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ESTIMATE PARAMETERS OF MICROCLIMATE AND AIR POLLUTION
DEPOSITION VELOCITY MODELS

by

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ABSTRACT

A method is described for estimating flux densities and deposition of gaseous pollutants for a period of a year or more, using data collected for a period of a few days. The estimates are based on models which characterize the transfer of gases from the atmosphere to the vegetation as a series of resistances. Linear statistical submodels based on experimental data are then used to relate the resistances to the surrounding environment. The models are shown to fit the experimental data reasonably well. Annual values calculated for a young loblolly pine plantation were evaporation 63.2 cm, carbon dioxide exchange 10.5 t/ha, and sulfur dioxide exchange 1.20 kg/ha.

INTRODUCTION

Most forest micrometeorological research is focused on short-term measurements, taken in a limited area, with the goal of understanding the processes which control the exchange of energy and matter between the forest and the atmosphere. On the other hand, many important scientific and technological environmental problems require information over long time periods. An example of this is the acid rain problem, where a knowledge of the dry deposition of sulfur compounds to forests is important in determining the relative role of dry deposition in the acidification of aquatic systems. The period of deposition of interest is on the order of years while most micrometeorological estimates of dry deposition are based on a few selected days of data. Models of long term deposition, using parameters derived from the shorter term measurements, have been used to construct longer term estimates of sulfur deposition (Sheih et al. 1979).

The models used for integration of the experimental data from forests are of many forms including time series models, completely empirical statistical models, and system models built

on submodels of the processes controlling the energy or material exchange. Each of these models have strengths and weaknesses for developing predictions. The time series model requires little knowledge about the internal workings of the system, however, it requires a long, continuous series of data for analysis (Ford and Milne 1981). The empirical statistical model does not require specific information about the underlying processes driving the system, but best results are obtained when enough is known to pick appropriate empirical relationships for statistical fitting. The strength of the systems approach is that information gained from experiments on parts of the system and from theoretical relationships can be included in the model. However, in many cases the submodels of the system are complex and have a number of site specific constants which must be evaluated. This leads to a very large number of constants for the entire model. In many cases the work involved in independently determining the constants of a system model by experiments is more than can be realistically accomplished. The number of constants also is too large to obtain meaningful values by fitting input/output data from less complete experiments. The model described in this paper is a systems model which includes empirical relationships in its submodels. The purpose of this approach is to construct a model that incorporates our knowledge of atmospheric science and vegetation physiology, but has a limited number of system constants to be evaluated.

The process of developing a model of this type has two steps: 1) defining the model and the unknown parameters of the model and 2) determining values of the parameters. The model described in this paper has been developed from the "big leaf" model of gas exchange. The model is a great simplification of the energy and gas exchange of the forest in that it simulates the forest as a single leaf with the average energy and gas exchange properties of all the leaves in the canopy. Gas exchange is modeled as driven by the concentration gradient of the particular gas which is limited by a series of resistances in the diffusion path. In this form the processes of turbulent transport from the atmosphere, through the canopy, to the leaf surface are characterized as a single aerodynamic resistance. Diffusion into the leaf is limited by a canopy resistance which is, largely, an integrated stomatal resistance. The sink or source strength for the gas in the leaf is treated as an apparent internal resistance to a zero sink concentration (Waggoner 1969) or through a submodel of the physiological processes.

The submodels of the big leaf model must provide estimates of the diffusion resistances and the sink or source strengths. The submodels in the model presented here are linear equations relating the resistances to measured environmental parameters.

The values of the linear coefficients are determined by multiple linear regression on data sets collected at the site of interest. In the cases presented here, the resistance values and the fluxes which were used to determine sink or source strength were calculated from energy balance flux-gradient measurements. However, the model is not constrained to use data from this type of measurement.

