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Chapter 1 - Outline of Model Structure (Bare Soil Component)

1.1 Introductory Comments

In this chapter a detailed description of the model will be given, specifically that for the bare soil component of the model. The model, now called Simsphere, deals with both the bare soil and vegetation components separately but then blends the fluxes from each at the top of the vegetation layer, weighted by the fractional vegetation cover. Strictly speaking, the vegetation component also takes account of the bare soil, but only that beneath the vegetation canopy, where the fluxes from that soil are mixed with those from the vegetation and then allowed to flow above the conopy where it is blended with the bare soil component. In this chapter, only the fluxes from the bare soil to the surface layer are unique to this chapter. The following equations governing the fluxes below the surface of the earth, within the surface layer defined as the layer governed by the Monin-Obukhov scaling theory (nominally up to 50 m), and those fluxes above the surface layer as well as those fluxes during the night time regime, apply to both the vegetation and bare soil components.

This chapter will include the sets of equations used, as well as the various micro-meteorological and numerical techniques employed in their solution. Appropriate references will be cited at various points in the discussion and these we hope, will help the reader understand the rationale of employing certain methods to solve specific parts of the model equations. However, in certain areas a more complete derivation or description will be given. This is done primarily when it is envisaged that a reference may be difficult to obtain or if the equation cited in the model formulation is difficult to relate to its counterpart in a text. The discussion though is structured in such a way that the reader may by-pass any lengthy discussion and still maintain an overall understanding of the model design.

1.2 Introduction

The purpose of the model is to predict changes in various meteorological variables, for example, substrate temperature, atmospheric temperature, wind speed and moisture; as a function of time. In order to accomplish this in the atmospheric surface layer and in the substrate, the underlying constraint in the model is taken as the balance between all the energy fluxes at the earth's surface, as expressed by equation [1]. Each term in this equation can be broken down further into constituent parts, the various equations listed below, and form a complete set which can be solved to obtain the variables T L_eE_o H_o G_o and T_{-1} (respectively, the temperature, evaporative flux, sensible heat flux, ground heat flux and the temperature at the first substrate level) ; given the measured temperature, specific humidity and wind speed at two levels. Note that the flux equations for H_o and L_eE_o are presented using the resistance notation as presented by Monteith (1975).

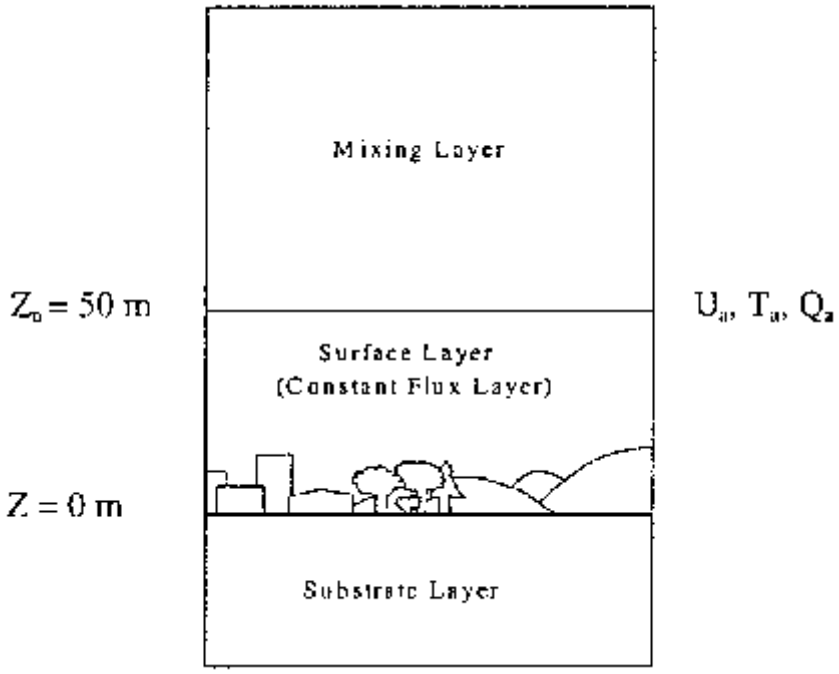

Figure 1

1.3 Model Structure

The structure of the bare soil component of the model consists of four layers:

1. Substrate layer Z_b - Z_φ
2. Transition layer Z_φ - Z_o
3. Surface layer Z_o - Z_a
4. Mixing layer Z_a - Hgt

The substrate layer varies in depth according to the user's choice of thermal inertia. It is usually between 1.5 and 3 metres and is assumed to have homogeneous thermal properties. There are, however, two water layers in the substrate. In the atmosphere, the shallow transition layer is viewed as a layer that contains many surface obstacles. Across this layer there is a variation between purely turbulent and purely molecular flow where radiation, conduction and turbulent transfer coexist in some fashion across which, diffusive fluxes at the interface are passed to the surface layer. When the vegetation component operates, the transition layer is replaced by the vegetation canopy. The surface layer or turbulent air layer extends from the top of the transition layer to a height of 50 metres. Fluxes of heat and water vapour are taken to be constant with height in the surface layer. Laws governing classical similarity theory apply in this layer. Finally a mixing layer is considered above the surface layer and its height depends on forcing from below, specifically the amount of sensible heat passed from the surface layer. Details of the physics in these layers are expanded upon below.

1.4 Model Components

If we begin by discussing Eq [1], the net available radiant energy (R_n) is seen to consist of three components; the absorbed solar flux at the ground (R_s), the downward longwave flux (Rd), and the outgoing longwave flux (Ru). These in turn are balanced by

the upward flux of sensible heat (H_o) and latent heat (L_eE_o) into the atmosphere and the flux of sensible heat into the ground (G_o).

$$Rn = Rs + Rd - Ru = Ho + LeEo + Go \qquad (1)$$

1.5 Solar Radiation Calculation

Initial forcing of the model then begins with the calculation of the solar radiation, ie, the R_s term of Eq [1] This is done using a simple one-layer radiative transfer model where the total down-welling irradiance absorbed in the substrate layer is given in terms of solar geometry, atmospheric transmission coefficients and the albedo for any particular time, day, month, year, latitude and longitude. The equation is of the form

$$R_s = S^* \frac{(1 - A)}{(1 - XA)} \qquad (2a)$$

and is analogous to Eq [2a].

where

R_s = Irradiance absorbed in the substrate layer.

S^* = Transmission function. This contains the solar constant (adjusted for solar distance) and products of various atmospheric transmission coefficients.

A = A weighted albedo.

X = A correction factor which accounts for the summations of internal reflections in the atmosphere.

The transmission function S^* is calculated as follows:

$$S^* = S_o T_a T_s + [S_k T_a (1 - T_s) (1 - T_b)] Sin(\alpha) \qquad (2b)$$

where S_o is the solar flux on a horizontal plane, modified for solar distance with no intervening atmosphere; T_a , T_s , T_b are transmission coefficients for absorption, scattering and back-scattering, S_k is the Solar constant and α the elevation angle.

Elevation angle (α) is a function of declination, local time and latitude and is programmed into the model along the lines of the steps outlined in Wolf (1972). Careful inspection of the curve of the Solar Declination (δ) and time of meridional passage (M) verses time of the year will reveal that there is a slight asymmetry due to the ellipticity of the earth's orbit.

This can be accounted for by the equation

$$d = \frac{[Number\ of\ days\ in\ year - 1]\ x\ 360}{365.242} \qquad (2c)$$

where d is the angular fraction of a year represented by a particular date and by substituting this into the equation

$$\sigma = C_1 + C_2 Sin(d) - C_3 Cos(d) + C_4 Sin(2d) - C_5 Cos(2d) \quad (2d)$$

the correction to the declination caused by the ellipticity of the earth's orbit can be obtained. The declination is then given by

$$D = Arcsin [(Sin23°26'37.8) Sin\ \sigma] \qquad (2e)$$

The next step involves the calculation of true solar noon,

$$M(hr) = 12 + C_1 \, Sin(d) - C_2 \, Cos(d) + C_3 \, Sin(2d) + C_4 \, Cos(2d) \quad (2f)$$

and finally the solar hour angle h, a measure of the longitudinal distance to the sun from which the calculation is being made -

$$h \, (deg) = (T - M) - L \quad (2g)$$

where T is the time in GMT and L is the longitude.

We now have the required information to calculate the solar elevation angle as -

$$\alpha = Sin^{-1} \, [\, Sin \, \varphi \;\; Sin \, D + Cos \, \varphi \;\; Cos \, D \;\; Cos \, h \,] \quad (2h)$$

We are also at the stage where we can calculate S_o, the amount of solar flux striking the earth with no intervening atmosphere

$$S_o = \frac{S_k \, [\, Sin \, d \, Sin \, \varphi + \, Cos \, D + Cos \, \varphi + Cos \, h \,]}{S} \quad (2i)$$

where S is the solar distance factor.

