A Soil-Canopy-Atmosphere Model: Description and Comparisons with Field Data

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Abstract: This report presents a full description of the Soil-Canopy-Atmosphere Model (SCAM) and a comparison of the predictions of SCAM with field measurements. SCAM is a model of land-atmosphere exchange processes suitable for use as a lower boundary condition in a primitive-equation atmospheric model at either regional or global scale, and for investigating the links between land-surface microclimate, hydrology and ecology. The model determines the temporal evolution of all the fluxes in the energy and water balances of an arbitrary terrestrial surface, separately resolving both the soil and vegetation components and fully resolving the diurnal cycle. The input information consists of time series for the meteorological forcing variables (radiation, temperature, humidity, wind speed, precipitation, pressure) on time steps of order 30 min, and a few parameters describing the soil and vegetation state, principally soil texture, soil depth, leaf area index and vegetation height. Output information includes the fluxes in the surface energy balance $F_N - F_G = F_H + F_E$ (the net irradiance, storage or ground heat flux, sensible heat flux and latent heat flux), the water fluxes making up the soil water balance, the radiative surface temperature, and other variables.

SCAM has several novel features. These include: (1) full allowance for microclimatic interactions between the vegetation and soil components of the landscape; (2) a sophisticated single-layer description of canopy aerodynamics, including incorporation of modern theory of canopy turbulence and a rational treatment of sparse canopies; and (3) a modular structure which enables comparative tests of alternative descriptions of processes relevant to land-air interaction, such as soil evaporation, infiltration, soil water storage and soil heat storage.

SCAM is described in detail and then compared with validation data from several major field experiments (Cabauw, HAPEX-MOBILHY, FIFE and OASIS). The comparisons are broadly satisfactory but indicate some areas where further effort is required. These include soil water storage (particularly the specification of the lower boundary condition), and canopy scale ecophysiology (where the incorporation of assimilation-based descriptions of physiological processes may be useful). A particular result is that modelled ground heat flux agrees with measurements (OASIS) provided that the measurements account for thermal storage effects.

SCAM is an evolving model, and will develop in the future. This report describes the present basis from which developments will occur.

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1. INTRODUCTION

This report describes Version C of the Soil-Canopy-Atmosphere Model (SCAM). The aim of SCAM is to determine the temporal evolution of all fluxes in the energy and water balances of an arbitrary terrestrial surface, separately resolving both the soil and vegetation components and fully resolving the diurnal cycle. The input information consists of time series for the meteorological forcing variables (radiation, temperature, humidity, wind, precipitation) on time steps of order 30 min, and a few parameters describing the soil and vegetation state.

The work is motivated by two general purposes: first, the provision of *terrestrial biosphere schemes for atmospheric models*. Global Climate Models (GCMs) and mesoscale models require specifications of the land-air fluxes of sensible heat, latent heat and momentum in terms of incident radiation, precipitation, and low-level wind, temperature and humidity. The second purpose is the exploration of *links between land-surface microclimate, hydrology and ecology*, including interactions between terrestrial microclimate (especially the energy and water balances for soil and vegetation) to the ecological state and development of the terrestrial biosphere. This goal will eventually require the coupling of models like SCAM to relatively simple models of carbon exchanges, and ultimately of ecological development.

SCAM has evolved through three quite different versions: SCAM-A, SCAM-B and SCAM-C, the present model. SCAM-A (Raupach 1991) was a "Simplified Canopy-Atmosphere Model" consisting of a bulk combination (Penman-Monteith) equation for the aggregated canopy-soil system, with simple specifications for bulk resistances. Its intention was to specify conceptually the few basic properties of land surfaces which are most important in determining land-air exchanges. It is now superseded. SCAM-B (Raupach and Finnigan 1995) was a "Simplified Canopy-Atmosphere Model" to calculate surface fluxes on the individual patches making up a heterogeneous landscape. Its aim was to permit detailed tests of the "scale insensitivity hypothesis" that regionally-averaged surface energy balances in heterogeneous terrain do not depend strongly on the scale of heterogeneity. Results obtained with SCAM-B supported this hypothesis (in dry conditions), basically for thermodynamic reasons (Raupach and Finnigan 1995).

SCAM-C (henceforth SCAM) is a model of the terrestrial biosphere in the form required for a lower boundary condition in an atmospheric model (global or mesoscale). The aim is to represent this system in the simplest possible way, with the minimum number of land-surface parameters, yet with adequate representation of all essential physical processes. SCAM includes one vegetation layer, in addition to the soil surface; a simplified aerodynamic conductance formulation for the turbulent transfer between soil, vegetation and atmosphere, accounting for thermal stability effects and the main features of turbulent exchanges within canopies; responses of the vegetation surface conductance to radiation, saturation deficit, temperature and soil water stress; and descriptions of soil temperature and moisture in two or more soil layers. A further intention is that the model be sufficiently modular to allow exploration of alternative descriptions of critical processes. For testing purposes, the present version includes alternative parameterisations for soil evaporation, infiltration, soil moisture storage and soil heat storage.

The structure of this report is as follows. Section 2 outlines the general principles of land-air energy and water exchanges, drawing out the implications of these principles for the logical and geometrical structure of a land-air exchange model. Section 3 presents the detailed description of all atmospheric constituents of the model, including vegetation and soil energy

exchanges, physiological processes, aerodynamic transfer and radiative transfer. Section 4 describes the modelling of soil processes, including soil heat storage, soil water fluxes and soil water storage. Several alternative parameterisations of each of these processes are presented and briefly compared (Section 4.4). Section 5 is an extensive comparison of the model with data from several major field experiments: Cabauw, HAPEX-MOBILHY, FIFE and OASIS.

2. GENERAL PRINCIPLES

A vegetated land surface consists of a number of types of surface element: the underlying soil surface, vegetation stems, and leaves in several canopy layers, possibly distinguished in each layer as sunlit or shaded and wet or dry. The surface elements are connected to a variety of heat and water stores, mainly in the soil. We are concerned with the energy and water balances for this system, which are coupled through the soil and plant evaporation terms.

2.1 Energy Balance

The energy balance for an arbitrary surface element is:

$$\begin{aligned} f_A &= f_H + f_E \\ &= (1-a)f_{S\downarrow} + ef_{L\downarrow} - e\sigma T_s^4 - f_G(T(Z)) \end{aligned} \tag{2.1}$$

Here f_H and f_E are the sensible and latent heat flux densities at the element surface, summing to the available energy flux density f_A ; f_G is the flux density into thermal storage (the ground heat flux if the element is the soil surface); $f_{S\downarrow}$ and $f_{L\downarrow}$ are the incoming shortwave (solar) and longwave (terrestrial) irradiances; a is the albedo; e the emissivity; σ the Stefan-Boltzmann constant; T_s the surface temperature; and $T(Z)$ the internal temperature distribution within the body of the element, a function of a position coordinate Z (we only indicate one space dimension explicitly though the problem is three-dimensional in general). The sensible and latent heat fluxes are specified by equations of the form

$$f_H = \rho c_p (T_s - T_r)/r_{aH} \tag{2.2}$$

$$f_E = \rho\lambda(Q_s - Q_r)/r_{aE} \tag{2.3}$$

where T and Q are air temperature and specific humidity; ρ is air density; c_p the isobaric specific heat of air; λ the latent heat of vaporisation of water; and r_{aH} and r_{aE} the aerodynamic resistances for heat and water vapour transfer from the surface ($T = T_s$, $Q = Q_s$) to an ambient reference location ($T = T_r$, $Q = Q_r$). These resistances include contributions describing molecular transfer through element boundary layers, and also (depending on the choice of reference location and spatial scale) turbulent transfer through the canopy and surface layers.

For each surface element i, the energy balance equations (2.1), (2.2) and (2.3) are to be solved for the three unknowns f_H, f_E and T_s. All other quantities are specified in ways described in detail later. This is a classical problem; however, it is not often made clear that the nature of the equations, and the approach to solving them, depends fundamentally on whether the storage heat flux f_G is significant or not.

Negligible thermal storage: Usually f_G is negligible (or nearly so) for vegetation elements. Then $f_G = 0$ in Equation (2.1), and Equations (2.1), (2.2) and (2.3) for f_H, f_E and T_s are *algebraic.* Physically, the system involves no storage terms and therefore has no "memory". An approximate solution is given by the combination or Penman-Monteith equation.

Non-negligible thermal storage: For the soil (or any other surface element with significant thermal mass), thermal storage is significant. Accordingly, the system has "memory" (dependence on prior history), and the equation set is *differential.* This is apparent from the downward storage flux f_G through a plane at depth Z:

$$f_G(Z,t) \quad = \quad -K_G(\partial T/\partial Z)_{Z=0} \tag{2.4}$$

where Z is depth into the soil (with $Z = 0$ at the surface) and K_G is the thermal conductivity of the soil. The most important storage flux is $f_{G0}(t) = f_G(0,t)$, the thermal flux into storage through the soil surface. Since f_G and f_{G0} depend on the internal temperature distribution $T(Z)$, it is necessary to solve for $T(Z)$ in addition to f_H, f_E and T_s. The governing equation for $T(Z)$ is the heat equation, written here without incorporating phase changes and advection of heat by the flow of liquid water (Fuchs *et al.* 1978, Cremer and Leuning 1985):

$$C_G \frac{\partial T}{\partial t} \quad = \quad -\frac{\partial f_G}{\partial Z} \quad = \quad \frac{\partial}{\partial Z}\left(K_G \frac{\partial T}{\partial Z}\right) \tag{2.5}$$

where C_G is the bulk volumetric heat capacity of the soil (J m^{-3} K^{-1}). The boundary condition at $Z = 0$ is a specification of $\partial T/\partial Z$, through Equations (2.1) and (2.4). In practice, this differential equation is normally solved in a highly simplified, spatially discrete form.