THE "BIG LEAF" MODEL

While the origins of the "big leaf" model of canopy energy and mass exchange can be traced to the earlier work of Penman (1948) and Raschke (1956), the model was first explicitly formulated by Monteith (1965). The "big leaf" model has been used extensively as a tool for understanding the characteristics of vegetation influencing exchange with the atmosphere (Stewart and Thom 1973, Thom 1975, Jarvis et al. 1976). The basic equation of the "big leaf" model is:

$$F = (s C_a - C_l) / [s (r_a + r_c) + r_x] \quad (1)$$

The gas (or energy) flux (F) of interest is assumed to be proportional to the gradient between the concentration of gas at some measured reference height external to the canopy (C_a) and the sink or source concentration inside the leaf (C_l). The flux is limited by a series of resistances which include the aerodynamic resistance (r_a), the canopy resistance (r_c), and the internal resistance (r_x). The solubility of the gas (s) is included because the sink inside the leaf is in the water filled cells.

Monteith used Equation (1) to describe water and sensible heat exchange in the canopy energy balance equation. In this case, the internal resistance is negligible and the concentration gradients are vapor density for water and sensible heat content for heat transfer. For other gases, such as carbon dioxide, sulfur dioxide or hydrogen fluoride, the effects of the sinks or sources in the leaves commonly are taken into account by defining the internal resistance as a virtual resistance to a zero sink ($C_l = 0$) or determining a relationship between the environment and the sink or source strength. Both formulations have been used successfully to predict net carbon dioxide exchange (Waggoner 1969, Sinclair 1976). For the zero sink case, the inverse of the sum of the resistances is equal to the deposition velocity (v_d) commonly used in atmospheric, pollution dispersion models.

$$v_d = C_a / F = 1 / (r_a + r_c + r_x/s) \quad (2)$$

Stewart and Thom (1973) showed how the big leaf model could

be a powerful means of interpreting data gathered by the energy balance/gradient method. They showed that the canopy resistance could be calculated from this data using the equation

$$r_c = [(d / g) B - 1] r_a + (B + 1) r_i \quad (3)$$

where B is the Bowen ratio, g is the psychrometric constant, and d the first derivative of the vapor pressure with respect to temperature. The climatological resistance (r_i) is defined as the resistance calculated as if all the heat load (H) on the canopy was used to evaporate water

$$r_i = q c_p de / (g H) \quad (4)$$

where q is the density of air, c_p the specific heat of air and de the vapor pressure deficit. The aerodynamic resistance can be calculated from the wind profile above the canopy as

$$r_a = u / u_*^2 + a u_* \quad (5)$$

where the wind speed (u) is measured at the reference height and the friction velocity (u_*) is found from the slope of the wind speed against the logarithm of height. The constant, a, has been found to be about 0.01 (Thom 1975).

Assuming that the aerodynamic resistance is known from the wind profile and the canopy resistance, and flux of the gas is known from the energy balance/water flux calculation, the internal resistance can be found from Equation (2)

$$r_x = (F / C_a) - r_a - r_c \quad (6)$$

The value of r_a will vary for different gases because the diffusion of gas into the leaf through the stoma is molecular. The variation is inversely proportional to the ratio of the molecular weight of the gases.

The above equations provide a means of determining the resistances to the diffusion of gases from the atmosphere to the canopy from very precise environmental measurements. The ability to predict gas exchange for periods other than those used in the experiments depends on the development of relationships which predict the resistances from routinely measured environmental data.

ESTIMATION OF RESISTANCES FROM CLIMATOLOGICAL DATA

Models can be developed for the resistances on the basis of theory and/or experiments which describe the functional

components of the resistances, by developing a lower order of models in the hierarchy of submodels. In the case of the aerodynamic resistance, this is the logical choice since an adequate model requires only the determination of roughness length and displacement height of the vegetation. These parameters are normally estimated in the procedure for determining the resistances experimentally.

However, as pointed out previously, the problem is that this approach often leads to a model that is too complex to be easily evaluated or used for prediction. The successful application of linear equations and standard statistical techniques to evaluate the coefficients depends on understanding enough about the mechanisms which control the resistances to choose the correct set of independent variables. It is also usually necessary to know enough about the form of the relationships to perform correct transformations on the data where necessary. Murphy et al. (1981) found that canopy resistance could be predicted from measured values of air temperature (T) and vapor density, and solar radiation (S). They found that the effect of seasonal changes in leaf area could be taken into account by multiplying the canopy resistance by the leaf area index to get an average leaf resistance. Leaf conductance (h_l), the reciprocal of leaf resistance was found to be linearly related to solar radiation. The relationship between leaf conductance and solar radiation was further strengthened by computing the average solar radiation incident on the leaves in the stand ($\bar{S}$).