1.5.1 Transmission Coefficients

The transmission coefficients (T_a, T_s, T_b) are no longer calculated as described by Augustine (1981) but instead, are selected from a look-up table (derived from the transmission equations), which contains solar spectrum entries for all the transmission coefficients. The model selects the appropriate transmission coefficients on the basis of the amount of precipitable water contained in the atmosphere. Primarily, the value of the precipitable water is used to calculate the appropriate transmission coefficients for absorption, both by solar and thermal radiation, and is based on a linear interpolation of

the precipitable water content. The relevant values for scattering and back-scattering are also taken at this stage. Once the appropriate values are taken from the table the actual values for the transmission coefficients have to be calculated for the path length for that particular time, day and month. This has to be done for both direct and diffuse solar radiation.

1.5.2 Direct Radiation

For direct radiation the path length is calculated on the basis of the declination angle taking the curvature of the earth into account and is expressed by the following equation.

$$PATH = \left(\frac{C_1}{(\alpha + C_2)^{C_3} + Sin\ \alpha} \right)^{-1} \qquad (2j)$$

where C_1, C_2 and C_3 are constants.

1.5.3 Diffuse Radiation

For diffuse radiation, the path length is set equal to 1.7, the so called diffuse path approximation. Given the values for PATH, the model calculates the transmission coefficients using scaling factors to interpolate between two successive path lengths in the table and another factor takes the depth of the atmosphere into account.

1.6 Sloping Terrain

Terrain slope and the azimuth of the slope are calculated from a knowledge of the heights of the corners of a grid square. Heights of the corner points and the trid spacing are read in the data file. The units should be identical for both height and grid spacing but

they can be specified in any units (e.g. meters) because slope and azimuth are independent of the units since only angles are actually computed in the code. Grid spacing is arbitrary. It does not refer to a real grid but is specified only to compute the relevant angles. The five numbers specified in the data are grid size and the heights of the four corner points, ZNW (upper left hand point), ZNE upper right hand point, ZSW (lower left hand point) and ZSE (lower right hand point). Slope and azimuth refer to the mean slope and azimuth of the grid square. Thus, if ZNW and ZSE are specified as 10 and ZNE and ZSW are specified as zero, the mean slope will be zero, although the terrain clearly has a valley running through it. If the grid size is entered as zero, the computation of slope azimuth and elevation performed in subroutine slope.for is bypassed and the terrain is considered to be horizontal.

It should be noted that the imposition of a non-zero slope will ultimately affect the surface turbulent energy fluxes which are specified in terms of Watts per unit of ground surface. Thus a vertical wall facing the sun will have a solar flux (and a sensible heat flux) per unit area of the wall surface even though the wall's projected area on on the horizontal surface is infinitely small. One would conclude from that argument that the real flux of surface sensible heat per unit horizontal surface area would be infinite, which is clearly an absurd result. In practice, one would need to consider the part of the horizontal surface shadowed by the vertical wall surface and to add the diffuse flux reaching the shadowed surface to the flux on the wall surface in order to compute the total flux of sunlight per unit surface horizontal area. The user is therefore advised to ponder such problems, as might arise in applying the model to steeply sloped terrain.

1.7 Long Wave Flux Determination

The conventional longwave radiation equations are used where σ is the Boltzman constant, T_a the near-surface air temperature, ε_g the emissivity of the ground (usually taken as 1.0), and ε_a, the emissivity of the atmosphere is calculated from a formula

suggested by Monteith (1961), in which thermal back radiation is represented as a function of the total precipitable water in an atmospheric column.

1.8 Albedo

Finally, all that is required now to complete the solution of R_s is the albedo. The model uses two albedos which can be either supplied or calculated. For the purposes of calculation, bare soil albedo is based upon the water content in the surface layer, increasing with decreasing soil water content, and is a modification of the form proposed by Deardorff (1978). For vegetation, it is based on the solar elevation angle, increasing with increasing solar elevation angle and is designed to fit the results as presented by Rauner (1976).

1.9 Net Radiation

At this stage then the net radiation can be evaluated as

$$R_n = R_s + R_L - R_l \qquad (3)$$

1.10 Cloud Cover

Normally, the model functions as if the sky were clear. This is because the original use of this model was in conjunction with satellite infrared surface temperature measurements, which could be obtained only when the sky was essentially free of cloud. The model does permit one to scale the solar and incoming long wave radiant energy by a certain amount so as to simulate the possible effects of cloud. Cloud is introduced as an initial parameter which varies from zero (clear sky case) to 10 tenths. Any relationship between real cloud and the actual attenuation of the radiant fluxes is purely accidental, however. A cloud

cover of ten tenths might reduce the solar fluxes by any amount from 20% to 80%, depending on the cloud type, thickness and altitude. The purpose of this cloud scaling parameter is simply to observe what happens to the surface energy fluxes and the temperature, humidity and wind speeds when the radiant forcing is reduced. If an actual air temperature measurement is available the user might wish to vary the cloud fraction until the measured and simulated air temperatures agree. In this way, one might find the correct cloud attenuation by trial and error and then proceed to examine the corresponding effects of this reduced solar forcing on the surface energy fluxes and other variables in the output.

In the latest version of the model, cloud cover is approximated very crudely by allowing the cover to vary from 0 to 100%. Even at 100%, however, some radiation is allowed to reach the ground, as is realistic for even a 100% cloud cover. The purpose of this function is merely to examine the effects of reduced net and solar radiation on the plant function.

1.11 Transition and Surface Layers

Next we have to consider the terms H_o and L_eE_o, Eq's [5a, 5b, 5c] in the energy balance equation (5a); where $(T_o - T_a)$ and $(q_{os}(T_o) - q_a)$ respectively refer to the vertical temperature between the effective surface and the top of the surface layer and specific humidity difference between a saturated surface at temperature T_o and the top of the surface layer. As previously mentioned these equations are given using the resistance notation of Monteith.

These resistance terms are calculated by integrating the generalized height-dependent resistance from the ground to the top of the surface layer. For momentum this resistance is R_m. The equation takes the form of the classical (Monin- Obukov) logarithmic integral (with a correction for the static stability, Panofsky, 1974) and is based on solutions presented by Paulson (1970) and Benoit (1977) as shown in Equations 4. The

lower boundary is not the ground but the roughness length. For heat and water vapour this resistance is subdivided into two components, referred to R_a and R_b ,R_a , whose form is shown in Equation 6b, extends from the roughness for momentum to the top of the surface layer and is, in all respects identical to that of momentum with the exclusion that the static stability correction pertains to heat flux. R_b , which represents a transition layer that includes molecular and turbulent exchange, extends from the roughness length for heat to that of momentum; this resistance is given in Equations (4). Note that this resistance depends both on the friction velocity and on the molecular conductivity. Justification for the use of molecular conductivities in this context is discussed by Garratt and Hicks (1973). This is often referred to as extra resistance. The resistance for water vapour flux between the roughness length and the top of the surface layer is identical to that for heat, but the resistance in the layer below pertain to a segment extending from the roughness length of water vapour to that for momentum. Note that appropriate molecular conductivity in the expression, Equation 4l is that for water vapour in air. Note also that this transition layer applies only to the bare soil component. As will be shown in the vegetation component, the solution takes both the bare soil component, specified as a fraction, and the remaining vegetation component and solves for them separately, blending the fluxes together at the top of the vegetation canopy.

For vegetation, the resistances between the surface of the vegetation and the reference level are subdivided differently than for bare soil. For momentum, the form of the equation and the limits are identical to that for R_a . For heat and water vapour the upper layer extends from a reference level, somewhat above the vegetation top of the surface layer. The integrals for determining these are similar to those of R_a where the friction velocity, roughness height for momentum and static stability corrections are used. The lower layer extends from the inter-leaf air space to the reference level. The resistance in this lower layer is calculated from a knowledge of the friction velocity and the amount of vegetation as given by the leaf area index.

Developing this topic further we consider neutral, unstable and stable stability profiles in the surface layer:

1.11.1 Neutral Solution

First we begin by considering the neutral case where u*, the friction velocity is derived using the well-known logarithmic wind profile:

$$u^* = k\,u\,\left(ln\,\frac{z_a}{z_o}\right)^{-1} \qquad (4a)$$

where k is the Kármán constant and u the wind-speed at 5O metres.

The resistance term is given by

$$R_a = ln\left(\frac{z_a}{z_o}\right)\,[\,ku^*]^{-1} \qquad (4b)$$

1.11.2 Unstable Solution

An unstable surface layer is somewhat different from the neutral case because the turbulent structure is affected by the presence of a heat flux. To account for this similarity theory is applied to obtain semi-empirical relations for the non-dimensional temperature gradient Φ_m and the dimensionless wind shear Φ_h as discussed in Panofsky (1974). However, since we use the integrated form of Φ_m and Φ_h the following definitions have been made as detailed in Nickerson (1979).

$$\xi_m = \left(\frac{1\ -\ 15\ z_{a;o}}{L}\right)^{\frac{1}{4}} \qquad (4c)$$

and

$$\xi_h = \left(\frac{1 - 9\, z_{a:o}}{L} \right)^{\frac{1}{2}} \qquad (4d)$$

where subscripts a,o respectively, refer to the top of the surface layer and the limits of the roughness height.