This is the most fundamental of many differences between the energy balance calculations for the vegetation and soil parts of a land-surface scheme (others include the method of specifying the surface humidity Q_s). The practical outcome is that the soil and vegetation energy balance calculations often appear quite different. This has led many land surface schemes to run entirely separate energy balance calculations for soil and vegetation, using a "two-patch" approach. If a land surface of area A is covered with uniform (but not necessarily dense) vegetation with fractional vegetation cover f_{veg} (in vertical projection), then the two-patch approach splits the surface into two separated patches: one of area $f_{veg}A$, covered with dense vegetation, and the other of area $(1\text{-}f_{veg})A$, covered with bare soil. Such a procedure ignores the fact that, on a partly vegetated surface, the soil and vegetation interact by modifying each other's microclimates, both radiatively and aerodynamically. In contrast, SCAM carries these interactions. Rather than calculating separate soil and vegetation energy balances, it calculates a combined energy balance for the composite soil-vegetation system, accounting for the radiative and aerodynamic processes by which each surface type influences the other. In other words, the vegetation is above the soil, rather than being horizontally separated from it.

2.2 Water Balance

The water balance is always strongly influenced by prior history ("memory") and therefore requires the solution of differential equations. This is so because of the importance of storage (which occurs almost entirely in the soil) and the close links between soil water stores and fluxes: soil moisture storage levels influence infiltration, deep drainage, soil evaporation and plant evaporation (transpiration).

Soil moisture changes are governed by the conservation equation:

$$\frac{\partial \eta}{\partial t} = -\frac{\partial q}{\partial Z} - S(\eta) \tag{2.6}$$

where $\eta(Z,t)$ is the volumetric soil moisture content ($m^3\ m^{-3}$), $q(Z,t)$ is the kinematic moisture flux ($m\ s^{-1}$, positive downward), $S(\eta)$ is the moisture sink due to vegetative transpiration via roots (s^{-1}), and Z is depth into the soil. From Darcy's law, $q(Z)$ is given by:

$$q(Z) = -D(\eta)\frac{\partial \eta}{\partial Z} + K(\eta) \tag{2.7}$$

where $K(\eta)$ is the hydraulic conductivity ($m\ s^{-1}$), and $D(\eta)$ the soil moisture diffusivity ($m^2\ s^{-1}$), given by $D = K\partial\psi/\partial\eta$ where $\psi(\eta)$ is the soil moisture potential (m). The functions $K(\eta)$ and $\psi(\eta)$ are intrinsic soil properties, determined by soil type. The first and second terms in Equation (2.7) respectively describe water fluxes due to capillarity and gravity. The combination of Darcy's law and the conservation equation gives Richards' equation (Richards 1931):

$$\frac{\partial \eta}{\partial t} = -\frac{\partial q}{\partial Z} - S = \frac{\partial}{\partial Z}\left(D(\eta)\frac{\partial \eta}{\partial Z}\right) - \frac{\partial K}{\partial Z} - S \tag{2.8}$$

which is the differential equation governing $\eta(Z,t)$. In terrestrial biosphere models, Richards' equation is not normally carried directly. Instead, simplified conservation equations are written for one or more soil layers, possibly using a simplified version of Darcy's law to represent water fluxes between the layers.

The boundary condition at $Z = 0$ is a specification of the water flux through the surface (q_0) due to infiltration and soil evaporation:

$$q_0 = q_{inf} - q_{Es} \tag{2.9}$$

where q_{Es} is the soil evaporative flux and q_{inf} is the water flux infiltrating downward through the soil surface. A boundary condition is also needed at the bottom of the resolved soil profile to specify the deep drainage flux q_{drain} (this is a critically important condition in practice). Since q_{Es}, q_{inf}, q_{drain} and the transpiration sink strength S all depend on η and its spatial distribution, the water balance must be solved differentially rather than algebraically. Like the heat equation, the moisture equation is normally solved in a simplified, spatially discretised form.

2.3 Geometrical and Logical Structure

In this report we present the description of most physical processes rather generally, for an arbitrary multilayer canopy, and then give the simplifications used in SCAM. The geometrical conventions used to define the multilayer structure are as follows (see Figure 2.1).

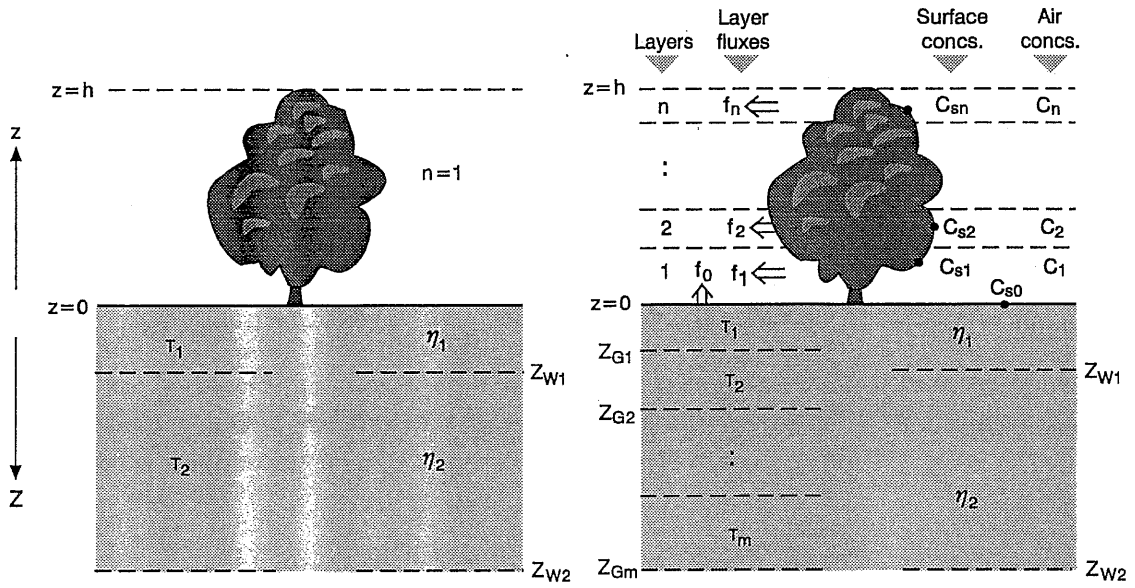

Figure 2.1: Geometrical structure of SCAM for a single and multi-layer canopy, and multi-layer soil.

Canopy layers: The canopy consists of n vegetation layers ($i = 1,\ldots, n$), together with a soil surface denoted by $i = 0$. The top of layer n is at $z = h$, the canopy height. (Later we consider $n = 1$, a single vegetation layer). For each vegetation layer ($i = 1,\ldots, n$), C_i is the layer-averaged concentration of an arbitrary scalar entity in the canopy air (outside element boundary layers), C_{si} the layer-averaged concentration on element surfaces, and f_i the layer-averaged scalar flux density into the air. The scalar flux density from the soil surface is f_0. Vegetation layer i has depth Δz_i, single-sided leaf area density α_i, and contains leaf area index $\lambda_i = \alpha_i \Delta z_i$. The total leaf area index of the vegetation is $\Lambda = \lambda_1 + \ldots + \lambda_n = \alpha_1 \Delta z_1 + \ldots + \alpha_n \Delta z_n$. Bulk vertical surface fluxes (vertical fluxes from the composite soil-vegetation system into the air) will be denoted F. The entity being transferred will be identified with a letter subscript, such as H or E for sensible or latent heat, respectively. It is convenient to normalise both bulk and layer fluxes with ground area rather than leaf or element area, so that bulk fluxes are unweighted sums of layer fluxes (including the contribution from the ground): $F = f_0 + f_1 + \ldots + f_n$.

Soil layers: We consider m soil layers bounded below by planes at depths Z_j, with $Z_0 = 0$ the soil surface. The number m and the layer depths Z_j may be different for soil heat (for which layers will be denoted $Z_{G,j}$) and soil moisture (layers $Z_{W,j}$). Then, if T_j is the average soil temperature in layer j, the heat conservation equation in that layer is:

$$\left(Z_{G,j} - Z_{G,j-1}\right) C_G \frac{dT_j}{dt} = -\left(f_{G,j} - f_{G,j-1}\right) \qquad (2.10)$$

where $f_{G,j}$ is the soil heat flux through the plane $Z_{G,j}$ (and in particular f_{G0} is the ground heat flux through the soil surface). This is a spatial discretisation of Equation (2.5), obtained formally by volume integration through layer j and application of the divergence theorem. Likewise if η_j is the average moisture content in layer j, the water conservation equation in that layer is

$$\left(Z_{W,j} - Z_{W,j-1}\right)\frac{d\eta_j}{dt} = -\left(q_j - q_{j-1}\right) - \left(Z_{W,j} - Z_{W,j-1}\right)S_j \qquad (2.11)$$

where q_j is the water flux through $Z_{W,j}$ (in particular $q_0 = q_{inf} - q_{Es}$) and S_j is the transpiration sink strength in layer j. This is a spatial discretisaton of Equation (2.6), also obtained by volume integration.

One layer canopy structure used in SCAM: The total surface energy balance in SCAM is:

$$F_N - F_G = F_H + F_E \qquad (2.12)$$

with F_N the bulk net irradiance, F_G the bulk ground heat flux, F_H the bulk sensible heat flux and F_E the bulk latent heat flux. Each of these bulk fluxes is the sum of a contribution from the soil (subscript 0) and the single vegetation layer (subscript 1) :

$$\begin{aligned} F_N &= (1-a_0)f_{S\downarrow 0} + (1-a_1)f_{S\downarrow 1} + f_{L\downarrow 0} - f_{L\uparrow 0} + f_{L\downarrow 1} - f_{L\uparrow 1} \\ F_G &= f_{G0} + f_{G1} \\ F_H &= f_{H0} + f_{H1} \\ F_E &= f_{E0} + f_{E1} \end{aligned} \qquad (2.13)$$

The net irradiance is described later in Equations (3.56)-(3.59). The thermal storage flux f_{GI} for the canopy is assumed to be negligible (therefore the canopy has no "memory"). The latent heat flux from the canopy (f_{E1}) has contributions from both the wet and dry parts of the canopy.

