface (E_g), and the transpiration rate (E_{tr}). For a known fractional vegetation cover, the evaporation rates from the wet parts of the canopy (Er) were also considered. Total water vapor loss from the surface was taken as sum of E_g, E_{tr}, and E_r, and was provided as a surface boundary condition to the atmospheric model as well as the feedback term for estimating Rc.

In the coupled model, Vd estimation was based on the Ball – Woodrow – Berry stomatal scheme (Ball et al., 1987, Niyogi and Raman, 1997) and the Collatz et al. (1991, 1992) photosynthesis scheme. Photosynthesis was taken as the residue of gross carbon assimilation (*Ag*) and loss due to respiration (*Rd*). Following Collatz et al. (1991, 1992),

*Ag = function {*rubisco limited *Wc,* radiation limited *We,* CO2 limited *Ws}*

The carbon assimilation limiting rates were estimated as a function of C3 and C4 photosynthesis pathway.

For C3 vegetation,

$$Wc = V_m \left\{ \frac{C_i - \Gamma}{C_i + K_c.\left(1 + O_2 / K_o\right)} \right\}$$

$$Ws = 0.5\ Vm$$

$$We = PAR.\ \varepsilon.\ (1-\omega_\pi).[(Ci - \Gamma)/(C1+2\Gamma)]$$

while for C4 vegetation,

$$W_c = V_m$$

$$W_E = PAR.\varepsilon.(1 - \omega_\pi)$$

$$W_s = \frac{20000.V_m.C_i}{P}$$

In the above, ε is efficiency for carbon dioxide uptake, and ω_π is the leaf-scattering coefficient for PAR (Sellers *et al.* 1996); *Vm*, is the maximum catalytic Rubisco capacity for the leaf, Γ is the CO_2 compensation point (Collatz *et al.* 1992), O_2 is oxygen availability for the leaf, and *Kc* and *Ko* are the Michaelis – Menten constant and the oxygen inhibition constant respectively; *P* is the atmospheric pressure, *PAR* is the component of the total radiation available for photosynthetic activities; *Ci* is the carbon dioxide concentration in the leaf intercellular spaces and was obtained through an iterative solution that included net assimilation (*An*), and stomatal conductance (g_s). The respiration loss *Rd* was estimated following Calvet *et al.* (1998) as,

$$R_d = 0.11 A_m$$

where, *Am* is the maximum assimilation rate (Schulze *et al.*, 1994) and it was limited via mesophyllic conductance (g_m) as,

$$A_m = A_{m,max}\,[1 - exp(-g_m(C_i - \Gamma)/\ A_{m,max})]$$

The mesophyllic conductance was related to the reactivity of the depositing gas (see

Wesley, 1989). The mesophyll also linked soil moisture, evapotranspiration and effectively their control on deposition. Thus *gm* was parameterized as (Calvet *et al*., 1998),

$$g_m = g_{m,max} \cdot 2^{Q_t} \cdot \frac{1 + exp(0.3(T_c - S_2))}{1 + exp(0.3(S_1 - T_c))} \cdot \frac{(w_2 - w_{wilt})}{(w_{sat} - w_{wilt})}$$

In the above, $g_{m,max}$ S_1 and S_2 are landuse based coefficients as described in Sellers et al. (1996), T_c is the surface temperature, and w_2, w_{wilt}, and w_{sat} are the deep (~ root level) soil moisture, and the wilting and saturation capacity of the soil. The gas concentration at the leaf surface *(Cs)* was estimated as

$$C_s = C_a - \frac{A_n}{g_b}$$

The equations were closed using an approach similar to that of Collatz et al. (1991), with η = 1.0 for ammonia(Wesley, 1989) as,

$$C_i = C_s - \frac{\eta A_n P}{g_s}$$

The converged gs values were estimated for both sunlit and shaded fraction of the leaf area and the effective canopy resistance was obtained (inverse of conductance). The Rb (inverse of gb and gm) were also obtained from the vegetation model, while Ra was estimated from the atmospheric surface layer parameterization (similarity theory based approach as described in Draxler and Hess 1997).