The stability functions for momentum and heat based on the solutions presented by Benoit are then

$$- \psi_m = ln \left(\frac{(\zeta_{mo}^2 + 1)\,(\zeta_{mo}^2 + 1)^2}{(\zeta_{ma}^2 + 1)\,(\zeta_{ma}^2 + 1)^2} \right) + 2 \left[Tan^{-1}\, \zeta_{ma} - Tan^{-1}\, \zeta_{mo} \right] \qquad (4e)$$

$$- \psi_h = 2\, ln \left(\frac{(1 + \zeta_{ho})}{(1 + \zeta_{ha})} \right) \qquad (4f)$$

These stability functions are then used to determine u* and the resistance term as follows:

$$u^* = ku \left[\ln\left(\frac{z_a}{z_o} \right) - \psi_m \right]^{-1} \qquad (4g)$$

$$R_a = \frac{0.74}{ku^*} \ln\left(\frac{z_a}{z_o} \right) - \psi_m \qquad (4h)$$

1.11.3 Stable Solution

In stable air, all measurements suggest

$$\Phi_m = 1 + 5 \frac{Z}{L} \qquad (4i)$$

Hence, ψ_m takes the simple form

$$\psi_h = \psi_m = -5\frac{Z}{L} \qquad (4j)$$

So the resistance term becomes

$$R_a = \frac{1}{ku^*}\left(\ln\frac{z_a}{z_o} - \psi_m\right) \qquad (4k)$$

The calculation of ustar will be discussed at a later stage in the night-time formulation.

The resistance terms in the transition layer are obtained as

$$R_{ch,cv} = \frac{ln\,(ku^*z_o + k_{h,v}) - ln\,k_{h,v}}{ku^*} \qquad (4l)$$

1.12 Dual roughness regimes: partial vegetation cover

The model allows for the specification of two roughness lengths in the partial vegetation or bare soil computation modes. This is to allow for a global and a patch-scale logarithmic wind profile, respectively above and below the tops of the surrounding obstacles, which may be trees or buildings. This option is futher explained in the section on partial vegetation cover.

1.13 Surface Moisture Availability

At this point the only term to be accounted for is the surface moisture availability M, . This is defined as $R_b = R_a + R_{cv}$ where R_s is a soil resistance. Generally, M

represents the fraction of potential evaporation at the temperature of the surface (T_o) Under saturated conditions R_s is essentially zero and evaporation is equal to the potential value. For a completely dry surface M is zero.

Moisture availability is a key parameter in the model. Strictly speaking, moisture availability is defined in terms of the soil surface resistance. Therefore, it is defined only in terms of the water content of the soil surface. It is also, by definition, the ratio of evaporation to potential evaporation at the radiometric temperature of the soil surface.

Note that this definition of moisture availability, in terms of the ratio of the atmospheric resistance to the sum of atmospheric and soil resistances indicates that the values of moisture availability will depend upon the values of atmospheric resistance. This dependency is not very strong, however, since the resistances in the numerator and denominator tend to vary throughout the day in a similar fashion. Thus, moisture availability tends to remain relatively constant throughout the day.

Further consideration to the moisture availability will be given later in the substrate and vegetation sections.

1.14 Heat and Evaporative Flux Solutions

We are now at the stage where we can determine the terms L_eE_o and H_o. The evaporative flux is solved directly and then the heat flux, Eq [5b, 5c], is solved by substituting the evaporative flux into equations 5b,c and the energy balance equation [5a] and this leads to an expression which resembles the Penman equation (Tanner and Pelton, 196O). Thus,

$$Rn\text{-}G = Ho + LeEo \qquad (5a)$$

$$LeEo = \rho LeMo\ (q_{os}(T_o) - q_a)/(Ra+Rch,cv) \qquad (5b)$$

where Mo is the moisture availability, defined as the fraction of field capacity in the soil, and Ra is the atmospheric resistance for water vapor or heat.

$$H_o = \frac{R_n - L_e E_o - A}{1 + B\,[R_a + R_{ch}]} \qquad (5c)$$

where

$$A = \frac{\lambda\,(T_a - T_{-1})}{\Delta Z} \quad \text{and} \quad B = \frac{\lambda}{\Delta Z\,\rho\,C_p} \qquad (5d)$$

The temperature at the first substrate level T_{-1} is initially taken from a vertical temperature profile based on a linear interpolation between the initial surface temperature (T_o) and the reservoir temperature (T_b). Thereafter, it is updated by solving a particular form of the diffusion equation; as detailed in the substrate layer discussion.

1.15 The Mixing Layer

It is also possible to obtain a value for T_o at this stage but it's worth mentioning that experiments carried out with this basic model formulation indicated the amplitude and phase lag of the temperature cycle, beyond solar noon, to be an under-estimation. As are result, a mixing layer formulation was embodied as an integral part of the model code. During the day the height of the mixing layer increases as the heat flux from below builds and a corresponding downward flux of heat is set up due to entrainment of unmixed air from above. This results in a higher air temperature than would otherwise be calculated if consideration was only given to a surface source of heat flux.

The mixing layer addition was developed by Tennekes (1973) and later modified by Tennekes (1974) and Zilitinkevich (1974). The Tennekes model essentially calculates the rate of change of potential temperature θ in an isentropic mixing layer of depth h (equivalent to Hgt). The Tennekes method relates the vertical flux convergence in the daytime mixed layer due to the upward fluxes of heat Ho incorporated in the top of the layer by mixing down stable air above Z = h. This method for computing potential

temperature assumes that the mixing layer is perfectly mixed with respect to potential temperature (but not moisture and momentum). Thus, the potential temperature at 50 metres is exactly equal to that everywhere within the mixing layer.

The equation is given below -

$$\left.\frac{\delta\theta}{\delta t}\right|_h = \frac{H_o + H_h}{\rho C_p h} - \delta\theta_r - \delta\theta_a \qquad (6a)$$

H_h is the downward heat flux.

The key issue here is the behaviour of the inversion strength Δ at the top of the boundary layer. This can be expressed mathematically as follows:

$$\frac{d\Delta}{dt} = \frac{\gamma h \frac{dh}{dt} - (\overline{\theta w})_o - \Delta \frac{dh}{dt}}{h} \qquad (6b)$$

This is used to evaluate the downward heat flux following the parameterization developed by Zilitinkevich (1974) -

$$-(\overline{\theta w})_i = C\,(\overline{\theta w})_o \left[1 + C_2 \frac{(\overline{\theta w})_o^{\frac{2}{3}}}{\left(\frac{g}{T_o h}\right)^{\frac{1}{3}} \Delta} \right]^{-1} \qquad (6c)$$

$\theta w_{(i,o)}$ are respectively, downward and upward heat fluxes where $\rho C_p \theta w_o$ ($\cong H_o$) is calculated from the surface layer equations. C and C_2 are constants.

In the process h is allowed to rise at a rate dependent upon $\frac{d\theta}{dt}|_h$, and upon the atmospheric lapse rate γ (= $\frac{d\theta}{dz}$) above z = h. The development of the above equations are shown in Appendix 1.

Within and above the mixing layer, long wave radiation (θ_r) is considered to cool the air at a rate of O.O6°C / hour. To this constant cooling is added the large-scale advective cooling (θ_a). The large-scale advection is based on the thermal wind equation and the vertical distribution of the geostrophic wind and is described in appendix 1. Note that small-scale advections, which occur as the result of horizontal gradients in atmospheric properties, due to spatial variations in the surface heating imposed by variations at the surface, are neglected.

1.16 The Eddy Diffusivities

Momentum and water vapour are calculated differently in the mixing layer than potential temperature. For these quantities, the model computes an arbitrary profile of eddy diffusivity, which has a maximum within the mixing layer, equals zero at the top of the mixing layer and is equal to the Monin-Obukhov eddy diffusivity at the top of the surface layer. The method for calculating these eddy diffusivities is discussed by O'Brien (197O).

In the surface layer we can specify eddy diffusivity at the top of the layer (5O metres) as -

$$K(Z_a) = \frac{ku^* Z_a}{1 + \Phi(Z_a)} \qquad (7a)$$

where $\Phi(z_a)$ is a stability function which is negative for unstable conditions, zero for neutral (adiabatic) conditions and positive for stable conditions. Note that this equation implies the log wind profile for neutral stability.

If we assume that at the gradient wind level (z_{top}), ie at the top of the mixing layer (Hgt), the eddy diffusivity (K) is small then it is possible to set up a parametric relationship, starting at the top of the surface layer and extending to the top of the mixing layer, which accounts for the eddy diffusivities throughout the layer. O'Brien shows that since K must increase monotonically with height in the surface layer, there must be a maximum value for the eddy diffusivity in the mixing layer through which a curve can be found that describes the eddy diffusion throughout the mixing layer. This curve has the form of a cubic polynomial and is given below:

$$K(z) = \left(K_{Ztop} + \frac{(z - z_{Ztop})^2}{\Delta z^2} \right) \left[K(z_a) - K_{Ztop} + (z - z_a) \left(K(z_{á}) + \frac{2K(z_a) - K_{Ztop}}{\Delta z} \right) \right] \quad (7b)$$

where the primed quantity denotes differentiation with respect to z. z is the height at which the diffusivity is being calculated and Δz is the thickness of the mixing layer.