The total water balance in SCAM is defined as

$$\Delta Z_{W1}\frac{\partial \eta_1}{\partial t} + \Delta Z_{W2}\frac{\partial \eta_2}{\partial t} = q_{pres} - q_{Es} - q_{Ev} - q_{drain} - q_{Hrun} - q_{DBrun,1} - q_{DBrun,2} \qquad (2.14)$$

with the left hand side denoting the change in water storage in a two layer soil moisture scheme with layer thicknesses ΔZ_{W1} and ΔZ_{W2}. The water fluxes into and out of the system are the precipitation (q_{pres}), the soil evaporation (q_{Es}), vegetative transpiration (q_{Ev}), the deep drainage (q_{drain}), the infiltration excess runoff or Hortonian runoff (q_{Hrun}), and the saturation excess runoff from the two layers, or Dunne-Black runoff ($q_{DBrun,1}$ and $q_{DBrun,2}$).

Logical structure: The above aspects of the energy and water balances have some implications for the overall structure of a terrestrial biosphere model, thence for SCAM. At any instant of time, all fluxes (both soil and atmospheric) are *algebraic* functions of the externally imposed meteorological variables (radiation, precipitation, wind speed, temperature, humidity and pressure) and the soil heat and water stores (specified by the temperature distribution T_j and the soil moistures η_j). That is:

$$\text{fluxes} = \text{function(weather variables, soil stores)} \qquad (2.15)$$

Therefore, all fluxes can be calculated from the state of the system at any instant (as specified by the weather variables and storage contents) irrespective of prior history. On the other hand, the evolution of soil heat and water stores is given by *differential* equations of the form

$$d(\text{store content})/dt \;=\; \Sigma(\text{fluxes entering store}) \qquad (2.16)$$

where the store content is understood to be the product of the layer thickness with $C_G T$ (for heat) or η (for water). Equations (2.10) and (2.11) are examples. The storage contents therefore depend on both prior history and current fluxes, and give "memory" to the system. This distinction between fluxes and storages suggests the following logic for each time step of a terrestrial biosphere scheme:

1. Specify storage contents and externally imposed meteorological variables at time t (either from the previous time step or as initially specified values on the first step).
2. Use Equation (2.15) to calculate fluxes at time t.
3. With these fluxes, integrate Equation (2.16) to obtain storage contents at the next time step, $t + \Delta t$.
4. Return to step 1.

This is the basic logic adopted in SCAM. One consequence is that it is straightforward to ensure exact conservation of energy and water. For later reference, a more detailed flow diagram for SCAM is given in Figure 2.2.

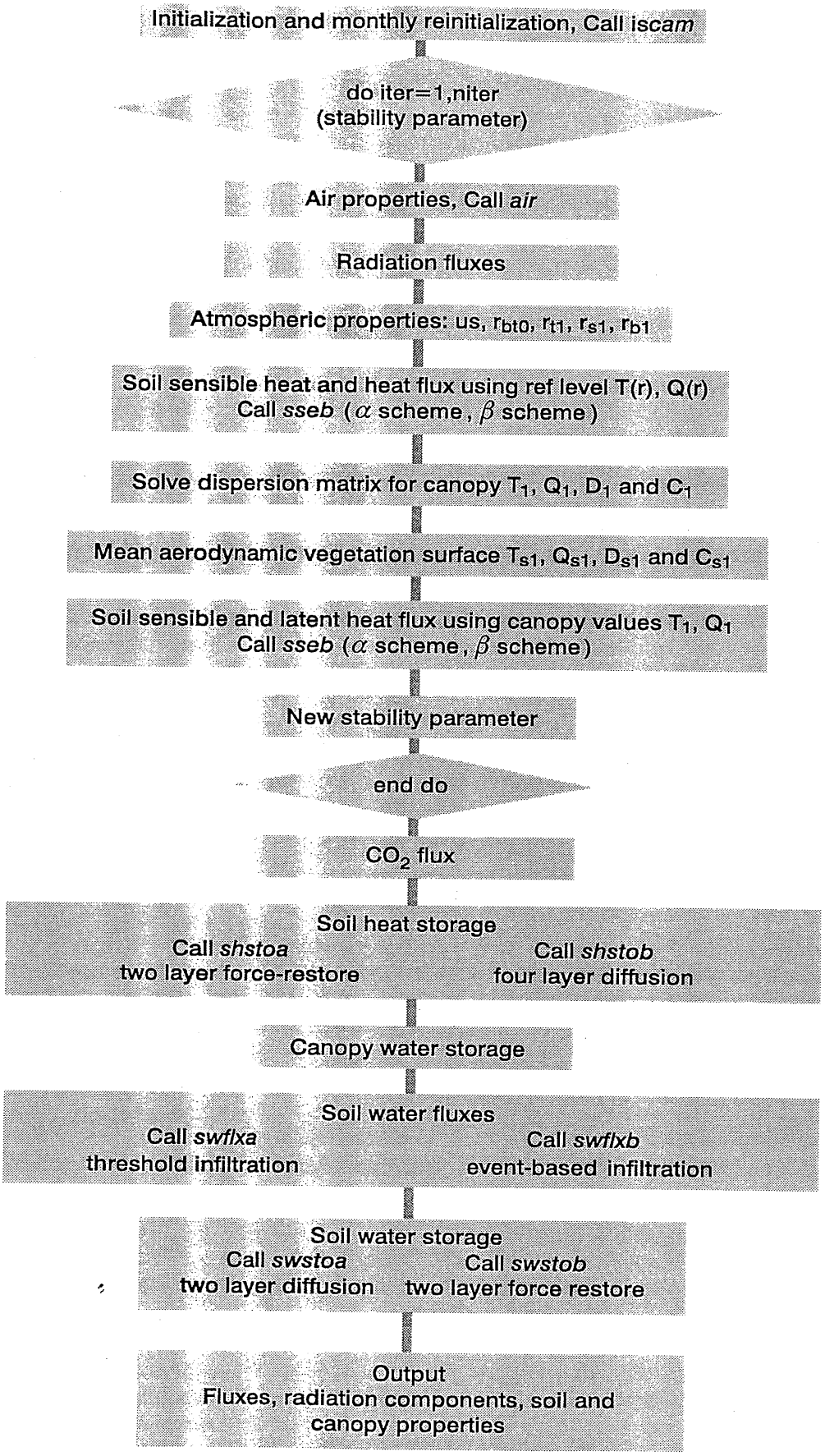

Figure 2.2: Schematic flow diagram of SCAM

3. ATMOSPHERIC FLUXES

3.1 Surface-to-Air Fluxes for Vegetation Elements

The sensible and latent heat fluxes from the vegetation to the air are calculated in SCAM from the Penman-Monteith or combination equation, a solution of the surface energy balance equations (2.1), (2.2) and (2.3) in which the surface temperature T_s is eliminated. This gives, for each vegetation layer ($i = 1,\ldots, n$):

$$f_{Ei} = \frac{\varepsilon r_{bi} f_{Ai} + \rho\lambda D_i}{(\varepsilon+1)r_{bi} + r_{si}} = \frac{\varepsilon r_{bi} f_{Ai} + \rho\lambda D_i}{r_{di}} \tag{3.1}$$

$$f_{Hi} = f_{Ai} - f_{Ei} \tag{3.2}$$

where $\varepsilon = (\lambda/c_p)\, dQ_{sat}/dt$ is the dimensionless gradient of the saturation specific humidity $Q_{sat}(T)$ with temperature; $D_i = Q_{sat}(T_i) - Q_i$ is the saturation deficit of the canopy air in layer i; r_{bi} and r_{si} are the boundary-layer and stomatal resistances for layer i, aggregated over all the elements in the layer (see below); and $r_{di} = (\varepsilon+1)r_{bi} + r_{si}$ is a resistance appearing as the denominator in the combination equation. The available energy flux f_{Ai} for layer i is given by

$$f_{Ai} = (1-a_i) f_{S\downarrow i} + e_i f_{L\downarrow i} - e_i \sigma T_{si}^4 \tag{3.3}$$

The resistances r_{bi} and r_{si} are aggregates for all surface elements (mainly leaves) in layer i. Even within a layer, these elements are not exposed to uniform conditions of radiation, temperature, saturation deficit and wind speed, and are physiologically variable for reasons such as variable leaf ages. Raupach (1995) discussed the aggregation of resistances in canopies with various radiation distributions (including the exponential distribution which we later use for radiation), by comparing a "flux-matching" averaging scheme with schemes based on parallel-sum definitions of the aggregated aerodynamic or surface resistances. The flux-matching scheme is based on linear averaging of scalar fluxes and matching of model form between scales, and is therefore better founded than parallel-resistance assumptions. Analytic forms for the aggregated resistances were derived under various averaging schemes. These showed that, for dry canopies (without free water on element surfaces), results from the flux-matching scheme are very close to those from parallel-resistance schemes. This information is used here in two ways: first to define the layer-aggregate stomatal and boundary-layer resistances, r_{si} and r_{bi}, separately for the dry and wet parts of each layer; then to amalgamate the dry and wet components.