The fit of the linear regression could be further improved by scaling the leaf conductance by the maximum (h_{mx}) and minimum (h_{mn}) conductances determined by leaf chamber experiments. Canopy resistance determined by the Bowen ratio method is most accurate at high fluxes when the resistances are small. The scaling forces the regression to predict reasonable values of conductance in the range of values where experimental error is highest.

The choice of temperature (T) and vapor density deficit as other parameters of the model was based on published observations that these variables affected leaf conductance (Gresham 1975, Lange et al. 1971). We were surprised that various measures of soil moisture did not correlate well with the leaf conductance. It may be that we have not had low enough soil moistures in our humid climate to produce this response or that the response to vapor pressure deficit decreases evaporation on days when the soil moisture is low and stress would be high. Closure due to vapor density deficit, in anticipation of high evaporative demand would avoid moisture stress throughout the entire tree.

The final form of the regression is

$$(h_1 - h_{mn})/(h_{mx} - h_{mn}) = a_1 \bar{S} + a_2 T + a_3 dv. \quad (7)$$

Similar equations can be used to estimate the internal resistances for specific gases. The success will depend on the ability to perform the proper transformations on the data.

RESULTS

Determination of Resistance

The results discussed in this section are based on a data set collected in the summer and fall of 1980 in a loblolly pine stand on the Savannah River Plant near Aiken, South Carolina. The data include energy balance and water balance data. The data are available as a Du Pont report to the Department of Energy (Murphy 1982). The full results will be published elsewhere at a later date. In this paper we will focus on the analysis of the data for use in predictive models.

The data set was used to calculate aerodynamic and stomatal resistance as described in Equations 3 to 5. Multiple linear regression procedures (SAS 1979) were used to fit scaled, leaf conductance as described above. The independent variables selected were solar radiation, temperature, water vapor density deficit, soil water tension, and carbon dioxide concentration in the air. The resulting coefficients are shown in Table 1. All of the variables were statistically significant at the 0.99 level except carbon dioxide concentration. However, soil water tension was positively correlated with conductance which was not expected. A closer look at the results reveals that the addition of soil water tension to the regression makes only a very small change in the squared regression coefficient (0.724 for the three parameter model versus 0.743 for the four parameter model), and thus, on the predictive capability of the model. Therefore, the three parameter model was judged to be the best model.

TABLE 1. Coefficients of linear models for leaf conductance (equation 7 and 8) and carbon dioxide exchange (equation 9) of a loblolly pine forest.

Parameter/ Equation	Vapor Density Deficit (dr) kg/m ³	Solar Radiation (S) mW/m ²	Temp (T) °C	S x dr	S x T	$h_1 \times T R^2$ m/s
(7)	-.03122	.0004340	.01397			.739
(8)		.0006120		-.00006323	.00002265	.755
(9)		3.992 x 10 ⁻⁶				.8143 .893

The form of this model can predict a leaf conductance lower than the specified minimum value if solar radiation is low and the vapor density deficit is high. This is not usually a problem because the vapor deficit is normally low when the solar radiation is low. However, it is reasonable to constrain the model to calculate no values of conductance lower than the minimum conductance when it is used for prediction. This problem can be lessened, but not eliminated by using a model of the form.

$$(h_1 - h_{mn})/(h_{mx} - h_{mn}) = a_1 S + a_2 S dv + a_3 S T. \quad (8)$$

This forces $h_1 = h_{mn}$ at zero solar radiation. The squared regression coefficient for this model is 0.736.