1.17 The Substrate Layer

To complete our discussion of the model structure per se, we consider the substrate layer: The substrate temperature is obtained by integrating a form of the diffusion equation over a number of substrate levels using the leap-frog method with a forward-differencing interval Δt of 3 minutes.

1.17.1 The Substrate Diffusivity

The substrate diffusivity K and the conductivity λ or thermal conductivity, density ρ_g and specific heat C_s (g $C_s = C_g$) of the substrate layer are combined to form a parameter called the thermal inertia P, where

$$P = \lambda K^{½} = \sqrt{\lambda C_g} \quad (8a)$$

This is a measure of the rate of heat transfer at the ground-air interface. As defined here, it can be shown (Lettau in Sellers, 1965) that P is inversely proportional to the amplitude of the first harmonic of the ground heat flux into the soil.

Tests with the model (Carlson and Boland, 1977) showed that the results are fairly insensitive to the exact choices of either λ or K for a given value of P. Thus, thermal inertia appears to be a fundamental measure of the ground conductivity or diffusivity, and can therefore replace both of these difficult to measure parameters. Since both λ and K are used explicitly in the model, a convention for equating them with P is adopted. This proved to be necessary because, although independent variations in λ and K generally yielded identical results for constant values of P when λ or K were assigned extreme values the results were no longer unchanged for the same value of P.

Accordingly, the formula

$$\lambda = -0.00013 + 0.0502\,P + 1.21\,P^2 \qquad (8b)$$

was used as a constraint on the value of λ. This equation was determined by fitting a second-order regression equation through 2O pairs of λ and P values listed in Sellers (1965) and the Manual of Remote Sensing, II (1975). The regression was found to explain 91% of the variance of λ about P in the dependent data sample, providing an empirical result which corresponds to a wide variety of surface materials. In fact, the actual surface may consist of materials which may not represent a truly diffusing or conducting medium, such as a mixture of structures and vegetation - trees, roads, houses, crops, etc.

P can be evaluated by convolution of the model (Chapter 3) and used along with λ to derive K according to the formulation.

$$K = \frac{\lambda^2}{P^2} \qquad (8c)$$

1.17.2 The Diffusion Equation

The transfer of heat through the soil is governed by the diffusion equation. Generally, the vertical profile of temperature in the substrate is such that the greatest change with height occurs near the surface. Thus, the vertical profile of temperature is similar to a logarithmic one. In order to analyze temperature T as a linear function, a logarithmic vertical scale Z is considered. This is accomplished by setting up a scale depth h where

$$h = ln\left(1 + \frac{Z}{\delta}\right) \text{ and } \delta \text{ is a constant.} \quad (9a)$$

$$\text{Let, } x = 1 + \frac{Z}{\delta} \;\therefore\; h = ln\, x \quad (9b)$$

By differentiating these two relationships we obtain

$$\frac{\delta x}{\delta Z} = \frac{1}{\delta} \text{ and } \frac{\delta h}{\delta x} = \frac{1}{x} \quad (9c)$$

When using a scale depth in place of an actual soil depth, the diffusion equation must be derived in terms of h instead of Z. In order to do this we begin with the classical form of the diffusion equation,

$$\frac{\delta T}{\delta t} = K \frac{\delta^2 T}{\delta Z^2} \text{ where T is the temperature and Z the depth.} \quad (9d)$$

Expanding the right hand side:

$$\frac{\delta T}{\delta t} = K \frac{\delta}{\delta Z} \frac{\delta T}{\delta Z} \quad (9e)$$

Now using the fact that

$$\frac{\delta T}{\delta Z} = \frac{\delta T}{\delta h}\frac{\delta h}{\delta Z} \quad \text{and} \quad \frac{\delta h}{\delta Z} = \frac{\delta h}{\delta x}\frac{\delta x}{\delta Z} \tag{9f}$$

Substituting these in the diffusion equation we get,

$$\frac{\delta T}{\delta t} = K\ \frac{\delta}{\delta Z}\frac{\delta T}{\delta h}\frac{\delta h}{\delta x}\frac{\delta x}{\delta Z} = K\ \frac{\delta}{\delta Z}\left[\frac{\delta T}{\delta h}\frac{1}{x}\frac{1}{\delta}\right] \tag{9g}$$

Factoring out $\frac{1}{\delta}$ and expanding the expression again becomes

$$\frac{\delta T}{\delta t} = \frac{K}{\delta}\frac{\delta}{\delta Z}\left[\frac{\delta T}{\delta h}\frac{1}{x}\right] = \frac{K}{\delta}\frac{\delta}{\delta h}\left[\frac{\delta T}{\delta h}\frac{1}{x}\right]\frac{\delta h}{\delta x}\frac{\delta x}{\delta Z} \tag{9h}$$

Again using relationships for $\frac{\delta h}{\delta x}$ & $\frac{\delta x}{\delta Z}$

$$\frac{\delta T}{\delta t} = \frac{K}{\delta^2 x}\left[\frac{\delta}{\delta h}\frac{\delta T}{\delta h}\frac{1}{x}\right] \tag{9i}$$

Differentiation by the chain rule must now be performed as x is a function of h, ie (x = exp h).

So,

$$\frac{\delta T}{\delta t} = \frac{K}{\delta^2 x}\left[\frac{\delta^2 T}{\delta h^2}\frac{1}{x} - \frac{\delta T}{\delta h}\frac{1}{x^2}\frac{\delta x}{\delta h}\right] \tag{9j}$$

and can take the form -

$$\frac{\delta T}{\delta t} = \frac{K}{\delta^2 x}\left[\frac{\delta^2 T}{\delta h^2}\frac{1}{x} - \frac{\delta T\, x}{\delta h\, x^2}\right] \qquad (9k)$$

Factoring out $\frac{1}{x}$ the diffusion equation becomes

$$\frac{\delta T}{\delta t} = \frac{K}{\delta^2 x^2}\left[\frac{\delta^2 T}{\delta h^2} - \frac{\delta T}{\delta h}\right] \qquad (9l)$$

Two aspects of the vertical temperature profile should be considered here. One is a correction, which accounts for a correction to the vertical derivative of temperature in the top layer. Since finite differences are used, the latter will tend to underestimate the temperature gradient at the soil surface. Secondly, as already mentioned, the initial vertical temperature profile is based on a linear interpolation between the initial surface temperature (T_o) and the reservoir temperature (T_b).

1.17.3 Substrate Moisture Content

Finally to conclude the substrate layer we have to consider the soil moisture status. This is based on the force restore treatment of ground soil moisture as described by Deardorff (1978). This uses the evaporative flux L_eE_o in the calculation of two soil moisture variables w_g and w_2 (respectively, the volumetric concentrations of soil moisture at the surface, and that at a depth below which the soil moisture flux is negligible). An intermediate soil moisture layer is also determined but its initial value is not specified but is taken as an average of that for the surface and substrate.

The variables w_g and w_2 are calculated according to the formulations presented by Deardorff, where

$$\delta w_g = - C_1 \frac{E_g}{\rho_w d_1'} - C_2 \left[\frac{w_g - w_2}{\tau_1} \right] \delta t \qquad (10a)$$

and

$$w_2 = \frac{- E_g}{\rho_w d_2'} \Delta t \qquad (10b)$$

t - Time.

τ_1 - Diurnal period.

E_g - Evaporation rate $\cong L_e E_o$ x Latent Heat of Vaporization.

$C_{1,2}$ - Coefficients for ground surface moisture.

$d_{1,2}$ - Soil depth influenced by daily and annual temperature cycles respectively.

The moisture availability M at the surface can then be updated as the ratio between w_g and w_{max} ; the maximum value for the soil moisture content, that is, the runoff value. Moisture availability also constitutes the vital link between the surface layer, the soil moisture resistance and the water content of the soil. The relationship between moisture availability and the soil water content of the surface layer is therefore empirical; that is, it is set equal to the ratio of the water content of the surface layer divided by the field capacity. This empirical relationship seems to be supported by observations, although other models may express the linkage between soil water content and moisture availability differently.

Recent modifications to this part of the model assign a moisture availability to the substrate as represented by $\frac{w_g}{w_{max}}$ This intermediate layer, where the root zone and transition substrate layers reside also dries slowly during the day, although the fraction of field capacity, though initialized as a deep-layer moisture availability, is never used as a

moisture availability and has no meaning as far as the atmospheric resistances are concerned.

In the model, surface moisture availability is allowed to vary somewhat, according to the amount of water in the surface soil layer. Once the initial moisture availability is declared, it will vary only with the change in the water content of the surface soil layer. For bare soil, evaporated water comes only from this surface soil layer. When the vegetation model is employed, evaporation still comes from the surface soil layer, but transpiration is distributed throughout two other soil layers, a deep root zone layer and an intermediate surface-root zone transition layer. Moisture availability is nevertheless defined only in terms of the surface evaporation. Typically, evaporation decreases the surface-layer water content (and moisture availability) by a small amount during the day. At night, water is allowed to percolate up from the deep layer to the surface, allowing the surface layer to moisten slightly between dusk and the next dawn. Moisture availability is otherwise not used at night, when evaporative fluxes are nil.