Stomatal resistance: Let r_s and $g_s = r_s^{-1}$ denote the stomatal resistance and conductance of an individual leaf (distinguished from the layer aggregates by roman rather than italic script). For wet leaves, $r_s = 0$. For dry leaves, a multiplicative "stress function" model (Jarvis 1976) is used to describe the dependence of r_s on ambient variables:

$$r_s^{-1} = g_s = g_{sx}\, s_S(f_{S\downarrow})\, s_D(D_s)\, s_T(T_s)\, s_\eta(\eta_r) \tag{3.4}$$

where g_{sx} is the maximum leaf stomatal conductance, and the empirical stress functions s ($0 \le s \le 1$) account for decreases in g_s caused by low solar irradiance $f_{S\downarrow}$, high leaf-surface

saturation deficit D_s, high or low leaf temperature T_s, or water stress caused by low relative soil moisture η_r (averaged over the root zone). The assumed forms are:

$$s_S(f_{S\downarrow}) = \frac{f_{S\downarrow}}{f_{S\downarrow} + f_{S\downarrow *}} \tag{3.5}$$

$$s_D(D_s) = \frac{1}{1 + D_s/D_*} \tag{3.6}$$

$$s_T(T_s) = 1 - \left([2T_s - (T_h + T_l)]/(T_h - T_l)\right)^2 \tag{3.7}$$

$$s_\eta(\eta_r) = \frac{\eta_r - \eta_{r\min}}{\eta_{r\max} - \eta_{r\min}} \tag{3.8}$$

where $f_{S\downarrow *}$, , D_*, T_h, T_l, $\eta_{r\min}$ and $\eta_{r\max}$ are empirical coefficients, and the extra constraint $0 \le s \le 1$ is imposed as necessary. All of T_h, T_l and T_s are in °C, and $\eta_{r\max}$ and $\eta_{r\min}$ are respectively the values of η_r at the onset of water stress and at wilting. The relative soil moisture η_r is defined from the volumetric soil moisture content η by $\eta_r = (\eta - \eta_{dry})/(\eta_{sat} - \eta_{dry})$, where η_{sat} and η_{dry} are the saturated and air-dry values of η.

The layer-aggregate stomatal resistance r_{si} can now be obtained from its individual-leaf counterpart under a parallel-sum definition:

$$g_{si} = r_{si}^{-1} = \int_0^{\lambda_i} g_s(\zeta)\, d\zeta \tag{3.9}$$

where λ_i is the leaf area index in layer i and ζ a coordinate traversing the area elements in layer i (in arbitrary order). Equations (3.4), (3.5) and (3.9) are integrated over all the leaves in a layer, with two assumptions: first, $f_{S\downarrow}$ is exponentially distributed with extinction coefficient c, so the transmission of layer i is $\tau_i = \exp(-c\lambda_i)$; and second, all other properties are set to uniform, average values within the layer. This gives (Saugier and Katerji 1991, Dolman and Wallace 1991, Raupach 1995 (canopy IVa in that paper)):

$$r_{si}^{-1} = g_{si} = \frac{g_{sx}}{c} \ln\left(\frac{1 + X}{\tau_i + X}\right) s_D(D_s)\, s_T(T_s)\, s_\eta(\eta_r) \tag{3.10}$$

where

$$X = \frac{f_{S\downarrow *}}{\left(\prod_{k=i+1}^{n} \tau_k\right) F_{S\downarrow}} \tag{3.11}$$

with $F_{S\downarrow}$ the solar irradiance above the canopy, so that the denominator is the solar irradiance incident on the top of layer i. The layer-aggregate stomatal resistance for dry leaves is

determined by this equation, the required values of the surface quantities T_s and D_s being found by iteration (see below).

Boundary-layer resistance: Flow over leaves in a canopy is almost always laminar, though unsteady, and is sustained by forced rather than free convection (Finnigan and Raupach 1987). Therefore, the individual-leaf boundary-layer resistance $r_b = g_b^{-1}$ can be estimated for most conditions from the Polhausen solution for scalar transfer by forced convection through a laminar boundary layer on a flat plate. This yields:

$$g_b = r_b^{-1} = (A_b/\kappa)(U_i l/\nu)^{1/2}(\nu/\kappa)^{1/3} \qquad (3.12)$$

where l is the leaf or element cross-stream dimension, U_i the ambient wind speed in layer i, κ the molecular diffusivity in air for the transferred scalar, and ν the kinematic viscosity of air. The theoretical (Polhausen) value of the dimensionless coefficient A_b is about 0.7, for single-sided transfer on a flat plate parallel to a laminar ambient flow at Reynolds numbers low enough to maintain a laminar boundary layer ($U_i l/\nu < 20\,000$). The Polhausen formula yields a plausible first estimate for real leaves in canopies under most practical conditions, despite at least four real-world complications: unsteadiness due to larger-scale turbulence, complex geometry, leaf flapping and mutual shelter. The first three of these effects tend to increase A_b (Chen *et al.* 1988a,b), and the last to decrease A_b. The net result is that $A_b = 0.7$ gives a reasonable first estimate of r_b, because of mutually opposing complications.

The layer-aggregate boundary-layer resistance r_{bi} is determined from its individual-leaf counterpart r_b by a parallel summation like Equation (3.9). Assuming an exponential wind profile $U(z) = U(h)\exp[c_U(z/h-1)]$ with attenuation coefficient c_U, this gives:

$$g_{bi} = g_b(U_i)\frac{2\alpha_i h}{c_U\, c_{shelter}} \qquad (3.13)$$

where α_i is the leaf area density in layer i, and $c_{shelter}$ is a shelter coefficient to account for the sheltering of individual leaves, typically about 0.5 (Landsberg and Thom 1973).

The coefficient c_U is determined by matching dU/dz at $z = h$ from in-canopy and above-canopy (roughness-sublayer) profiles (see Section 3.7). This gives

$$c_U = \left[(kU_h/u_*)c_w(1-d/h)\right]^{-1} \qquad (3.14)$$

where k (= 0.4) is the von Karman constant, U_h the wind speed at canopy height ($z=h$), u_* the friction velocity, d the zero-plane displacement and $c_w = (z_{ruff}-d)/(h-d) \approx 2$ is a coefficient specifying the upper height limit z_{ruff} of the roughness sublayer (Raupach 1992, 1994).

The aggregation of dry and wet vegetation in layer i is done through a wet area fraction a_{wet} for the layer. Dry and wet latent heat fluxes f_{Ei}(dry) and f_{Ei}(wet) are calculated using Equation (3.1) with r_{si} given by Equations (3.4) to (3.11) for dry vegetation, $r_{si} = 0$ for wet vegetation, and r_{bi} for both dry and wet vegetation given by Equations (3.12) to (3.14). The fluxes are then combined with area weighting as required on conservation grounds (Raupach 1995):

$$f_{Ei} = (1-a_{wet})f_{Ei}(\text{dry}) + a_{wet}f_{Ei}(\text{wet}) \quad (3.15)$$

The sensible heat flux is then calculated from Equation (3.2). The wet area fraction a_{wet} is defined as W_{can}/W_{cansat}, where W_{can} is the canopy store (intercepted water held on the foliage) and W_{cansat} is the saturated value of this store (interception storage capacity). A bucket-style differential equation governs W_{can}: water is added to the canopy store from precipitation and withdrawn by evaporation at a rate governed by f_{Ei}(wet), with overflow to the soil whenever W_{can} exceeds W_{cansat}.

3.2 Surface-to-Air Fluxes for Soil

Soil-to-air fluxes are determined in part by the contents of the soil stores, especially the soil surface temperature T_{s0}. For the algebraic determination of fluxes during a time step, these store contents are treated as given, by values at the beginning of the time step. The soil-to-air sensible heat flux is determined by T_{s0} and the air temperature T_1 in the lowest canopy layer:

$$f_{H0} = \frac{\rho c_p (T_{s0} - T_1)}{r_{bt0}} \quad (3.16)$$

where r_{bt0} is the resistance from the ground to z_1 (the centre of layer 1). Unlike the boundary-layer resistances r_{bi} (i = 1 to n) for the vegetation layers, which represent laminar pathways only, r_{bt0} includes both laminar and turbulent pathways, as indicated by its notation. Its evaluation is dealt with in Section 3.7.

The soil-to-air latent heat flux (evaporation) is modelled by one of three alternative formulations (Mahfouf and Noilhan 1991), the "alpha", "beta" and "threshold" forms:

$$f_{E0} = \rho\lambda \frac{\alpha(\eta_{r1})Q_{sat}(T_{s0}) - Q_1}{r_{bt0}} \quad (3.17)$$

$$f_{E0} = \rho\lambda\beta(\eta_{r1}) \frac{Q_{sat}(T_{s0}) - Q_1}{r_{bt0}} \quad (3.18)$$

$$f_{E0} = \min(f_{E0}(\text{atm}), f_{E0}(\text{soil})) \quad (3.19)$$

where α and β are empirical functions (constrained to $0 \le \alpha \le 1$ and $0 \le \beta \le 1$) of the soil moisture content η_1 in the topmost soil layer. In the "alpha" and "beta" forms, f_{E0} is determined by the soil surface humidity and the humidity Q_1 in the lowest canopy layer (similar to f_{H0}). In the threshold form, f_{E0}(atm) is an atmospherically-limited rate (for instance, the potential rate $\alpha = \beta = 1$) and f_{E0}(soil) is a soil-limited rate determined by the upward diffusion rate of water through the soil, the actual soil evaporation being the lesser of the two (Philip 1957a). At this stage, the threshold form is not yet implemented in SCAM. Many forms for $\alpha(\eta_{r1})$ and $\beta(\eta_{r1})$ have been suggested (Mahfouf and Noilhan 1991). This is not surprising, given the empirical nature of the equations. Noilhan and Planton (1989) use an "alpha" scheme with:

$$\alpha(\eta_{r1}) = 0.5(1 - \cos(\pi\eta_{r1})) \quad (3.20)$$

where $\eta_{r1} = (\eta_1 - \eta_{dry})/(\eta_{sat} - \eta_{dry})$ is the relative water content in the topmost soil layer. This form is used for the "alpha" option in SCAM. For the "beta" option, we use a form which embraces several previous suggestions:

$$\beta(\eta_{r1}) = \min(\beta' \eta_{r1}, 1) \tag{3.21}$$

where β' is the slope of $\beta(\eta_{r1})$. Deardorff (1978) proposed $\beta' = 4/3$, while Kowalczyk *et al.* (1991) suggest forms dependent on soil type, which for most soils are approximated by $\beta' = 8$.