The model was configured over the Phillips et al. (2004) study site. This was done by prescribing the geographical locations, surface characteristics, and the initial surface meteorological observations. The model simulated ammonia deposition velocity for the Spring 2002 field campaign. The model was run for: April 28, May 1-2, May 7, and May 9-10.

Figure 5a-b shows the observed and simulated ammonia Vd values as a time-series and a scatter plot. Results indicate several key features. First, the measurements show significant bi-directional exchange. That is, ammonia is both deposited as well as emitted from the surface. This feature is not anomalous to this particular study site and is consistent with prior ammonia deposition flux studies conducted in Europe (e.g. Sutton et al. 2001, Nemitz et al. 2001). In general, the model results show poor overall agreement with the observations, though for periods dominated by deposition (as against emissions) the agreement is relatively better. The model results conspicuously missed two features seen in the observations: the negative Vd values (emissions) of ammonia from the surface, and the relatively high Vd values (both positive as well as negative). In that the modeled values range between 0 to 4 cm/s while the observations have a much larger range (about -5 to 8 cm/s). These results suggest that: (i) the default ecological modeling approach, which yielded good results for ozone Vd, has a significantly deteriorated performance for a active gas such as ammonia; (ii) a bi-directional exchange component needs to be added to test whether the ecological scheme would be able to simulate the exchange better and improve the model performance.

One approach for introducing the bi-directional exchange is by incorporating a compensation point in the flux – deposition calculation. The photosynthesis scheme inherently considers a CO_2 compensation point formulation (which typically allows the carbon source / sinks studies in climate models, for instance). The default ecological deposition velocity formulation was therefore modified to consider a simple ammonia compensation point formulation. The ammonia compensation point (Ccp) was calculated following the framework proposed by Sutton et al. (1998) and Nemitz et al. (2003). In this, the compensation point concentration can be generalized as: Ccp = Cr + *F* (Ra+Rb), where Cr is the ammonia concentration at height at which winds are measured and *F* is the total exchange flux.

By definition the compensation point shows a conservation of flux between cuticles and stoma and including soil emissions considerations,

$$Ccp = [Cr /(Ra + Rb) + Ccps/ Rc] . [1/(Ra + Rb) + 1/ Rc + 1/ Rw]^{-1}$$

In the above, Ccps is the stomatal compensation point, and Rw is a resistance term estimated via Henry's constant and temperature variations as discussed in Sutton et al. (1998).

The modified model was run for the same cases and the results are plotted in Figure 6 a-b. In the figure, both the original model results as well as those after adding the ammonia compensation point are compared with observations. With the addition of the compensation point, the model results follow the observations much more closely. In particular, the model exhibits the observed bi-directional exchange. Further, the range of variability in the model results is also much closer to that seen in the observations (Fig 6b). Note that there are still some periods for which the model results are qualitatively different than observations. These are attributed to two factors: (i) the micrometeorological features and microscale variability that is not resolved by the modeling system, and (ii) lack of sufficient realism in the model parameterization (e.g. soil emission).

Note that the results were developed with a default variable values representative of a mixed natural grassland ecosystem (i.e. no tuning was performed). The results, with the addition of the compensation point formulation, showed significant agreement with the observations. Since the field results themselves show significant variability due to the proximity to a animal waste lagoon and other advective features which were not considered in our model, there no specific attempt was made to systematically evaluate the model.

5 Conclusions

The model Vd results are sensitive to the choice of the vegetation / canopy scheme in the model. Our results indicate that a photosynthesis – based / ecological Vd estimation scheme can be successfully adopted in coupled air quality – mesoscale modeling system. The photosynthesis scheme based Vd results show significant variability and responsiveness to the environmental conditions as well as to the changes in the model formulations.

The results suggest there are distinct advantages in including ecological concepts in deposition velocity / air quality model. Future studies would be directed towards additional verification with additional field observations and for developing sensitivity studies to understand the various nonlinear feedback that can affect Vd calculations from the ecological scheme. Additional future developments that could improve the model performance include coupling a detailed soil biogeochemistry model for soil emissions. Overall, the results suggest that the ecological / photosynthesis based model paradigm can be applied for developing deposition velocity estimates for gaseous compounds.