As Jarvis et al. (1976) have pointed out, the modeling of carbon dioxide exchange (net photosynthesis) with the approach outlined above has been difficult. They present a nonlinear empirical model where the independent variables are solar radiation and vapor pressure deficit. It is likely that most of the effect of vapor pressure deficit is an effect on the canopy resistance in the diffusion path for carbon dioxide. Therefore, a model including leaf conductance and solar radiation should apply equally well. The form we used was

$$(P_n + R)/P_{mx} = a_1 S + a_2 h_1 T. \quad (9)$$

The respiration of the stand (R) includes both canopy respiration and soil respiration. Daytime respiration was calculated from night measurements of respiration by extrapolating to daytime conditions, assuming a Q_{10} of 2.0 for temperature. The maximum gross respiration is an arbitrarily high value that is not likely to be exceeded ($15 \text{ mgm/m}^2/\text{s}$). The resulting coefficients are found in Table 1. The squared regression coefficient is 0.804. It is surprising that the linear regression fits these data so well when the response of individual needles of loblolly pine is very nonlinear. However, the photosynthetic response of whole canopies to solar radiation may not be as nonlinear as single needles. Even though the photosynthetic capacity of sunlit needles becomes saturated as the solar radiation increases, the shaded needles may not have reached saturation. In this case, the photosynthesis of the entire canopy will continue to increase as radiation intensity increases.

Another gas for which we have measured fluxes and air concentration is sulfur dioxide. These data indicate that, for the conditions under which the measurements were made, i.e., low sulfur dioxide concentrations, the internal resistances are low and nearly constant throughout the season. This is the simplest case for making predictions using our model.

Calculation of Seasonal Flux Densities

We have set as our objective the estimation of long-term exchange of gases between the atmosphere and the vegetation. The means of making these estimates is the model developed above. One of the reasons for taking this approach has been to simplify the process of making the estimates. Figure 1 shows the results of simulating the exchanges of water vapor, carbon dioxide, and sulfur dioxide for the loblolly pine plantation.

The model is basically the same as that used above to derive the resistances and their relationship to the environment. There is one important exception, the values of all the parameters in the model were derived from half hour averages of the measured parameters, while the model was run with daily (daytime) averages of the climatological inputs. This may not be reasonable for all types of vegetation or climates, but because the relationships derived for this model are all linear, linear averages should not cause great bias. We have tested for bias in the calculation of

Figure 1. Model estimates of the annual variation in the monthly flux density of water vapor, carbon dioxide and sulfur dioxide for a pine forest.

daily fluxes for the energy balance components of the "big leaf" model. Given the response curves for loblolly pine and meteorological inputs for selected days, we found very small differences in the average flux densities based on hourly inputs and the flux densities based on average daily inputs.

Table 2 shows the results of the integrated flux densities for the year 1980. The evaporation is about 65% of the rainfall which seems reasonable for this vegetation type under the prevailing climatic and soil conditions (this was one of the driest years on record in this region). The carbon dioxide exchange is in line with what one might expect. The sulfur dioxide exchange is somewhat lower than reported in some areas, but this is a function of the relatively low atmospheric concentration of sulfur dioxide in this area.

SUMMARY AND CONCLUSIONS

For the transport of several important gasses between the atmosphere and vegetation, annual flux densities have been estimated from experiments of a few days duration scattered throughout the year. The means of extrapolation between measurement periods has been a model that is a systems model in the sense of having a hierarchy of modeling statements. The lowest level in the hierarchy is a system of linear statistical models. The results appear to be satisfactory, but are yet to be tested by independent means such as water balance estimates of evaporation or growth estimates of carbon exchange.

While this methodology appears to be a means of using short time span data to extrapolate over long periods, it would also be desirable to use this type of model to extrapolate to other stands of vegetation of the same or even other species. Use of the model for other sites, having the same species, is probably possible for water exchange. It is, therefore, also likely to give reasonable estimates of exchange of pollutant gases at air concentrations below the level where the gases begin to affect physiological processes of vegetation. However, the uptake of gases, such as carbon dioxide, which are metabolically active will depend on the physiological activity of the vegetation which

TABLE 2. Model Estimates of the Flux Density of Gaseous Transport for Water Vapor, Carbon dioxide and sulfur Dioxide

<u>Water</u> <u>cm/yr</u>	<u>Carbon Dioxide</u> <u>t/ha/yr.</u>	<u>Sulfur Dioxide</u> <u>gm/ha/yr</u>
63	10.5	1270

depends on factors not taken into account in this model, such as mineral nutrition. While significant steps have been taken in this direction (Luxmoore et al. 1978, Landsberg 1981) it is likely to be some time before we are able to produce wood volume yield tables from these models.

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