Strategies for Micrometeorological Modeling: from Big-Leaf to Large-Eddy Simulation

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Abstract

A review is presented of the range of schemes used to mathematically model the microclimate of vegetation canopies and the exchanges of momentum, heat, water vapor and other scalars between the living tissue of plants and the atmospheric surface layer. In order, are considered bulk expressions which do not take into account distinct strata within the canopy, Eulerian diffusion models employing either parallel and series resistances or eddy diffusivities, higher-order closure schemes, and large-eddy simulation. Differences primarily involve the degree to which aerodynamic characteristics of the air flow through and above vegetation are treated. The simplest models have utility in offering estimates of exchange rates that may be applied to large geographic areas, while the most advanced models are used for more fundamental studies of environmental physics.

Key words: micrometeorology, mathematical models, large-eddy simulation.

1. Introduction

Representations of the exchanges of water vapor and carbon dioxide between green tissue and the surrounding air are essential components in any treatment of transpiration and photosynthesis. While diffusion of gaseous material through stomata and the thin boundary layer of the leaf is primarily molecular, transport through the bulk of the air surrounding the vegetation is turbulent. Mathematical models (representations) of gaseous exchange may generally be classified according to the extent to which they treat the turbulent aspects of the air layers.

So-called big-leaf models and large-eddy simulations are at opposite ends of the spectrum in this regard. The simplest models are often the most useful, and the only option in many cases, but they ignore the extremely complex distribution of sources within a canopy. The Penman-Monteith formula is one of the best known and includes aerodynamic influences through an aerodynamic resistance term. Other early models were also based on an Ohm's law analogy in which different layers of a canopy are linked through aerodynamic resistances. The first attempts at solutions to the basic governing equations involved K-theory (gradient-diffusion) approximations to the turbulent fluxes, despite some fundamental inconsistencies. Such models were followed by second- and higher-order closure, procedures which make predictions of turbulence statistics as well as of mean wind speed, temperature, and gaseous concentrations. Recently, large-eddy simulation (LES) has been applied to canopy air flow. The output is a time dependent, three-dimensional flow field, yielding simulations of the aerodynamics of vegetation at an unprecedented level. This paper is a review of the various Eulerian schemes that have been employed to model the atmospheric environment of plants.

2. Single Leaf Models

Evaluating the exposure of a single leaf to its aerial environment, Raschke (1956) combined the physical principles of energy conservation and molecular and turbulent diffusion.
to formulate a model for heat and water vapor exchange. Neglecting the thermal capacity of
the leaf, the energy balance can be expressed as

\[ R_n = H + \lambda E \]  

(1)

where \( R_n \) is the net radiative flux towards the leaf, \( H \) is sensible heat and \( \lambda E \) is evaporative
flux, both positive when directed away from the leaf surface. Recognizing that the diffusion of
heat and vapor between leaf and air is controlled to a large extent by molecular conduction
within the stomatal cavity and in the viscous layer adhering to the leaf surface, Raschke
expressed sensible and latent energy fluxes in terms of diffusion resistances such that

\[ H = \rho C_p \left( T_i - T_a \right) / r_a \]  

(2)

and

\[ \lambda E = \frac{\rho C_p \left( e_i - e_s \right)}{\gamma \left( r_a + r_s \right)} \]  

(3)

where \( \rho \) is air density, \( C_p \) is specific heat at constant pressure, \( T \) is temperature with the
subscripts referring to that of the leaf and that of the air, \( e \) is vapor pressure, and \( \gamma \) is the
psychrometric constant. The quantities \( r_a \) and \( r_s \) are diffusion resistances, with units of
inverse velocity, between the external leaf surface and the air, and through the stomatal
opening, respectively. Raschke assumed that the air adjacent to the interior cell walls was
saturated such that the vapor pressure \( e_s \) is specified according to the leaf temperature as
\( e_s(T_l) \).

The specification of diffusive exchange in terms of resistances (or their inverse:
conductances) has provided the basis for much of what has followed on the subject of
environmental physiology, and expressions of a format similar to (2) and (3) are in wide use
today.