1.18 The Night-time Formulation

Up until now we have solved the model to obtain the variables T_0, L_eE_0, H_0, G_0, and T_{-1} for conditions that are either near neutral or under free convection. However, we still have to deal with stable conditions which occur predominantly, although not exclusively during nightfall. The discussion then must continue with the so-called night-time regime and therein, the alternative solutions to some of the above variables. It is also worthwhile at this stage to show how the vertical profiles of temperature, humidity and winds are predicted at night and compare their calculation with the daytime method.

During the day, specifically under unstable conditions where $H_o > O$, when there is solar heating of the surface layer the surface layer stability profile is largely determined by the intensity of surface heating and by the constraints of Monin-Obukhov scaling. When the solar flux diminishes to the point where H_o becomes negative, the turbulence represented by the friction velocity u* begins to diminish rapidly. During stable conditions, the temperature profile is strongly affected by the longwave radiational

cooling and by the vertical wind shear near the surface. Heat flux is no longer determined directly by net radiation but becomes passively dependent on the lapse rate. As the surface layer becomes more stable with time, the downward heat flux and u* both tend to vanish or become intermittent.

At night the critical Richardson number formulation of Blackadar (1979) is used to calculate the temperature and wind speed tendencies in the surface layer and turbulent layers with an additional equation for the temperature tendency imposed near the surface. The surface temperature T_o is determined as a quasi-equilibrium value at each time step from the afore-mentioned set of equations. Solutions quickly approach radiative equilibrium after sunset with the vanishing of turbulence, except under windy conditions when turbulent episodes may still occur

1.19 The Blackadar Scheme

In detail then, in the Blackadar scheme, the maintenance of turbulence under nocturnal conditions is governed by a bulk Richardson number (Ri_b) which in the surface layer, is given by

$$Ri_b = \frac{g\, Z_a}{\bar{\theta} w_a^{\,2}} \left((\theta_a - \theta_s) + T^* \ln \frac{Z_a}{Z_1} \right) \qquad (11a)$$

where w_a is the total wind speed at Z_a, Z_1 is at 1 metre, $\bar{\theta}$ is the average temperature in the surface layer, g the gravitational constant and θ_s a 'shelter' height temperature (nominally at 1 metre) which is predicted using the equation.

$$\frac{\delta \theta_s}{\delta t} = a\,(\theta_a - \theta_s) - b \left(\frac{H_o}{\rho C_p Z_a} \right) \qquad (11b)$$

This empirical relationship incorporates two terms on the right hand side. The first term simulates radiation conduction and radiational cooling in the lowest metre. The

second term simulates a temperature change due to turbulent flux itself. At equilibrium the two values cancel, heat flux convergence balancing radiative divergence.

Monin-Obukhov scaling is used to define T* and u* where:

$$T^* = \frac{(\theta_a - \theta_s)}{\ln \frac{Z_a}{Z_1} - \psi_h} \qquad (11c)$$

$$u^* = \frac{k w_a}{\ln \frac{Z_a}{Z_1} - \psi_m} \qquad (11d)$$

$$H_o = - k \rho C_p u^* T^* \qquad (11e)$$

where θ_a and Z_a have their usual meaning for the surface layer. Here, ψ_h and ψ_m are the non-dimensional profiles for temperature and wind, the functional forms of which are dependent upon stability, and k is the von Kármán constant.

There are three stability classifications for which the physics in the surface layer are dissimilar. The distinction is made on the basis of both the bulk and the critical Richardson numbers. These are as follows:

I $Ri_b < O$ Unstable

II $O < Ri_b < Ri_c$ Stable, Turbulent

III $Ri_b > Ri_c$ Stable, Non-turbulent

Note that neutral stability criteria are used if the static stability between 1 and 5O metres is zero or within a small range of zero.

A screen level temperature is calculated at night in a somewhat different manner, unlike the daytime screen temperature which is computed from the logarithmic

temperature profile, it relies upon a time dependent equation. The latter contain two terms, one containing a radiometric flux and the other a sensible heat flux.

1.19.1 Vertical Profiles

The interpolation routine operates once at the end of the daytime heating when the nighttime regime is invoked, to collapse the turbulent layer to the lowest 5OO metres by interpolating between the 250 metre daytime levels.

The vertical profiles of temperature and wind from 5O to 5OO metres are provided through the integration of the u and v momentum equations, and the thermodynamic equation, expressed as

$$\frac{\delta u_i}{\delta t} = f(v_i - u_{gi}) + \frac{k_{mi+1}}{\Delta Z^2}(u_{i+1} - u_i) - \frac{k_{mi}}{\Delta Z^2}(u_i - u_{i-1}) \qquad (12a)$$

$$\frac{\delta \theta_i}{\delta t} = \frac{k_{hi+1}}{\Delta Z^2}(\theta_{i+1} - \theta_i) - \frac{k_{hi}}{\Delta Z^2}(\theta_i - \theta_{i-1}) + \frac{\theta_a - \theta_r}{\Delta t} \qquad (12b)$$

where f is the Coriolis parameter, Z the layer depth in the atmosphere (50 m), $\theta_{r,a}$ are corrections for radiative cooling and advection respectively, and subscript i is the level index which varies from 1 (at $Z = Z_a = 50m$) to 10 (at $Z = 500m$). The v momentum equation is analogous to the u equation. The temperature is analogous to these but for the fact that k_h and k_m differ by a component of radiative mixing, which is included in the former diffusivity. For specific humidity, the equation is analogous to that for temperature except that there is no radiative component in the diffusivity, which is therefore equal to k_h. The lowest 50 metre layer must be treated differently within the context of the logarithmic profile laws which incorporate turbulent exchange through the underlying surface. As such, the lower and upper boundary conditions for these equations are slightly different, taking account of the similarity theory constraints in the surface layer.

Accordingly, the last term in these equations must be replaced by $\frac{-u^{*^2} u_1}{w_a DZ}$ and $\frac{H_o}{C_p r DZ}$ respectfully, which are the surface boundary flux conditions above the mixing or surface layer.

1.19.2 The Night-time Eddy Diffusivities

Except for the radiative mixing effect, the eddy diffusivity coefficients k_h and k_m are assumed to be equal in the stable nocturnal boundary layer and are expressed by the function

$$k_i = \frac{l^2 S_i (Ri_c - R_i)}{R_c} \qquad (12c)$$

which was found by Blackadar (1979) to fit the data of Mellor and Yamada (1974) for second order closure theory where

$$S_i = \frac{\sqrt{(u_i - u_{i-1})^2 + (v_i - v_{i-1})^2}}{\Delta Z} \qquad (12d)$$

and l was arbitrarily chosen at 28 metres in the surface layer. In the layer above the surface, the local Richardson number is calculated as

$$R_i = \frac{\frac{g}{\bar{\theta}} \Delta Z (\theta_i - \theta_{i-1})}{S_i^2} \qquad (12e)$$

while the critical Richardson number (Ri_c) is calculated as a function of the geostrophic wind speed using the empirical result suggested by Blackadar,

$$Ri_c = 0.5542\ exp\ -\ 0.2129\sqrt{u_{gi}^2 + v_{gi}^2} + 0.2 \qquad (12f)$$

where u_{gi} and v_{gi} are the geostrophic wind speed components in metres per second. When the local Richardson number exceeds the critical value, which is typically a little larger than 0.2 , turbulent exchange will cease at that height and k_i in the model is set to zero.

This should be contrasted with the way the model simulates the vertical distributions of wind, temperature and humidity throughout the surface and mixing layers during the day. In the mixing layer, temperature is calculated from the Tennekes (1973) formulation for conditions of free convection during the day. Wind-speed and specific humidity are calculated from the time-dependent momentum equations, including the effects of Coriolis force and vertical mixing, the latter being determined by specifying the vertical distribution of the mixing coefficients in the mixing layer as a function of height (O'Brien, 1970).

As the resistances in equations 5a and 5b become undefined when turbulence ceases, the surface temperature T_o has to be solved directly as an equilibrium solution to the energy balance equation when H_o becomes negative. L_eE_o is calculated using equation 5b until it become negative but the resistances R_a , R_{ch} and R_{cv} are constrained from becoming zero by setting 1.0 centimetres per second as a lower limit for u*.

Solving for T_o in Eq [1] yields the quartic equation -

$$A' T_o^4 + B' T_o + C' = 0 \qquad (12g)$$

where

$A' = \varepsilon_g \sigma$

$B' = \dfrac{\lambda}{\Delta Z}$

$$C' = \frac{\lambda T_{-1}}{\Delta Z} + H_o + L_e E_o - \varepsilon_a \sigma T_a^4 + R_s$$

At each time step, Newton's iteration technique for finding real zeros of a polynomial is used to solve for T_o.

1.20 Initial Conditions

The model requires for execution, a set of initial atmospheric conditions which are provided by radiosonde measurements. The measurements (air-temperature, atmospheric pressure, dewpoint depression, wind speed and wind direction) at each sounding level, are used to calculate sounding heights at each of the pressure levels as read in. It also calculates potential temperature and mixing ratio values and computes their gradients. Wind-speed and wind direction at the sounding levels are converted into their u and v components.