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FIGURE CAPTIONS

Figure 1 Surface resistance pathways for the deposition gases. Inverse of the total resistance offered by Ra, Rb, and the Rc term yields deposition velocity (Vd). [After Baldocchi et al. 1988]

Figure 2 Sample time history of simulated aerodynamic (Ra), boundary layer (Rb), and canopy (Rc) resistances using a photosynthesis – based biophysical model. Effects of stability changes and the dominance of the canopy resistance term is clearly seen.

Figure 3. Changes in the MM5 simulated latent heat fluxes for three different values of Rcmin (40, 150, and 300 s/m) representative of the grassland. Also, shown are the observed values: LHF(Obs), and the calibrated Rcmin based latent heat flux: LHF.

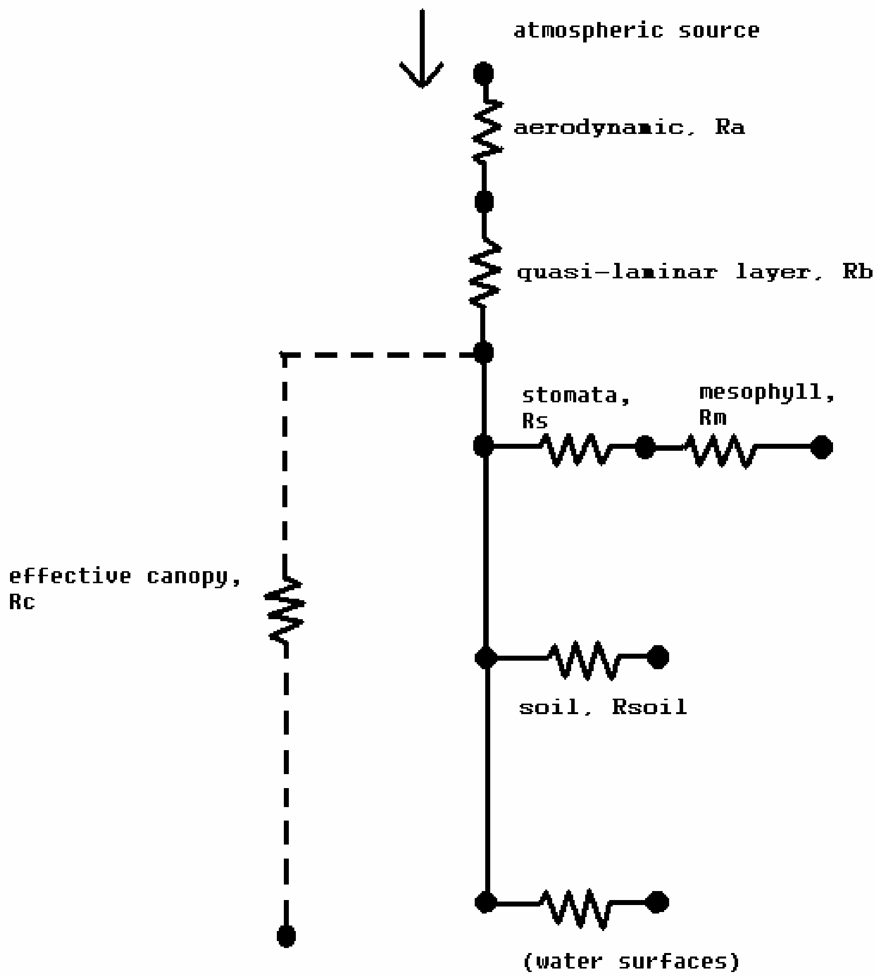
Figure 4. Observed and a photosynthesis model based ozone deposition velocity over a fully grown agricultural field. (Adapted from Niyogi et al. 2003, A photosynthesis based deposition velocity modeling approach, Water, Air and Soil Pollution, Kluwer Press, The Netherlands).

Figure 5a. Observed (circle, dashed line) and model simulated (square) ammonia deposition velocity (cm/s) over a short grass vegetated landscape near an animal agricultural experimentation facility in Raleigh, NC.

Figure 5b. Observed (X-axis) versus modeled (Y-axis) ammonia deposition velocity (cm/s) corresponding to Fig. 5a.

Figure 6a. Same as Fig. 5a. O= observations (closed circles), G= default model run (open circles), GC = the ecological model with compensation point (squares).