### 3. Extension to Canopies

The combination of energy balance and aerodynamic principles extends readily to
surfaces covered with vegetation as long as there is sense to the specification of a
representative canopy temperature and bulk diffusion resistances. Based on the well-
established Penman equation (Penman, 1948), which was formulated for evaporation from a
wet surface, Monteith (1965) expressed latent energy flux for a canopy of vegetation in the
following manner:

\[ \lambda E = \frac{\Delta \left( R_n - G \right) + \rho C_p \left[ e_s(T_a) - e(z) \right]}{\Delta + \gamma \left( r_{av} + r_s \right) / r_{ol}} \]  

(4)

where \( \Delta \) is the slope of the saturation vapor pressure curve, \( G \) is heat flux into the soil, \( e(z) \)
is atmospheric vapor pressure at reference height \( z \), and other terms are equivalent to those in
(3) except that separate aerodynamic resistances are included for sensible heat and for water
vapor, and the resistances relate to the vegetation as a community with no consideration for
canopy morphology (hence the term “big-leaf”). Combining energy balance and diffusion
equations in this manner allowed Penman and those who followed to eliminate surface
properties, specifically surface temperature, from the expression. The result was a valuable suite of formulae that have gained widespread acceptance.

4. Gradient-Diffusion Models

Models such as those described so far preclude any consideration of the distinct microclimates of different stands of vegetation, or of the separation of soil surface and layers of canopy as distinct sources or sinks of heat and mass. They also disallow consideration of the influence of atmospheric stability or of advective effects. In answer to this, Philip (1964) applied gradient transfer to the diffusion of air within the canopy space. Gradient transfer draws an analogy to Fick's law of diffusion by which a flux density is expressed as the product of a diffusion coefficient (turbulent or eddy diffusivity) and the gradient of the time average of the quantity of interest as in the following examples:

\[ H = -\rho C_p K_h \frac{dT}{dz} \]  
\[ \lambda E = -\rho \lambda K_w \frac{dq}{dz} \]

where \( H \) and \( \lambda E \) are energy fluxes per unit horizontal area (flux densities), \( q \) is specific humidity, and the overbars signify time averages. Incorporated into conservation equations for heat and water vapor, these expressions have formed the basis of many simulations of the plant-atmosphere interaction. Another early version is represented by the model of Waggoner and Reifsnyder (1968), which was formulated as a layer model using a resistance network to represent aerodynamic transfer. The resistances appearing in such a model are simply the integrals of the reciprocals of the eddy diffusivities through the strata.

Discussing the accuracy of descriptions of diffusive exchange formulated in this manner, Waggoner (1975) suggested that "the greatest shortcoming seems the specification of diffusivity \( K \)" and that "the cure is, of course, a proper understanding of \( K \)". The shortcoming, as we now realize, is that fundamental problems with these formulations are particularly critical in the canopy environment. Turbulent diffusion is not a local phenomenon, yet (5) and (6) employ local gradients, while eddy sizes most important to exchanges with the canopy can be many times larger than scales associated with the distribution of sources and sinks of heat, water vapor, and \( \text{CO}_2 \). One consequence is that the direction of a flux cannot always be determined from the sign of the gradient, as in the case where an open trunk space creates a secondary maximum in the wind speed profile.

Examples of first-order but non-local closure are transilience theory (Stull, 1984) and spectral diffusivity theory (Berkowicz and Prahm, 1979) but neither is in common use in the plant environment, perhaps because information needed to prescribe model coefficients is not easily obtained. Yet another class of model, of a quite different nature, employs Lagrangian techniques in which a large number of "particles" are released numerically, allowed to drift in the downwind direction, and forced to diffuse vertically by a velocity created with an equation containing persistence and random components. The "particles" can represent heat or water vapor released by leaves at different canopy levels. The unique features of Lagrangian models have been used to advantage in the plant environment (e.g., Wilson et al., 1981; Raupach, 1989) but they must be driven by Lagrangian statistics which are rarely available from direct observations and, as a consequence, they will not be discussed further here.
5. Higher-Order Closure