In addition to this, a spline routine, Price and Mac Pherson (1973) is invoked to interpolate the data obtained at the sounding levels to yield, at regular grid intervals, the u and v components of the wind as well as vertical humidity and temperature profiles.

The next stage in the initialization process is to generate vertical profiles of the u and v components of the geostrophic winds, for the initial daytime, as is required for the momentum equations and other formulations used in the model. This can be accomplished by three different methods:

1.20.1 The Thermal Wind

Hess (1959, pg. 191) shows that the thermal wind equations yield geostrophic wind gradients as:

$$\Delta v_i = \frac{\delta v}{\delta Z} = \frac{g}{fT}\left[\frac{\delta T}{\delta x}\right]_o \qquad (13a)$$

and

$$\Delta u_i = \frac{\delta u}{\delta Z} = - \frac{g}{fT} \left[\frac{\delta T}{\delta y} \right]_o \qquad (13b)$$

These expressions have been transformed to obtain an average gradient form.

$$\Delta v_i = \frac{Z_g}{R_d} \bar{T} \frac{\delta T}{\delta x} \frac{R_d}{f} \frac{1}{Z} \qquad (13c)$$

and

$$\Delta u_i = \frac{Z_g}{R_d} \bar{T} \frac{\delta T}{\delta y} \frac{R_d}{f} \frac{1}{Z} \qquad (13d)$$

where $\frac{Z_g}{R_d} \bar{T}$ = Pressure Difference across 4° Latitude which is 0.061875 at $\bar{T}$= 273.2°K.

Δv_i and Δu_i are calculated for the night-time from $\bar{T}$ = 273.2°K and for the daytime from T = T_3 (obtained from the sounding). Z is an arbitrary height which is factored out. The geostrophic wind gradients Δu_i and Δv_i are used to calculate daytime and night-time geostrophic wind profiles at 250 metres and 50 metres steps, respectfully.

1.20.2 Interpolation

As already described, the vertical profile of the observed winds can be broken down into the constituent u and v components at reported wind observations and interpolated (using cubic splines) at regular grid intervals. By examining a vertical plot it

is possible to extrapolate the trend of the geostrophic winds down to the surface to obtain a value for the surface geostrophic u and v components.

Using the geostrophic wind components obtained at the surface for u and v and those obtained from the spline routine at 1050 metres, the model linearly interpolates the geostrophic wind between 50 and 1050 metres. We assume that from 1050 metres on up the winds to be geostrophic.

1.20.3 Default

A default routine is also available in the event that the user is unsure of the surface geostrophic winds or the horizontal temperature gradient. This routine simply lets the geostrophic winds at 1050 m be constant at all levels between 1050 m and the surface. Note that at and above 1050 m, the geostrophic winds are always equated with the real winds. It should be emphasized as a warning to the user that if the actual and geostrophic winds differ greatly, the computed wind speeds may oscillate wildly (and in some cases uncontrollably). Since the real and geostrophic winds are likely to be similar above the first several hundred meters, it is advisable to use the interpolation method, which maintains relative closeness between actual and geostrophic winds. Note that the default case implies no geostrophic temperature advection.

1.21 Additional Comments

The reader's attention should be drawn to the fact that many models take account of a displacement depth. In this model there is no explicit reference to displacement depth. It is understood, however, that all height levels included in the logarithmic profile equations refer to the height above the displacement height. Typically, the displacement height is about 0.65 the depth of a uniform vegetation canopy. The potential temperature is also taken with reference to the displaced height origin, rather than 1000 mb as is customary. Omission of displacement depth should not matter in the results unless one wishes to use actual wind, temperature or moisture measurements for validation of the

results. Since the displacement height is typically only a few tens of centimetres or less, the differences between modelled height and actual height with respect to the ground surface will have little importance except very close to the ground.

As already explained, the atmospheric part of the model operates quite differently during the day and at night. For a smooth transition between day and night certain arbitrary decisions must be made. As a result day and night are defined in terms of the sensible heat flux H_o and in terms of the net radiation R_n or both. For example, if H_o is less than zero it is night, and if greater than a very small positive value it is day. The neutral case is expected to occur only at the start of the program when H_o is initialized to zero before it is calculated for the first time.

There are two times when the model does not fit exactly into the day or night mode. During the first iteration some variables have not yet been calculated and so are initialized (usually to zero). In this iteration neither the "day-only" or the "night-only" routines are called (because H_o equals zero certain routines may be called twice, as long as the net radiation is greater than zero). The other time when it may not be properly day or night, such as at the start of the simulation time -- in the early morning when H_o may be less than zero. However, a flag to set the model definitely into the daytime mode will not yet have been set. This prevents the calling of the routines which set up the night-time vertical wind profiles, thus a partial night mode is simulated where the Blackadar scheme is used to calculate H_o. Note that the mixing layer formulation is not executed until daytime heat flux becomes positive. Also note, that it is inadvisable to run the model for more than 24 hours, as the model has no way of treating the change in the atmospheric structure with time due to advection in the mixing layer. Doing this will just cause the model to heat up every day. We recommend that the model be started at dawn and terminated during the small hours of the morning. We have found that, after years of trial and error, adjustments and fixing, the model is now quite stable and reliable.

Chapter 2 - Vegetation

2.1 Introduction

As stated in Chapter 1, the vegetation component is computed separately and the fluxes blended above the canopy with those coming from the bare soil alone, weighted by the fractional vegetation cover. Otherwise, the fluxes beneath the soil surface and above the vegetation canopy – the surface and mixing layers – are the same as in Chapter 1 and will not be repeated here.

In order for the user to fully understand the vegetation parameterizations employed in the model a good understanding of certain concepts would be beneficial. As mentioned before, electrical analog notation is used as a concept to formulate the movement or transfer of particular model variables, notably those of moisture and heat, through the various model layers. Following on from this then, we reintroduce the idea of a resistance to transfer and present the concept of water potential which is used implicitly in the plant canopy equations.

2.2 The Vegetation Parameterization

The vegetation component closely follows the description given by Taconet et al. (1986; *J. Appl. Meteor.*), Lynn and Carlson (1990; *Ag and Forest Meteor.*), and Olioso et al. (1996: *Ag. And Forest Meteor.)* with some later modifications. Essentially, the model accounts for a layer of vegetation between the atmospheric surface layer and the ground surface. Heat and moisture fluxes are exchanged between the foliage and the inter-plant airspaces and between the ground and the inter-plant airspaces through resistances in the leaf (for water vapour) and the air. The transition layer is replaced by a shallow air layer just above the vegetation canopy.

2.3 Radiation Partition

Radiative energy penetrates the canopy to or from the leaves and to or from the ground. Relative amounts absorbed in the vegetation layer or at the surface are governed by a function that depends upon the leaf area index. The radiative temperature of the canopy is determined by a long-wave radiative balance equation that takes into account the temperatures of the foliage and the ground.

2.4 Flux Partition

The partitioning of flux between the ground and the canopy is parameterized as a function of the canopy characteristics, using conductance and resistance formulations.

2.4.1 Sensible Heat Flux

The sensible heat formulation has two components; ie, the sensible heat flux above the canopy, comprising that to or from the canopy and that to and from the ground.

The part originating from the ground is obtained as for bare soil where the analogous equations to that of bare soil are substituted into the energy balance equation resulting in a similar expression which resembles the Penman equation.

However, the sensible heat flux from the canopy is written as:

$$H_f = \frac{\rho C_p (T_1 - T_{af})}{r_{af}} \qquad (1a)$$

where r_{af} (inter-leaf airspace resistance) is the reciprocal of the conductance (the conductance Ch_f is defined in Taconet et al); C_p stands for the specific heat of air, ρ the density, T_1 & T_{af} are respectively the temperatures of the leaf and the inter-leaf airspaces.

2.4.2 Latent Heat Flux

Similarly, latent heat transfer has two elements to it. Originating from the ground is formulated as:

$$L_eE_g = \frac{\rho L_e M \{q_s(T_g) - q_{af}\}}{r_{ag}} \qquad (1b)$$

In this equation the factor M, ie, the moisture availability at the surface of the ground is assumed to be a fraction of the field capacity; $q_s(T_g)$ & q_{af} respectively represent the saturation mixing ratio at the temperature of the ground and in the inter-leaf airspaces, r_{ag} is the resistance between the soil surface and the canopy.

The contribution to the total furnished by the vegetation, ie the transpiration, is given by equation and is unlike that presented in Taconet et al.

$$L_eE_f = \frac{\frac{C_p}{\gamma} V}{r_1 + r_{af}} \qquad (1c)$$

V being the difference between saturation vapor pressure at the temperature of the leaf and the leaf-air boundary vapor pressure. $\gamma = \frac{PC_p}{0.622\, L_e}$ where P is the ambient pressure. r_1 is the leaf resistance. r_{af} is calculated from a knowledge of the friction velocity (ustar) and the size of the leaf (Goudriaan 1977).

It is important to note that L_eE_f is calculated first, so that H_f is really a residual between R_n (the foliage component) and L_eE_f , this can lead to a negative H_f if the demand for a large LE_f occurs.