Figure 6b. Same as Fig. 5b except that the data are based on Fig. 6a. G (open circle) = default model; GC (closed circles) = modified model with the compensation point consideration.



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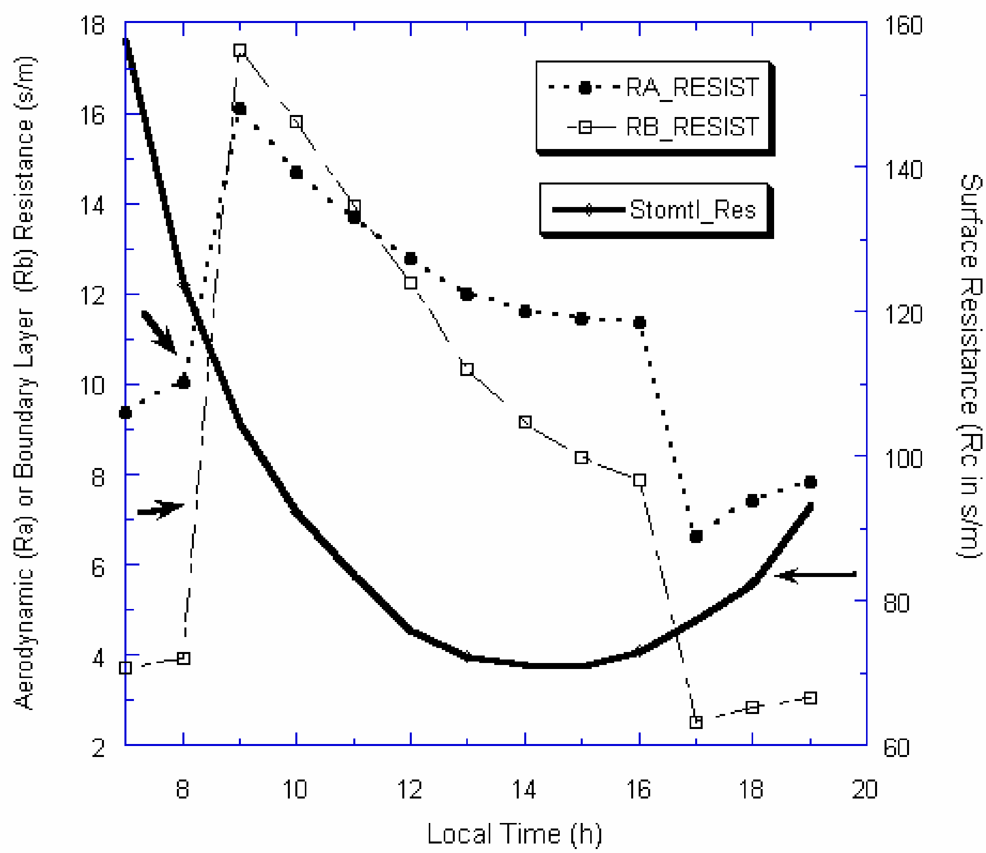

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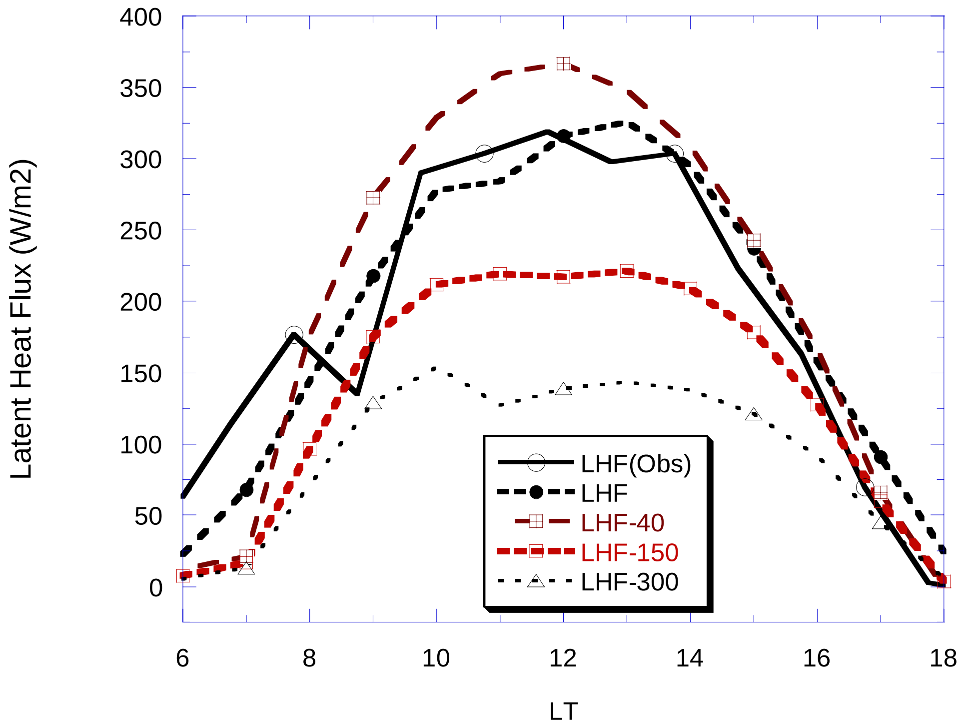