Some of the difficulties with gradient-diffusion are alleviated by further manipulation of the basic conservation equations (for momentum, heat, water vapor, CO₂, etc.) to create equations for the time rate of change of the fluxes themselves. This is a straightforward mathematical procedure which, in itself, does not introduce any new physics into the problem but allows a more direct treatment of the turbulent nature of the flow. As an example, the following two equations represent, in order, the time rate of change of temperature, and the time rate of change of kinematic heat flux.

\[
\frac{\partial \theta}{\partial t} = -\frac{\partial w' \theta'}{\partial z} + Q_h \tag{7}
\]

\[
\frac{\partial w' \theta'}{\partial t} = -w^2 \frac{\partial \theta}{\partial z} + \frac{g}{\theta} \theta'^2 - \frac{\partial w'^2 \theta'}{\partial z} + \frac{p'}{\rho} \frac{\partial \theta}{\partial z} \tag{8}
\]

Here, \( \theta \) is potential temperature, \( w \) is vertical velocity, \( w' \theta' \) is the vertical kinematic heat flux \((H/\rho C_p)\), \( Q_h \) is source strength for heat input to the air per unit volume from plant material, \( g \) is gravitational acceleration, and \( p' \) is fluctuation in static pressure. Both equations are posed under the assumption of horizontal homogeneity, and both equate to zero under steady state conditions. Molecular diffusion is neglected relative to turbulent diffusion.

Adopting gradient transfer as the closure procedure (first order closure), the kinematic heat flux would be expressed in terms of the gradient of potential temperature, as in (5) and the heat source would be related to the temperature difference between the air and leaves at different levels in the canopy. With second order closure, the heat flux is not parameterized but, rather, additional equations, such as (8), are included. The terms on the right hand side of equation (8) represent processes which act to increase, decrease, or physically move the quantity equal to the kinematic heat flux and are, in order, gradient production, buoyant production, turbulent transport, and return-to-isotropy. This latter term is the primary sink for kinematic heat flux and expresses the rate at which the flow becomes scrambled and vertical velocity and temperature become decorrelated.

Now, to close the equation set, we have to either parameterize the higher order terms that appear on the right or write a set of even higher order equations (one can easily see that this is a never-ending process). Gradient-diffusion has often been selected for the turbulent transport term (Wilson and Shaw, 1977) but others have elected to add a rate equation for this term (Meyers and Paw U, 1987) and close at a higher level. Additional levels of sophistication can be found in the works of Wilson (1988) and others.

While holding many advantages over first-order closure, higher-order techniques are still "local" and, as such, remain deficient in their predictive abilities because they are unable to account for the fact that turbulence scales are generally quite large compared with the scale of the distribution of plant elements.

6. Large-Eddy Simulation

The procedures discussed up to this point have progressed in a manner of increasing detail in the treatment of turbulent diffusion. Accompanying this progression is an unavoidable increase in computational power to obtain solutions to the various equation sets. Nevertheless, the output of the simulations are expressed in terms of time averaged statistical
properties of the air flow. A further considerable increase in computational (though not mathematical) complexity is introduced by a more direct, time-dependent solution to the basic conservation equations. Simulation of all scales of motion present in turbulent atmospheric flows (DNS - Direct Numerical Simulation) is not possible because such flows are generally of very high Reynolds numbers but a suitable compromise is presented by Large-Eddy Simulation (LES).

LES was pioneered by Deardorff (1972) and is now employed extensively in many fields of engineering and environmental fluid dynamics. The compromise of LES is that the largest eddies are resolved by a three-dimensional grid network, while parameterizations are applied only to the smallest scales (SGS - subgrid-scale), which remain unresolved. The grid network is designed such that the resolved scale eddies are responsible for most of the kinetic energy content of the flow, leaving only a small contribution from SGS motions (Figure 1). SGS parameterizations are generally either K-theory or second-order closure.