Examination of this equation highlights the importance of the resistance terms in the denominator, which play an important role in the magnitude of the latent heat flux and in particular, the part stomatal resistance plays in the overall leaf resistance. This is central to the plant canopy structure and will occupy much of the discussion that follows:

2.5 The Stomatal Resistance

The stomatal resistance constitutes an essential element of the vegetation parameterization. Essentially it expresses the efficiency of the vegetation to transpire. The energy partition between sensible and latent heat is adjusted by the magnitude of R_{st} per se. Many physiological and climatological factors are involved in the foliage resistance to transpiration. The primary ones include the variation in daylight, the evaporative demand imposed by atmospheric forcing, the water supply to the plant's roots and the phenology and type of vegetation.

2.5.1 Deardorff Formulation

To take account of these effects the model employs two stomatal parameterizations. The first is the Deardorff formulation which captures the gross aspects of stomatal behaviour as affected by soil water content and sunlight. Yet it is important to state that it ignores plant hydraulics which account for significant shifts in transpiration rate over the diurnal period. These important variations in transpiration rate are manifested by a change in the stomatal resistance and can be correlated with variables that reflect the physiological status of the plant. At this point in the discussion the reader needs to become acquainted with the concepts of water potential, vapour pressure deficits and osmosis. A relatively straight-forward survey of plant physiology is presented in Raven et al (1981), which may help those unfamiliar with the field.

2.5.2 Plant Canopy Formulation

The development of stomatal resistance then begins with a model conception as suggested by Jarvis (1976) and futher developed by Lynn and Carlson. Here the stomatal resistance (r_s) is calculated from the product of two functions f(S) and $f(\psi_e)$, according to the relationship:

$$r_s = r_{min}\, f(S)\, f(\psi_e) \qquad (2a)$$

where r_{min} is the minimum stomatal resistance that can be observed; defined as that occurring with full sunlight and at saturation leaf water potential. The functions $f(\psi_e)$ and f(S) represent the stomatal resistance initiated due to leaf potential and solar flux.

The solution for $f(\psi_e)$ is analytical and is a function of soil moisture, vapour pressure deficit, inter-foliage resistances and plant internal resistances.

The resistance structure of the plant is shown in Figure 2.

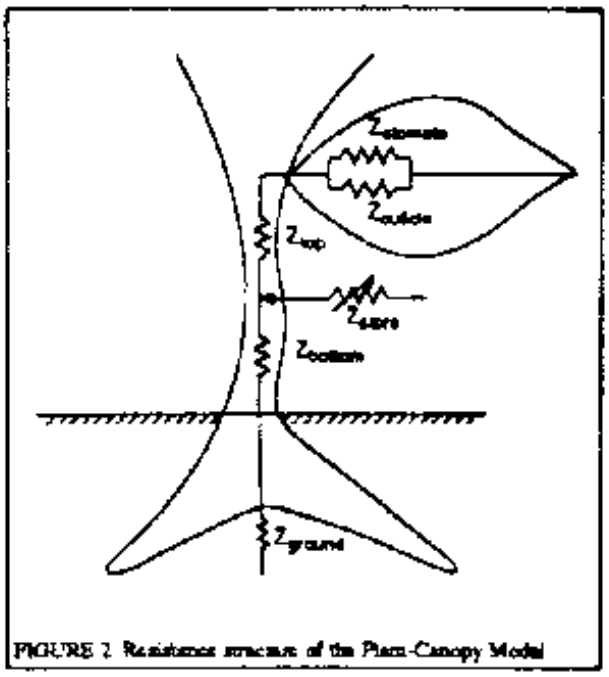

FIGURE 2 Resistance structure of the Plant-Canopy Model

Figure 2

Attention is drawn to the fact that a variable resistor (Z_{store}) is drawn at the mid-point along the stem of the plant, which is an analogy representing the ability of the plant to store water in its tissue (root, stem or leaf). This resistance pertains to the flow of water to or from storage and governs the ability of the plant to store water in its tissue (root, stem or leaf). This capacity to store water, termed in our electrical analogy

scheme as the capacitance can be modelled such that any flux of water resulting from storage is directly related to the position of the resistor. For example, if the resistor (branch point) is situated at the top of the plant, the implication is that most of the stored water comes from the leaves. The choice of the branch point position is left up to the user.

2.5.3 Solutions for f(S) & f(ψ_e)

The solution then to f(ψ_e) is two fold. The first is designated "steady-state" and implies that there is no water storage in the plant or simply, any water entering the plant at the roots is leaving through the leaves. The second implies that water storage in the plant is a contributing factor to the eventual transpiration at the leaves and is called "capacitance".

The functions f(S) and f(ψ_e) exhibit exponential behaviour which can be represented simply by a pair of straight lines whose intersection defines sub-critical and super-critical regions separated by a critical value of S or ψ_e . We term this a "discontinuous linear" model and maintain that it captures the fundamental form of the functions without any great loss of accuracy.

The equations are of the form:

$$f(\psi_e) = \frac{r_{min} + b_1 \psi_e + b_2 (\psi_e - \psi_c) \delta_\psi}{r_{min}} \qquad (3a)$$

$$f(S) = \frac{r_{min} + c_1(S_o - S) + c_2(S_c - S)\delta_s}{r_{min}} \qquad (3b)$$

Key $f(\psi_e)$

b_1 Slope of sub-critical part of $f(\psi_e)$; $f(\psi_e) > f(\psi_c)$: where ψ_c is the intersection point which defines the critical value.

b_2 Slope of super-critical part of $f(\psi_e)$; $f(\psi_e) < f(\psi_c)$

$f(\psi_c)$ is the critical leaf water potential; intersection point of lines b_1 and b_2

$\delta_\psi = 0$ $\psi_e > \psi_c$; $\delta_\psi = 1$ $\psi_e < \psi_c$ and $\psi_e = \psi_c$ in first term on the RHS of the equation

Key $f(S)$

c_1 Slope of f(S) between S_o and S_c: subscript $_c$ defining the critical value

c_2 Slope of f(S) between S_c and S where $S < S_c$

S_c is the solar radiation threshold; intersection between c_1 and c_2

S_o is a maximum solar radiation value, loosely defined as the value at which light saturation of the leaves is reached

$\delta_s = 1$ $S < S_c$ and $\delta_s = 0$ $S > S_c$; $S = S_c$ in first term on the RHS of the equation.

The solution for f(S) is straight-forward where the solar flux (S) is obtained from the radiation component of the model.[i] However, the function defined by $f(\psi_e)$ requires greater elaboration.

For steady-state situations, transpiration from the leaves is considered equal to the flux of water from the root zone. It is therefore, possible to combine these equations into the form -

$$a\psi_e^2 + b\psi_e + c = 0 \quad ; \quad a \neq 0 \qquad (3c)$$

where the coefficients a b and c contain all of the independently specified or calculated variables listed in the equations. This quadratic equation is then solved for ψ_e to yield two roots -

$$\psi_e = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \qquad (3d)$$

the negative root specifying the correct value for ψ_e.

All that remains now is to establish whether ψ_e is above or below the threshold value to determine the value of δ_ψ. This is accomplished by defining a critical ground water potential (ψ_{gc}) as that minimum ground water potential which can meet the evaporative demand without ψ_e becoming less than ψ_c. This is done by setting the leaf water potential to that of the threshold water potential, at which point r_s is equal to a critical resistance r_{ct}. We define sub-critical simply to refer to the region where stomatal resistance varies slowly with S or ψ_e. Super-critical signifies the region where r_s varies rapidly with S or ψ_e.

The critical value can be obtained by arranging the equations to yield the expression:

$$\psi_{gc} = \frac{(\psi_c - \beta V) - V\sigma Z_t}{r_{af} + \frac{r_{cut}\, r_{ct}}{r_{cut} + r_{ct}}} + H \qquad (4)$$

where β is a constant describing the difference between the mesophyllic and leaf epidermal water potential divided by the vapor pressure and Z_t is the sum of the resistances from ground to, but not including, the leaf. $\sigma = \rho L_e$ and the critical and cuticular resistances are r_{ct} and r_{cut} respectively.

If the critical ground water potential is less than the value of the soil water potential, the sub-critical solution is correct as ψ_e is greater than ψ_c. Moreover, when the

critical ground water potential is greater than the value of the soil potential, ψ_e is less than ψ_c, necessitating the super-critical solution.

The additional water supply from the plant's storage can be an important contribution to the transpiration. The capacitance solution though takes the same form but with the inclusion of substantially more terms which account for the storage resistance, initial storage volume and placement of the variable resistor. Further elaboration on the capacitance parameterization is to be found in Carlson and Lynn (1991).

2.6 The Canopy Resistance

It is possible to define a canopy moisture availability, which is the ratio of evapo-transpiration to the potential evaporation from a surface with radiometric surface temperature calculated by the model. Indeed, if one chooses to ignore vegetation and use the bare soil model (which, strictly, is a general canopy model rather than a specific bare soil model), the moisture availability is then the canopy moisture availability. Given this definition of the canopy moisture availability, that is, the ratio of evapo-transpiration to potential evaporation and the atmospheric resistance, one can define a canopy resistance (instead of a soil resistance). This canopy resistance is that which is often measured over vegetation.