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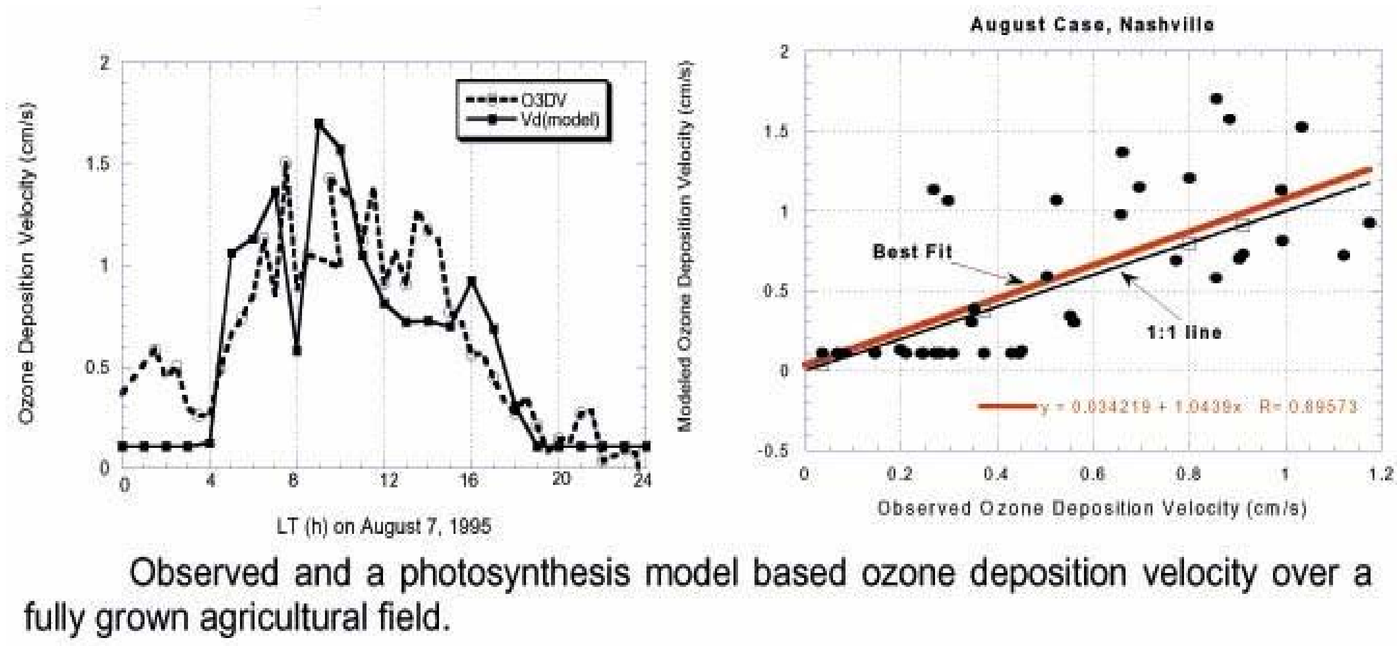

Figure 4. Observed and a photosynthesis model based ozone deposition velocity over a fully grown agricultural field. (Adapted from Niyogi et al. 2003, A photosynthesis based deposition velocity modeling approach, Water, Air and Soil Pollution, Kluwer Press, The Netherlands).