![Figure 1. Spectral energy content showing resolved and subgrid-scales.](image)

Shaw and Schumann (1992) were first to apply LES to the canopy environment in attempts to reproduce characteristics of the flow through and above a deciduous forest. The code numerically solves the basic conservation equations for momentum and heat with options for additional scalars. For canopy flow, the momentum equation, written in index notation because the flow is three-dimensional, appears in the following manner:

\[
\frac{\partial \bar{u}_i}{\partial t} + u_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} + \frac{g}{T} \bar{\rho} \delta_{ij} + F_i
\]  

(9)

where the canopy drag force is parameterized as \( F_i = -C_d a \bar{V} \bar{u}_i \), and \( \bar{V} \) is the scalar wind speed. The overbars used in equation (9) have a different meaning from those in equations (7) and (8). In the latter equations, Reynolds averaged quantities refer to time averages, where the averaging period is long compared to time scales of the turbulence. Single primes in those equations indicate departures from such averages. In (9), an overbar refers to a resolved variable whose value changes from grid point to grid point and from time step to time step.
through the numerical integration. Double primes denote unresolved SGS contributions. In this example, $u_i u_j$ represents an SGS contribution to the turbulent stress, which must be parameterized. Additional equations are written to describe scalar quantities such as temperature and humidity. They will include also terms representing SGS fluxes.

Shaw and Schumann (1992) chose to model SGS terms using a second-order scheme but more recent work (Patton et al., 1994; Cho et al., 1995) has used gradient-diffusion theory based on code originally designed by Moeng (1984). In order to provide sufficient resolution of the major aspects of the canopy, the computational domain has been restricted to only a few canopy heights. For example, Patton et al. (1994) adopted a 96x96x30 (x,y,z) grid system with the lowest 10 grid points being used to represent the canopy layer. Future simulations are planned in which a high resolution surface layer is nested within a coarser grid network encompassing a deeper atmospheric boundary layer. Lateral boundaries to the domain are necessarily periodic.

LES output is a three-dimensional, time-dependent flow and scalar field, and simulations are computationally demanding to the point where codes are generally run on supercomputers. The results are unique in reproducing the turbulent flow field and its interactions with a layer of vegetation. An example is presented in Figure 2, which shows an x,z slice of the resolved scale streamwise velocity within and above a forest at a single time step during the simulation by Shaw and Schumann (1992).

![Figure 2. Instantaneous streamwise velocity over an x,z slice. Horizontal line indicates the top of the canopy.](image)

It is expected that simulations will capture the large coherent eddies that are characteristic of the surface layer in contact with plant canopies (Gao et al., 1989). The aerodynamic aspects can be coupled to heat and mass exchange under the constraint of energy balance (Su et al., 1995), however, at this stage, exchanges between the air and individual leaves are still SGS processes as far as LES is concerned.
7. Discussion

There exists a wide range of possibilities for mathematically representing the links between plants or their components and the atmosphere to which they are exposed. The overall governing principles that determine canopy microclimates and heat and mass exchange are basic conservation laws for thermodynamic energy, momentum, and mass. Within a framework based on these principles, this review has discussed various methodologies that have been employed to represent mathematically the turbulent diffusion of heat, mass, and momentum between a vegetation canopy and the lowest layers of the atmosphere.

The simplest strategies have employed resistance networks to express the diffusing power of the atmosphere, either in bulk fashion, as in the Penman-Monteith equation, or within a series of strata. The governing aerodynamic equations are non-linear and must be closed in appropriate fashion. The most common scheme is K-theory but fundamental problems limit its applicability for the canopy environment. Higher-order closure provides some answers and, presumably, greater accuracy in reproducing flow and scalar statistics but closure is still local, and fundamental characteristics of the penetration of large eddies into the canopy are excluded from possibility. Large-eddy simulation is the closest to reproducing, from fundamental conservation principles, the turbulent properties of the air flow because only the small, unresolved scales need to be modeled. There is strong evidence that such scales have little impact on diffusion processes. Due to its great computational expense and consequent limitations in domain size, LES of the canopy currently suffers from unrealistic boundary conditions. Regardless of this, the technique is likely to become a valuable tool in studies of the plant environment.

While this review has ordered modeling strategies from the conceptually simplest to the most exacting numerically, there is no implication that any one level of representation of aerodynamic exchange is correct for all situations. Indeed, the cost of large-eddy simulation is prohibitive and LES, or other turbulence models, serve no purpose when limitations to accuracy in expressing exchange rates are determined by physiological rather than physical processes. Choice of modeling scheme is to be determined with the specific purpose in mind.

References