3.3 Dispersion Matrix Formulation for Turbulent Transfer

Aerodynamic transfer of heat, water vapour and CO_2 occurs over both laminar (element-boundary-layer) and turbulent pathways. The laminar pathway has been described in Section 3.1. We now treat turbulent transfer, which links the scalar concentration profile in the air, $C(z)$, to the profiles of source strength $S(z)$ and bulk vertical flux $F(z)$ (note the difference between the vertical flux $F(z)$ through a plane at height z, and the scalar flux from a canopy layer of thickness dz, $f(z) = S(z)dz$). In a horizontally uniform canopy without atmospheric storage, S and F are related through scalar conservation, by $S = dF/dz$ or $Sdz = f = dF$. However, relating C to either S or F requires a physical parameterisation of turbulent transfer.

It is useful to separate the "forward" problem (finding C from a specified S), the "inverse" problem (finding S from C) and the "implicit" problem (finding both S and C when they are linked by a specified relationship). The forward and inverse problems are defined by Raupach (1989b). The implicit problem arises as follows: for many scalars of interest, including heat and water vapour, $S(z)$ depends on the scalar concentration $C(z)$ itself. Such a dependence is implied by Equation (3.1), as the evaporation (water vapour source strength) depends on the saturation deficit in the canopy air and therefore on humidity (water vapour concentration). It is useful to suppose that this type of dependence can be expressed, sufficiently generally, by the linear relationship

$$f(z) = S(z)dz = A(z) - R(z)C(z) \tag{3.22}$$

The specified functions $A(z)$ and $R(z)$ are, respectively, a concentration-independent source strength (A) and a decay rate constant (R) for a sink (negative source) of strength ($-RC$). The forward and inverse problems are then linked implicitly because S and C are mutually dependent.

In discrete form, a solution to the forward problem expresses the air concentrations C_i (at levels z_i in the canopy) in terms of the source density profile and properties of the turbulence. Such a solution is linear (because of the superposition principle) and can be written in the general form (Raupach 1989a,b):

$$C_i' = C_i - C(r) = \sum_{j=0}^{n} M_{ij} f_j = \sum_{j=0}^{n} M_{ij} (S\Delta z)_j \tag{3.23}$$

where C_i is the concentration at z_i (the centre of canopy level i), $C(r)$ is the concentration at the reference height z_r above the canopy, C_i' is the concentration difference $C_i - C(r)$, and M_{ij} is the

"dispersion matrix", defined as the concentration difference C_i' produced in layer i by a unit source in layer j ($f_j = 1$) with zero source in all other layers. The source-profile index (j) runs from 0 to n (with $j = 0$ denoting the ground source f_0) while the concentration-profile index (i) runs from 1 to n (with C_1 being the concentration in the canopy layer adjacent to the ground). The elements of M_{ij} have the dimension of resistance. They parameterise the turbulent transfer in the sense that they depend solely on the properties of the turbulence inside the canopy, and fully describe the effect of the turbulence on the mean scalar field.

Our interest is in the inverse and implicit problems rather than the forward problem. Because of the interdependence between S and C, a solution requires that the number of concentration layers (i) and source layers (j) be the same, or that the matrix M_{ij} be square rather than ($n \times (n+1)$) as in Equation (3.23). To achieve a square M_{ij}, we lump the sources from the ground and the lowest canopy layer together, defining a lumped layer flux $\hat{f}_j$ (for $j = 1,\ldots,n$) as:

$$\hat{f}_1 = f_0 + f_1; \qquad \hat{f}_j = f_j \text{ for } j = 2,\ldots,n \tag{3.24}$$

We can now write a relationship between concentrations and fluxes which involves a square ($n \times n$) dispersion matrix. In formal tensor notation, using the convention of summation over repeated indices, this is

$$C_i' = M_{ij}\hat{f}_j \tag{3.25}$$

Henceforth, M_{ij} will be a ($n \times n$) square matrix defined by this equation.

In terms of the lumped layer fluxes, the generic linear source-sink relationship (Equation (3.22)) can be written (with summation convention) as

$$\hat{f}_j = A_j - R_{jk}C_k \tag{3.26}$$

where R_{jk} is nonzero when $j = k$, and zero when $j \neq k$. It is useful to express this equation in terms of the concentration differences $C_i' = C_i - C(r)$:

$$\hat{f}_j = \hat{f}_j(r) - R_{jk}C_k' \tag{3.27}$$

where

$$\hat{f}_j(r) = A_j - R_{jk}e_k C(r) \tag{3.28}$$

with e_k being the n-vector (1,1,...,1). Physically, $\hat{f}_j(r)$ is the lumped-layer flux computed from Equation (3.26) when the actual layer air concentration C_j is replaced by the reference-level concentration $C(r)$, retaining the layer values for A_j and R_{jk}.

The solution to the implicit problem can now be written easily. Putting Equation (3.27) into Equation (3.25), we obtain:

$$C_i' = M_{ij}\left[\hat{f}_j(r) - R_{jk}C_k'\right] \tag{3.29}$$

This can be rearranged to an inhomogeneous linear system in C_j':

$$\left[\delta_{ik} + M_{ij}R_{jk}\right]C_k' = M_{ij}\hat{f}_j(r) \tag{3.30}$$

where δ_{ij} is the Kronecker delta ($\delta_{ij} = 1$ when $i = j$, 0 otherwise). This linear system can be solved readily for C_i' once $\hat{f}_j(r)$, R_{jk} and M_{ij} are specified.

3.4 Dispersion Matrix for Coupled Heat and Water Vapour Transfer

For coupled heat and water vapour transfer with n vegetation layers and one soil surface layer, Equation (3.25) becomes a system of $2n$ equations:

$$\begin{aligned} T_i' &= T_i - T(r) = M_{ij}\,\hat{f}_{Hj}(T_j', Q_j')/\rho c_p \\ Q_i' &= Q_i - Q(r) = M_{ij}\,\hat{f}_{Ej}(T_j', Q_j')/\rho\lambda \end{aligned} \tag{3.31}$$

where T_i' and Q_i' are the departures from reference level conditions. The problem is coupled in the sense that the source strength for T depends not only on the concentration field T but also on the concentration field of another scalar (Q). Likewise the source strength for Q depends on both Q and T. Thus, there is "crosstalk" between T and Q. This will lead to a matrix R_{jk} in which off-diagonal elements are not always zero, as they are for the single-scalar problem.

The task is now to find the dependence of the layer fluxes f_{Hj} and f_{Ej} (and thence the lumped fluxes $\hat{f}_{Hj}$ and $\hat{f}_{Ej}$) on T_j' and Q_j', in the linearised form used in Equation (3.26). This can be done seeking expressions of the form

$$\begin{aligned} f_{Hj} &= f_{Hj}(r) + \rho c_p\left(a_{Hj}T_j' + b_{Hj}Q_j'\right) \\ f_{Ej} &= f_{Ej}(r) + \rho\lambda\left(a_{Ej}T_j' + b_{Ej}Q_j'\right) \end{aligned} \tag{3.32}$$

(without tensor summation) for both the vegetation ($j \geq 1$) and soil ($j = 0$) layers. Here, $f_j(r)$ are layer fluxes (not lumped-layer fluxes) calculated using the reference-level temperature, humidity and saturation deficit (T_r, Q_r and D_r) in place of in-canopy values (T_j, Q_j and D_j) in Equation (3.1). The coefficients a_j and b_j can be evaluated as follows. For vegetation layers ($j \geq 1$), the layer water vapour flux can be written from Equation (3.1) as

$$\begin{aligned} f_{Ej} &= \frac{\varepsilon r_{bj} f_{Aj} + \rho\lambda(Q_{sat}(T_j) - Q_j)}{(\varepsilon+1)r_{bj} + r_{sj}} \\ &= \frac{\varepsilon r_{bj} f_{Aj} + \rho\lambda[Q_{sat}(T_j) - Q_{sat}(T_r) + Q_{sat}(T_r) - Q_r + Q_r - Q_j]}{r_{dj}} \\ &= f_{Ej}(r) + \frac{\rho\lambda}{r_{dj}}\left(\frac{c_p\varepsilon}{\lambda}T_j' - Q_j'\right) \end{aligned} \tag{3.33}$$

This, together with the equivalent expression for f_{Hj}, shows that the coefficients a_j and b_j for vegetation layers ($j \geq 1$) are:

$$a_{Hj} = \frac{-\varepsilon}{r_{dj}}, \quad b_{Hj} = \frac{\lambda}{c_p r_{dj}}, \quad a_{Ej} = \frac{\varepsilon c_p}{\lambda r_{dj}}, \quad b_{Ej} = \frac{-1}{r_{dj}} \tag{3.34}$$

$$\begin{bmatrix} 1+r_{t1}(a_{H0}+a_{H1}) & r_{t1}(b_{H0}+b_{H1}) \\ r_{t1}(a_{E0}+a_{E1}) & 1+r_{t1}(b_{E0}+b_{E1}) \end{bmatrix} \begin{pmatrix} T_1' \\ Q_1' \end{pmatrix} = \begin{pmatrix} r_{t1}(f_{H0}(r)+f_{H1}(r))/\rho\, c_p \\ r_{t1}(f_{E0}(r)+f_{E1}(r))/\rho\, \lambda \end{pmatrix} \quad (3.39)$$

which can be cast in the form

$$\begin{aligned} A_H\, T_1' + B_H\, Q_1' &= C_H \\ A_E\, T_1' + B_E\, Q_1' &= C_E \end{aligned} \quad (3.40)$$

The solution is

$$T_1' = \frac{C_H B_E - B_H C_E}{A_H B_E - B_H A_E}, \qquad Q_1' = \frac{A_H C_E - C_H A_E}{A_H B_E - B_H A_E} \quad (3.41)$$

From these canopy temperature and humidity values, the layer fluxes can now be calculated using Equations (3.1), (3.16) and (3.18).