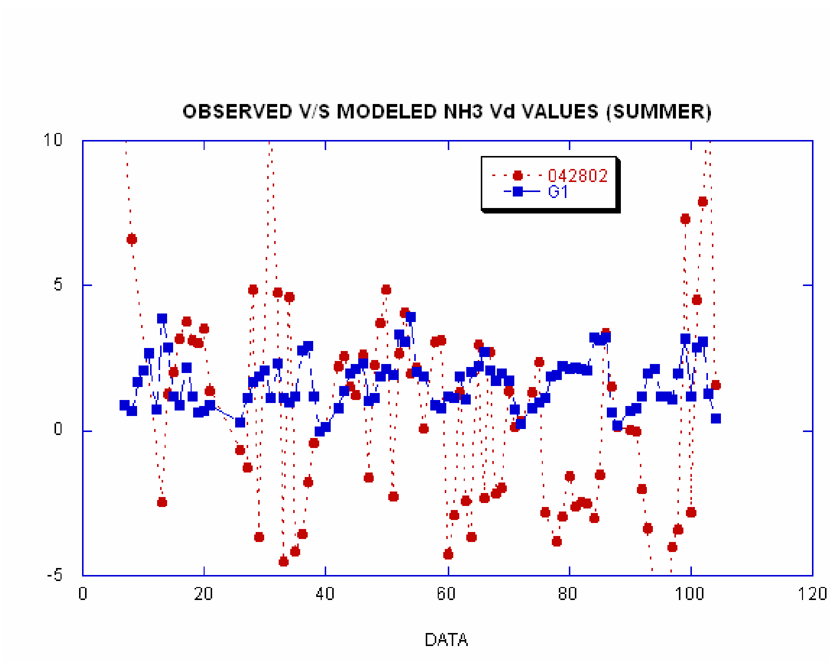

Figure 5a. Observed (circle, dashed line) and model simulated (square) ammonia deposition velocity (cm/s) over a short grass vegetated landscape near an animal agricultural experimentation facility in Raleigh, NC.

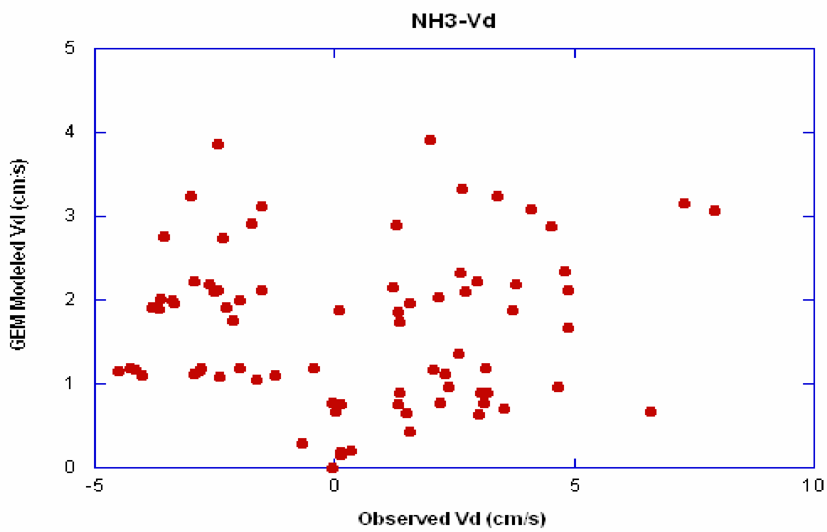

Figure 5b. Observed (X-axis) versus modeled (Y-axis) ammonia deposition velocity (cm/s) corresponding to Fig. 5a.