2.6.1 Partial Cover

In some cases, as with sparse vegetation, the user may wish to blend in the bare soil and vegetation models. This is done by setting a fractional vegetation cover in addition to the leaf are index, the latter, however, pertains to the entire mixture of bare soil and vegetation. At the level of the canopy, the model then operates separately (bare soil and vegetation) and blends the radiometric surface temperatures and the atmospheric fluxes above the canopy according to the bare soil and vegetation fractions. The parital

routine is useful for studying the change in radiometric surface temperature as a function of fractional vegetation cover. Fractional vegetation cover is thought to be closely related to the normalized difference vegetation index (NDVI) in the range of fractional vegetation cover below 100%.

2.7 Dual Roughness Regimes

When a stand of vegetation or other obstacles obstructs the flow of air over surrounding clearings the logarithmic wind profile in the air above the obstacles behaves differently from that below the obstacles. Guyot and Seguin (**Ag. And Forest Meteor.**, 1978, p 411) show that widely separated tree rows can influence the logarithmic wind profile in the spaces between the rows such that the wind speed above the average height of the trees responds to the average roughness height of the trees, which is typically about 0.1 times the tree height. We will refer to this roughness as the "global" roughness. Below the tree level, the wind profile responds to the average roughness length of the surface elements between the trees, e.g. the grass. We will refer to this roughness as the "patch" roughness. Thus, two roughness regimes exist at one point even when the trees are separated by a distance several times the height of the trees and the latter occupies only a small fraction of the surface area in a larger region consisting of trees and surrounding bare or grassy terrain. The importance of specifying two roughness regimes is that the option will allow the surface temperature of clearings to become more elevated because the roughness of the clearing will be much less than that for the vegetation; an analogous situation exists for the heating of the surfaces between buildings in urban areas, where the obstacles are buildings rather than trees. For vegetation, clearings may simply constitute the bare soil between rows of a crop such as corn.

We generalize the result of Guyot and Seguin to include obstacles such as trees, bushes or buildings, that may be surrounded by flatter patches such as bare soil.. Five cases can be specified: flat bare soil, bumpy urban landscape, uniform vegetation, uniform vegetation but uses a patch roughness and trees and grass (or urban with vegetation and). The users should first decide if they want to have a dual roughness

regime and whether the obstacles are due to vegetation or buildings. The obstacle height and a roughness are specified in the eighth and ninth slot in the data statement, immediately after the parameter omega, which is the precipitable water amount.

If no obstacle height is specified, the model assumes that there is no dual roughness regime and uses only one roughness value, even if a partial vegetation cover is indicated. This roughness height must be specified in the slot for the roughness parameter. A single roughness height would apply to the case of a bumpy bare soil regime or a vegetation canopy with no clearings or for partial vegetation cover if the user wanted to ignore the dual roughness option. If both a zero roughness height and a zero obstacle height are specified the model will fail.

If an obstacle height is specified the model assumes that the global roughness is 0.1 times the obstacle height, e.g. 10 cm if the obstacle height is 1 m; (obstacle height is specified in meters). The user should note that the roughness length still should be specified. If this parameter is specified as zero, the model uses 0.1 times the obstacle height as the roughness height and proceeds as if there were only one roughness regime.

Although this is not yet made available in the on-line version of Simsphere, it is possible to calculate the fluxes for vegetion in the case where two roughness regines are present, say with a layer of short grass within a layer of brush or short vegetation within an urban environment having buildings several meters high. One is treated as the usual roughness and the other is called the obstacle height. Assuming that the option becomes available on line, if the user specifies an obstacle height and a roughness height, the model assumes that there is a dual roughness regime. In this case global roughness is computed as 0.1 times the roughness height and patch (clearing) roughness is specified by a value in the roughness parameter slot. Note, however, that the model will fail if the obstacle height is less than 10 times the specified roughness parameter. A typical example would be for a forest canopy with partial bare soil patches. If the trees are 5 meters high, an obstacle height of 5 meters is specified and the global roughness would be calculated as 50 cm. If the tall grass surrounding the forest is 10 cm high (essentially bare soil but with a sparse grass cover), one might wish to specify a roughness of 1.2 cm, for example. The model will then calculate the fluxes in the partial vegetation mode (if

the partial mode is activated in the data statement) or for an urban type setting if bare soil is indicated, using the global and patch roughnesses. This option is present in the model code and could be made available in the on line version by allowing the obstacle height to be selected by the user.

If the partial vegetation mode is not activated, the model proceeds as if there is a 100% vegetation cover or bare soil (if LAI = 0), and uses the specified roughness parameter if obstacle height is not specified and otherwise uses 0.1 times the obstacle height as the roughness parameter if the roughness parameter is not specified. If both roughness length and obstacle height are specified for the case of vegetation, but the partial vegetation mode is turned off, the model still calculates a dual roughness regime, although this option is a bit artificial. However, the user may wish to apply the dual roughness regime calculations to the case of bare soil, e.g. urban areas, where buildings constitute the obstacles. In that case, no partial vegetation mode is called for. The user would specify bare soil conditions (zero LAI), an obstacle height to represent the average height of the buildings and a roughness height, which would apply to the spaces between the buildings.

One could consider a vegetated urban area in which the obstacle height would be that of the buildings, but a vegetation fraction and other vegetation parameters would be specified and the model would execute in the partial vegetation and dual roughness modes. Note that a vegetation height must be specified in the vegetation mode, but that parameter has nothing to do with roughness, being used only to calculate the water flow through the plant.

Finally, the user should note that the dual roughness concept may be inapplicable if, for example, the percent of vegetation is so small as to not influence the wind regime in the clearings. A good rule of thumb might be that the vegetation must be greater in height than about 0.1 the spacing between vegetation clumps in order to affect the wind in the clearings. The existence of a dual roughness regime depends on the wind direction with respect to the roughness elements. A row of trees may not affect the wind in the surrounding clearing if the wind blows along the direction of the row rather than across it. Conversely, one would expect the logarithmic profile laws to become invalid in the

spaces between vegetation clumps as the percentage of vegetation approaches 100%. In that case a representative wind speed between the vegetation elements is the interleaf wind speed, UAF, which is calculated in VEGVEL.for. A fuller development of the obstacle height concept was employed in a paper by Lynn et al. (2009: *J. Appl. Meteor*.)

2.8 Carbon Dioxide Flux

Carbon dioxide flux from the leaves is calculated in a similar manner to that of transpiration, see Goudriaan (1977). Stomatal and boundary layer resistances are scaled from those of water to accommodate the differing diffusivity of CO_2. The gradients of the CO_2 between the mesophyll and above the canopy must be specified; As of 1991, the external concentration $[C_a]$ is about 330 ppmv (parts per million per volume) and the internal concentration $[C_i]$ is thought to be about 120 ppmv for C_4 plants and 210 ppmv for C_3 plants. The fluxes are output in $Kgm^{-2}s^{-1}$, typically of the order of 100×10^{-8}. They are scaled by the leaf area index divided by the shelter factor to convert to fluxes per unit horizontal surface area.

2.9 Ozone Fluxes and Concentrations within a Plant Canopy

Ozone is destructive of plant tissues. Destruction occurs when the ozone enters the leaf cells. The result is a reduction in yield and in green leaf area and an increase in the root mass. Fluxes of ozone to the plant consist of fluxes through the stomates and through the cuticle. Fluxes also occur through the ground beneath the big leaf and in the bare soil areas. One assumption is that the contact concentration in side the leaf and at the ground is zero. It is also assumed that no ozone is destroyed at the leaf surface outside the stomates and the cuticle. In fact, the efficiency of ozone destruction at dry surfaces is probably not 100%.

Ozone fluxes from atmosphere to leaf move through an atmosphere and canopy air resistance and then a leaf boundary layer, where they split in parallel to go through the

stomates and the cuticle. A third branch bypasses the leaf and goes into the ground. Concentration inside the canopy is calculated from a fixed ozone concentration at 50 m. Ozone density is taken as 1.9 kg m^{-3}, similar to that of carbon dioxide. Molecular diffusivities are assumed to be identical to those for carbon dioxide.

Ozone concentrations calculated in the model are assumed to be in the plant canopy, roughly near the top of the vegetation. Ozone concentration is prescribed at 50 m in units of parts per million by volume (ppmv); a typical value is 0.08. (In reality, ozone tends to be created in the boundary layer during the day as the result of photochemical effects on NO_2, so that the maximum occurs during the early afternoon.) Even with the assumption of constant concentration at 50 m, that at canopy level tends to maximize at mid day because of increased turbulent transport. Fluxes are expressed in kg m^{-2} s^{-1}; a typical value is about 1. Output is for both the plant fluxes alone and for the global fluxes, which includes that in the non-vegetated part of the canopy. In reality, the fluxes in the non-vegetated areas are overestimated due to the assumption of zero contact concentration.

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[i]As of the beginning of 1993, the coefficients in the stomatal resistance function (b_1,b_2,c_1,c_2) are defined differently than expressed in the text. Henceforth the new coefficients are calculated as the old ones divided by $r_{min.}$ Thus, the new expressions do not contain the minimum stomatal resistance in eqch of the individual functions f(S) etc.

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