3.6 LNF Theory for the Dispersion Matrix

The technique used here for evaluating M_{ij} is a simplified form of the Localised Near-Field (LNF) theory (Raupach 1989a,b). This theory can accomodate the non-diffusive nature of the turbulence in the canopy, associated with the fact that the eddies responsible for most scalar transfer in a vegetation canopy have a vertical length scale that is a large fraction of the canopy height, and therefore larger than the vertical scale over which dC/dz changes significantly. The theory approaches the forward problem (finding C from S) by breaking C into two components: $C = C_f + C_n$. The "far-field" component C_f obeys a gradient-diffusion relationship between flux and concentration, while the "near-field" component C_n does not. Thus, C_f obeys

$$F(z) = -K_f(z)\frac{dC_f}{dz}, \qquad K_f(z) = \sigma_w^2(z) T_L(z) \quad (3.42)$$

where $\sigma_w(z)$ is the vertical velocity standard deviation, $T_L(z)$ the Lagrangian time scale for vertical velocity and K_f the far-field eddy diffusivity. The near-field component C_n accounts for the non-diffusive character of near-field dispersion; it is calculated by assuming the turbulence to be locally (but not globally) homogeneous, and then applying classical Lagrangian methods (Taylor 1921) to describe the near-field dispersion process. The full expressions for C_f and C_n are given in Raupach (1989a).

Recalling its definition, the dispersion matrix M_{ij} may be split into a far-field term and a near-field term in the same way that C is split into two terms $C_f + C_n$, so that:

$$M_{ij} = M_{ij}^{(f)} + M_{ij}^{(n)} \quad (3.43)$$

where all elements are functions only of $\sigma_w(z)$ and $T_L(z)$. The far-field matrix $M_{ij}^{(f)}$ describes the part of the concentration field which is given by the gradient-diffusion equation, (3.42). The

For the soil layer ($j = 0$), use of Equation (3.16) for f_{H0} and the "beta" form for f_{E0} (Equation (3.18)) shows the coefficients to be:

$$a_{H0} = \frac{-1}{r_{bt0}}, \quad b_{H0} = 0, \quad a_{E0} = 0, \quad b_{E0} = \frac{-\beta}{r_{bt0}} \tag{3.35}$$

A linear system of the form of Equation (3.30), containing $2n$ coupled equations, can now be written for T_i' and Q_i'. In this system, the vectors C_j' and $\hat{f}_j(r)$ become

$$C_j'^{(2)} = \begin{pmatrix} T_1' \\ T_2' \\ \vdots \\ T_n' \\ Q_1' \\ Q_2' \\ \vdots \\ Q_n' \end{pmatrix}; \quad \hat{f}_j^{(2)}(r) = \begin{pmatrix} (f_{H0}(r) + f_{H1}(r)) / \rho c_p \\ f_{H2}(r) / \rho c_p \\ \vdots \\ f_{Hn}(r) / \rho c_p \\ (f_{E0}(r) + f_{E1}(r)) / \rho\lambda \\ f_{E2}(r) / \rho\lambda \\ \vdots \\ f_{En}(r) / \rho\lambda \end{pmatrix} \tag{3.36}$$

and the matrices R_{ij} and M_{ij} become

$$R_{ij}^{(2)} = \begin{bmatrix} a_{H0} + a_{H1} & 0 \cdots & 0 & b_{H0} + b_{H1} & 0 & 0 \\ 0 & \ddots & 0 & 0 & \ddots & 0 \\ 0 & 0 & a_{Hn} & 0 & 0 & b_{Hn} \\ a_{E0} + a_{E1} & 0 & 0 & b_{E0} + b_{E1} & 0 & 0 \\ 0 & \ddots & 0 & 0 & \ddots & 0 \\ 0 & 0 & a_{Hn} & 0 & 0 & b_{Hn} \end{bmatrix}; \quad M_{ij}^{(2)} = \begin{bmatrix} M_{ij} & 0 \\ 0 & M_{ij} \end{bmatrix} \tag{3.37}$$

where M_{ij} is the ($n \times n$) dispersion matrix for a single scalar defined by Equation (3.25), and the (2) superscript denotes the coupled system of $2n$ equations. Because of the dependence of layer heat and water vapour fluxes on both temperature and humidity, the matrix $R_{ij}^{(2)}$ is no longer diagonal as it is in the case of a single scalar, and has two nonzero diagonals located n elements off the principal diagonal which account for the "crosstalk" between T and Q.

3.5 The Case of a Single Vegetation Layer

SCAM is based on a single vegetation layer ($n = 1$). The dispersion matrix M_{ij} in this case is simply the number (1×1 matrix) $r_t(1,r)$, henceforth shortened to r_{t1} and defined later in Section 3.7. Equation (3.31) for temperature and humidity becomes:

$$\begin{aligned} T_1' &= r_{t1}(f_{H0} + f_{H1}) / \rho c_p \\ Q_1' &= r_{t1}(f_{E0} + f_{E1}) / \rho\lambda \end{aligned} \tag{3.38}$$

and the linear equation system (3.30) becomes

elements of $M_{ij}^{(f)}$ can be expressed as aerodynamic resistances, by defining $r_t(j,r)$ to be the turbulent aerodynamic resistance from z_j (the centre of level j) to the reference level z_r above the canopy. Thus, for the general (n-level) case,

$$r_t(j,r) = \int_{z_j}^{z_r} \frac{dz}{K_f(z)} = \int_{z_j}^{z_r} \frac{dz}{\sigma_w^2(z)T_L(z)} \tag{3.44}$$

and $M_{ij}^{(f)}$ is given by

$$M_{ij}^{(f)} = \begin{bmatrix} r_t(1,r) & r_t(2,r) & \cdots & r_t(n,r) \\ r_t(2,r) & r_t(2,r) & \cdots & r_t(n,r) \\ \vdots & \vdots & \ddots & \vdots \\ r_t(n,r) & r_t(n,r) & \cdots & r_t(n,r) \end{bmatrix} \tag{3.45}$$

where columns (i = 1,..., n) represent concentration levels and rows (j = 1,..,n) represent lumped-source levels. In the case of a single vegetation layer (as used in SCAM), $M_{ij}^{(f)}$ reduces to a single element $r_t(1, r) = r_{t1}$.

3.7 Parameterisation of Turbulence Within and Above the Canopy

For thermally neutral flow within a vegetation canopy, the turbulence properties $\sigma_w(z)$ and $T_L(z)$ are governed by a single turbulent velocity scale and a single turbulent length scale, for which convenient choices are the friction velocity u_* and the canopy height h. These two scales approximately collapse observed profiles of many turbulence moments in both field and wind tunnel model canopies (Raupach 1988; Kaimal and Finnigan 1994; Raupach *et al.* 1996). The turbulence in the canopy also depends on the leaf area density profile $\alpha(z)$, but in practice it is reasonable to reduce this dependence to one on the leaf area index $\Lambda = \int_0^h \alpha(z)dz$.

To obtain the friction velocity u_*, we use the reference-level wind speed U_r (at reference height z_r) together with the canopy roughness length z_0:

$$u_* = \frac{kU_r}{\ln((z_r-d)/z_0) - \psi_M((z_r-d)/L_{MO}) + \psi_M(z_0/L_{MO})} \tag{3.46}$$

where d is the zero-plane displacement, k is the von Karman constant, L_{MO} is the Monin-Obhukov length and ψ_M is the diabatic influence function for the velocity profile (Garratt 1992). The last term in the denominator is often ignored, but is retained here because there is no assumption that the canopy roughness length is small compared with L_{MO}.

Within and just above the canopy, we adopt the following parameterisation for $\sigma_w(z)$:

$$\sigma_w(z)/u_* = a_3 \min\left[\exp(c_{sw}\Lambda(z/h-1)), 1\right] \tag{3.47}$$

where z is height above ground, h the canopy height, u_* the friction velocity, a_3 the ratio σ_w/u_* in the inertial sublayer above the canopy, and c_{sw} a constant determining the rate of decrease of

$\sigma_w(z)$ with depth in the canopy. This form is based on a simplified, analytic second-order closure model of canopy turbulence by Weil (personal communication). It allows for a decrease in $\sigma_w(z)$ within the canopy with increasing Λ, while holding $\sigma_w(z)$ constant at $a_3 u_*$ above the canopy. Values adopted for the constants are $a_3 = 1.25$, $c_{sw} = 1.0$. The former is derived from common surface-layer observations (Garratt 1992), and the latter by fitting Equation (3.47) to the model of Weil.

The parameterisation adopted for $T_L(z)$ is:

$$T_L(z) = \begin{cases} \dfrac{k(z-d)}{a_3^2 u_* \phi_H\left((z-d)/L_{MO}\right)}, & z \geq z_{ruff} \\ f_{sparse}(\Lambda)\, c_{TL} h/u_* , & d \leq z \leq z_{ruff} \\ f_{sparse}(\Lambda)\, (c_{TL} h/u_*)\, (z/d) , & 0 \leq z \leq d \end{cases} \qquad (3.48)$$

where d is the zero-plane displacement; k is the von Karman constant; c_{TL} is a number determining the magnitude of T_L within and just above the canopy; and ϕ_H the Monin-Obukhov stability function for the scalar profile gradient in the inertial sublayer (a function of the stability parameter $(z\text{-}d)/L_{MO}$). The "sparseness factor" $f_{sparse}(\Lambda)$, fully described below, is a monotonically increasing dimensionless function (between 0 and 1) of the leaf area index Λ, which is 1 for medium to dense canopies. It accounts for the requirements of the sparse-canopy limit. Values adopted for the constants are $k = 0.4$, $c_{TL} = 0.4$. The normalised displacement height d/h is a function only of Λ, given by Raupach (1994). Equation (3.48) for $T_L(z)$ is based on the following ideas:

- *Roughness-sublayer depth:* z_{ruff} is the point where the canopy time scale matches the outer canopy time scale. Ignoring stability effects, this is

$$z_{ruff} = d + \left(\frac{a_3^2 f_{sparse}(\Lambda)\, c_{TL}}{k} \right) h \qquad (3.49)$$

- *Inertial sublayer:* Above the roughness sublayer (which extends to height z_{ruff} above the ground), T_L takes on the inertial-sublayer value given by equating the expressions $\sigma_w^2 T_L$ and $ku_*(z\text{-}d)/\phi_H$ for the scalar eddy diffusivity.