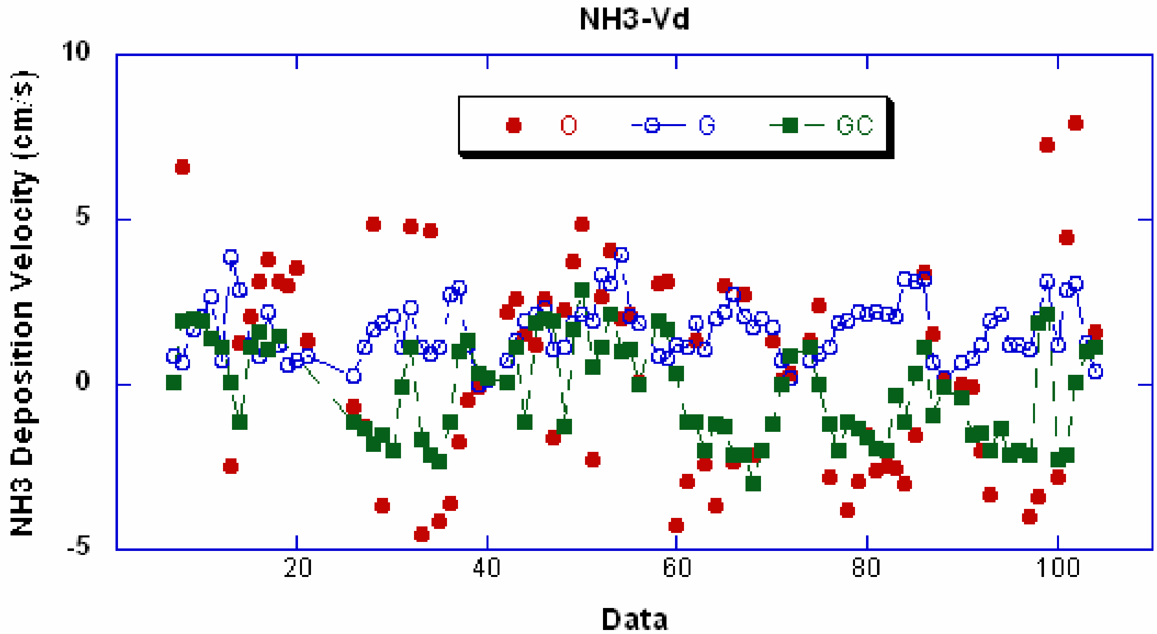

Figure 6a. Same as Fig. 5a. O= observations (closed circles), G= default model run (open circles), GC = the ecological model with compensation point (squares).

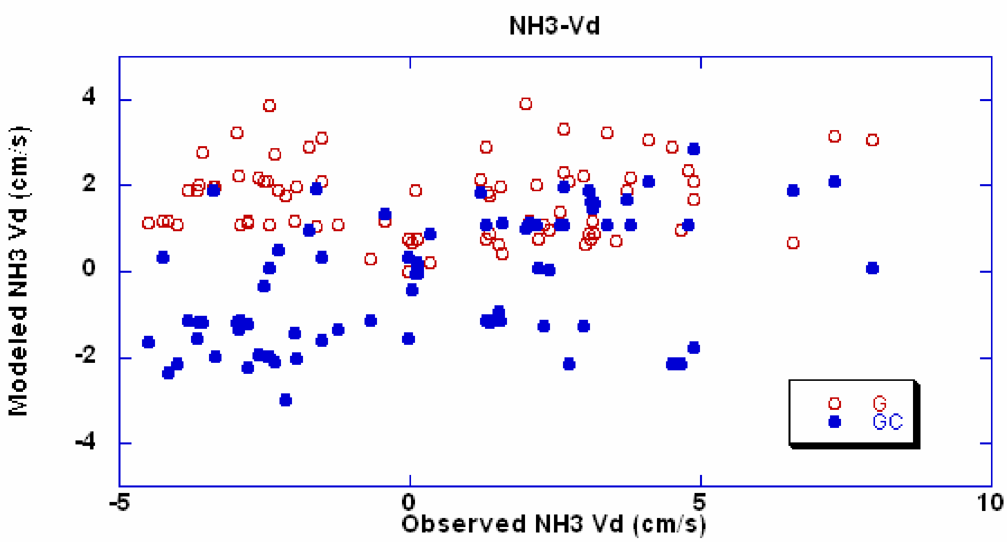

Figure 6b. Same as Fig. 5b except that the data are based on Fig. 6a. G (open circle) = default model; GC (closed circles) = modified model with the compensation point consideration.