- *Upper canopy and roughness sublayer:* In the layer $d \leq z \leq z_{ruff}$, the form for T_L is based on the hypothesis that the turbulence is patterned on a plane mixing layer rather than a surface boundary layer (Raupach *et al.* 1989, 1996). This implies that $T_L(z)$ should be roughly constant, rather than increasing linearly with height. The height-independent value $T_L = c_{TL} h/u_*$ is assumed (except in sparse canopies where $f_{sparse} < 1$), with $c_{TL} = 0.4$ (Raupach *et al.* 1992). Stability effects are ignored in this region and lower in the canopy. [Note: in future versions, an expression of the form $T_L = c_{TL2}(h\text{-}d)/u_*$ will be used.]

- *Lower canopy:* It is probable that T_L decreases in the lower canopy as the ground is approached, such that $T_L \propto z$ near the ground. We assume that T_L decreases linearly from $z = d$, to zero at $z = 0$.

Sparse-canopy limit: The limit $\Lambda \rightarrow 0$ implies vanishing leaf area index, or a vanishingly sparse canopy of finite height. This requires special consideration, because the canopy turbulent transfer should then approach the bare-ground limit. The limit of d as $\Lambda \rightarrow 0$ is $d \rightarrow 0$, but h remains constant and nonzero in the sparse-canopy limit, so both z_{ruff} and T_L remain nonzero as $\Lambda \rightarrow 0$ if there is no sparseness factor applied (that is, if $f_{sparse} = 1$). This implies that the model retains a "ghost" canopy as $\Lambda \rightarrow 0$. To avoid this problem, a sparseness factor $f_{sparse}(\Lambda)$ is included in the formulation for T_L in the canopy layers, such that $f_{sparse}(\Lambda) = 1$ for medium to dense canopies and $f_{sparse}(\Lambda) \rightarrow 0$ as $\Lambda \rightarrow 0$. By definition, this factor also appears in the expression for z_{ruff}, Equation (3.49). This ensures that $z_{ruff} \rightarrow 0$ as $\Lambda \rightarrow 0$, and that in the layer of constant $T_L(z)$ within the canopy, both the value of T_L and the depth of the layer becomes negligible as $\Lambda \rightarrow 0$. The physical reason why it is necessary to introduce $f_{sparse}(\Lambda)$ is that the canopy T_L profiles in Equation (3.48) are based on an analogy between flow in the upper canopy and a plane mixing layer (Raupach *et al.* 1989, 1996), a flow with only one dimension of inhomogeneity (z). This analogy, like any one-dimensional description, breaks down in the sparse-canopy limit because the wakes associated with individual canopy elements become strongly three-dimensional. We take $f_{sparse}(\Lambda) = \min[(3d/2h), 1]$, in which the dependence on Λ appears through d. The choice of the fraction in this expression determines the Λ at which f_{sparse} falls below 1 with decreasing Λ (that is, the Λ at which "sparseness" sets in). For the chosen fraction ($d/h = 2/3$), $f_{sparse} < 1$ below $\Lambda = 1.1$.

From the expressions for $\sigma_w(z)$ and $T_L(z)$, we can write the turbulent aerodynamic resistance $r_t(j,r)$, and thence the dispersion matrix M_{ij}, using Equations (3.44) and (3.45). For the case of a single vegetation layer ($n = 1$), the effective centre of the layer is taken to be $z = d$ and the following expressions are obtained for $r_t(1,r)$ (denoted by r_{t1}):

$$r_t(1,r) \quad = \quad r_{t1} \quad = \quad r_{t1(a)} + r_{t1(b)} + r_{t1(c)} \tag{3.50}$$

where the three terms represent, respectively, resistances over pathways from d to h, h to z_{ruff}, and z_{ruff} to z_r. They are given by:

$$u_* r_{t1(a)} = \int_d^h \frac{dz}{a_3^{\,2} \exp[2 c_{sw} \Lambda (z/h - 1)] f_{sparse} c_{TL} h} = \frac{\exp[2 c_{sw} \Lambda (1 - d/h)] - 1}{(a_3^{\,2} f_{sparse} c_{TL})(2 c_{sw} \Lambda)} \quad (3.51)$$

$$u_* r_{r1(b)} = \int_h^{z_{ruff}} \frac{dz}{a_3^{\,2} f_{sparse} c_{TL} h} = \frac{z_{ruff} - h}{a_3^{\,2} f_{sparse} c_{TL} h} \quad (3.52)$$

$$u_* r_{t1(c)} = \int_{z_{ruff}}^{z_r} \frac{\phi_H((z-d)/L_{MO})\, dz}{k(z-d)} = \frac{1}{k}\left[\ln\left(\frac{z_r - d}{z_{ruff} - d}\right) - \psi_H\left(\frac{z_r - d}{L_{MO}}\right) + \psi_H\left(\frac{z_{ruff} - d}{L_{MO}}\right)\right] \quad (3.53)$$

The aerodynamic (turbulent plus boundary-layer) resistance from the ground to the centre of layer 1, r_{bt0}, is required for the calculation of the soil-to-air sensible and latent heat fluxes, Equations (3.16) - (3.18). This depends on the roughness of soil, characterised by a soil roughness length $z_{0\,soil}$. Then:

$$u_* r_{bt0} = \int_{z0\,soil}^{d} \frac{dz}{a_3^{\,2} \exp[2 c_{sw} \Lambda (z/h - 1)]\ f_{sparse} c_{TL} h\, z/d} \approx \ln\left(\frac{d}{z_{0soil}}\right) \frac{\exp[2 c_{sw} \Lambda] - \exp[2 c_{sw} \Lambda (1 - d/h)]}{(a_3^{\,2} f_{sparse} c_{TL})(2 c_{sw} \Lambda)} \quad (3.54)$$

3.8 Radiation

Radiation in SCAM is treated very simply at present. Both the shortwave and longwave radiant energy fluxes (irradiances) are computed by assuming the canopy to be a turbid medium in which extinction is described by Beer's law. The following equations cover only the case n = 1, a single vegetation layer with leaf area index Λ. The fraction of incident radiation reaching the ground, or canopy transmission, is

$$\tau = \exp(-c\Lambda) \quad (3.55)$$

where c is an extinction coefficient. No distinctions are carried between different parts of the shortwave spectrum, direct and diffuse beams, or sunlit and shaded leaves. At this coarse level of description, a typical average value of c is 0.6 (Denmead 1976). The incoming and outgoing beams (both shortwave and longwave) are treated with a "single-scattering" approximation in which multiple scattering is ignored explicitly, though implicitly it is parameterised by τ. Thus, the canopy is treated as a screen with transmission (optical porosity) τ, a view consistent with the single-layer treatment of the canopy. In this approximation, the following equations specify the incoming and outgoing irradiances to the ground and the vegetation layer, in terms of the bulk incoming shortwave and longwave irradiances $F_{S\downarrow}$ and $F_{L\downarrow}$, which are externally specified. The radiation model is illustrated in Figure 3.1.

Shortwave: The bulk incoming shortwave irradiance $F_{S\downarrow}$ above the canopy is partitioned between vegetation (subscript 1) and soil surface (subscript 0) according to:

$$\begin{aligned} f_{S\downarrow 1} &= (1-\tau)F_{S\downarrow} \\ f_{S\downarrow 0} &= \tau F_{S\downarrow} \end{aligned} \tag{3.56}$$

The net (incoming less outgoing) shortwave irradiance on vegetation and ground is then:

$$\begin{aligned} f_{S\downarrow 1} - f_{S\uparrow 1} &= (1-a_1)f_{S\downarrow 1} \\ f_{S\downarrow 0} - f_{S\uparrow 0} &= (1-a_0)f_{S\downarrow 0} \end{aligned} \tag{3.57}$$

with a_1 and a_0 the vegetation and ground albedo, respectively. The albedo values are bulk (areally-averaged) rather than single-element values, noting that the two can be very different because of multiple scattering (Dickinson 1992).

Longwave: For the ground, the incoming and outgoing longwave irradiances are:

$$\begin{aligned} f_{L\downarrow 0} &= \tau F_{L\downarrow} + (1-\tau)e_1\sigma T_{s1}^4 \\ f_{L\uparrow 0} &= e_0\sigma T_{s0}^4 \end{aligned} \tag{3.58}$$

where e_1 and e_0 are the vegetation and ground emissivities, and T_{s1} and T_{s0} the vegetation and ground surface temperatures. In the equation for $f_{L\downarrow 0}$, the first term on the right hand side represents the part of the incoming longwave sky irradiance $F_{L\downarrow}$ that reaches the ground, and the second the downward longwave radiation emitted from the vegetation. The incoming and outgoing longwave irradiances for the vegetation layer are:

$$\begin{aligned} f_{L\downarrow 1} &= (1-\tau)F_{L\downarrow} + (1-\tau)e_0\sigma T_{s0}^4 \\ f_{L\uparrow 1} &= 2(1-\tau)e_1\sigma T_{s1}^4 \end{aligned} \tag{3.59}$$

Here the first and second terms of the first equation represent, respectively, the contributions to longwave irradiance on the vegetation from the sky and the ground, respectively. The factor 2 in the outgoing longwave radiation equation accounts for fact that the vegetation emits longwave radiation both upward and downward.

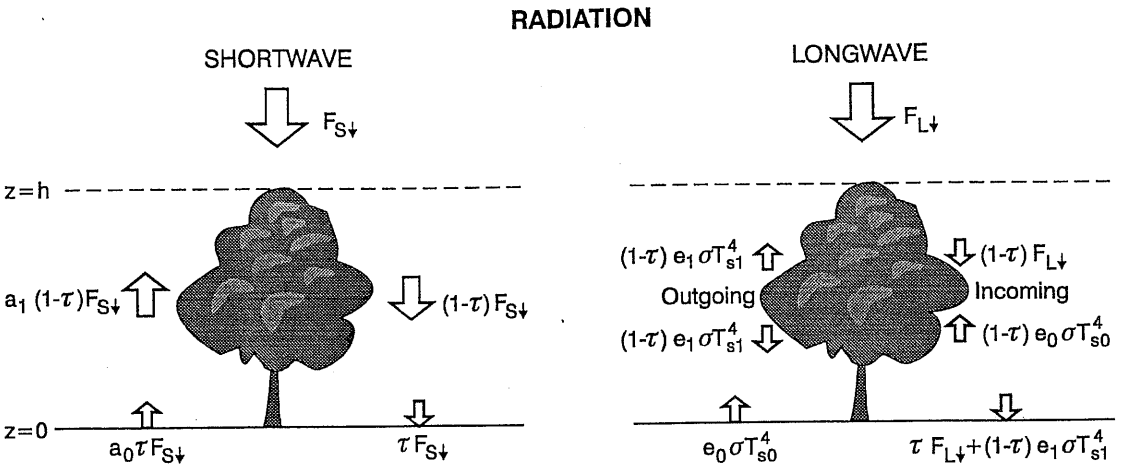

Figure 3.1: Shortwave and longwave radiation for the ground and vegetation.

3.9 Iteration for Surface Concentrations and Stability Parameter

Description of the calculation procedure for the atmospheric fluxes is now almost complete. Specified variables are the weather variables ($F_{S\downarrow}$, $F_{L\downarrow}$, T_r, Q_r, U_r), which are externally given; and the soil store contents (T_{s0} and η_1), which are determined by solving the differential equations given in Section 4 and are treated as fixed (at their values at the beginning of each time step) for calculating atmospheric fluxes. However, variables yet unspecified in the atmospheric flux calculation are the vegetation surface temperature T_{s1} and saturation deficit D_{s1}, and the stability parameter $\zeta = (z_r - d)/L_{MO}$ (where L_{MO} is the Monin-Obukhov length). Of these, T_{s1} affects the net radiation fluxes; both T_{s1} and D_{s1} influence the stomatal resistance r_{s1}; and ζ influences the turbulent resistances. To find these variables, an iterative method is necessary.

The most difficult aspect of this iteration procedure is the determination of

$$\zeta = \frac{z_r - d}{L_{MO}} = -\frac{kg(z_r - d)(F_H + 0.07F_E)}{\rho c_p T_r u_*^3} \qquad (3.60)$$

A direct iteration procedure would be: calculate F_H, F_E and u_* using an intial assumed value of ζ (say $\zeta = 0$); calculate ζ from these fluxes using Equation (3.60); recalculate fluxes using the new ζ; iterate to convergence. However, this procedure is often unstable and diverges rapidly. The reasons for this fact, and its consequences, are the subject of a paper in preparation. Therefore, in SCAM, the following simple 2-step iteration procedure is used to determine T_{s1}, D_{s1} and ζ at each time step. The iteration step (at any time step) is denoted by the superscript k (Roman).

(0) To start the procedure (k = 0), neutral stability within the canopy layer is assumed, so $\zeta^{(k=0)} = 0$, $T_{s1}{}^{(k=0)} = T_r$ and $D_{s1}{}^{(k=0)} = D_r$.

(1) First-iteration values (k = 1) are calculated for the soil and vegetation fluxes f_{H0}, f_{E0}, f_{H1}, f_{E1}, the bulk fluxes F_H, F_E and the friction velocity u_*. First-iteration values of $T_{s1}^{(k=1)}$, $D_{s1}^{(k=1)}$ and $\zeta^{(k=1)}$ are then found from the first-iteration fluxes.

(2) On the second and final iteration, the stability parameter is assumed to be a constant fraction of $\zeta^{(k=1)}$:

$$\zeta = c_\zeta \zeta^{(k=1)} \text{ with } c_\zeta = 0.4 \tag{3.61}$$

All atmospheric fluxes are then determined, using this ζ and $T_{s1}^{(k=1)}$, $D_{s1}^{(k=1)}$.

This procedure is quick, numerically stable and provides quite a good approximation to the exact solution (which can be obtained by using the bisection method to find ζ, a robust but very inefficient method). The value 0.4 for c_ζ has been found to be a reasonable approximation, especially on the unstable side. On the stable side it slightly overestimates ζ (work by the present authors, in preparation).

4. SOIL AND CANOPY STORAGE OF HEAT AND WATER

To determine changes in the soil and canopy heat and water stores, together with associated fluxes, it is necessary to solve differential equations of the general form of Equations (2.10) and (2.11). Several alternative schemes have been developed; all are described here.

4.1 Soil Heat Storage

Two schemes for solving the soil heat balance equation have been tested and are available in SCAM: a two-layer force-restore scheme (Section 4.1.1) and an m-layer diffusion scheme where m can be arbitrary (Section 4.1.2). We recall that soil thermal layer j lies between depths $Z_{G,j-1}$ and $Z_{G,j}$ (j=1 denoting the top layer) and that the average temperature in layer j is T_j (with $T_0 = T_{s0}$ being the surface temperature). Thus,

$$T_j = (Z_j - Z_{j-1})^{-1} \int_{Z_{j-1}}^{Z_j} T(Z)\, dZ \tag{4.1}$$

4.1.1 Soil Heat Storage by Force-Restore Method

The "force-restore" scheme (Bhumralkar 1975; Blackadar 1976; Deardorff 1977, 1978; Dickinson 1988) simplifies the soil heat equation (2.5) to two coupled ordinary differential equations, one for the soil surface temperature T_0 and the other for the bulk soil temperature T_2 averaged over the layer ($0 \le Z \le Z_{G2}$). These equations describe the soil heat balance in two overlapping layers: a shallow layer ($0 \le Z \le Z_{G1}$), and a deep layer ($0 \le Z \le Z_{G2}$). There is zero flux through Z_{G2}. The layer depths Z_{G1} and Z_{G2} are the propagation depths for sinusoidal daily and annual temperature waves, respectively, given by:

$$\begin{aligned} Z_{G1} &= Z_{G,day} = (\kappa_G\, t_{day} / \pi)^{1/2} \\ Z_{G2} &= Z_{G,year} = (\kappa_G\, t_{year} / \pi)^{1/2} \end{aligned} \tag{4.2}$$

where κ_G is the soil thermal diffusivity, t_{day} = 1 day, and t_{year} = 1 year. The equations for T_0 and T_2 are:

$$\begin{aligned} \frac{dT_0}{dt} &= c_{T1} \frac{f_{G0}}{C_G Z_{G1}} + c_{T2} \frac{(T_2 - T_0)}{t_{day}} \\ \frac{dT_2}{dt} &= \frac{f_{G0}}{C_G Z_{G2}} \end{aligned} \tag{4.3}$$

where C_G is the soil heat capacity (J m^{-3} K^{-1}), f_{G0} is the ground heat flux (into the soil surface), and c_{T1} and c_{T2} are dimensionless coefficients. The ground heat flux is determined from the soil surface energy balance $f_{G0} = f_{N0} - f_{H0} - f_{E0}$, with f_{N0} the net irradiance on the soil surface. The coefficients c_{T1} and c_{T2} are chosen so that the solution of Equation (4.3) matches the exact solution of Equation (2.5) for T_0 and T_2, for sinusoidal temperature oscillations of periods 1 day and 1 year. This gives $c_{T1} = 2$ and $c_{T2} = 2\pi$. These two periods are chosen because they are the most prominent in the temporal spectrum of soil temperature.

4.1.2 Soil Heat Storage with m-Layer Diffusion Equation

The m-layer soil heat storage scheme is based on Equation (2.10):

$$\frac{dT_j}{dt} = \frac{-\left(f_{G,j} - f_{G,j-1}\right)}{C_{G,j}\left(Z_{G,j} - Z_{G,j-1}\right)}, \qquad j = 1,\ldots,m \tag{4.4}$$

where $C_{G,j}$ is the heat capacity of layer j and $f_{G,j}$ is the heat flux across $Z_{G,j}$ (the interface between layers j and j+1). There is no equation for the soil surface temperature T_0, which is inferred by making the first layer thin enough to assume that $T_0 = T_1$. The heat flux is calculated from a temperature gradient derived from the layer-averaged T_j:

$$f_{G,j} = \frac{-\alpha_j\left(T_{j+1} - T_j\right)}{0.5\left(\dfrac{Z_{G,j+1} - Z_{G,j}}{K_{G,j+1}} + \dfrac{Z_{G,j} - Z_{G,j-1}}{K_{G,j}}\right)} \tag{4.5}$$

where $K_{G,j} = C_{G,j}\kappa_G$ is the thermal conductivity of layer j, and α_j is an enhancement factor accounting for the use of layer-averaged temperatures in computing dT/dZ at the interface between layers j and j+1. The factor α_j is calculated following McGregor *et al.* (1993), by assuming that the soil temperature profile has an exponential form:

$$T(z) = \overline{T} + \Delta T e^{-\gamma z} \tag{4.6}$$

where γ is an attenuation coefficient. By comparing the exact and numerically approximated gradients for this profile, it is found that (temporarily shortening $Z_{G,j}$ to Z_j):

$$\alpha_j = \frac{\gamma^2 \exp(-\gamma Z_j)\,0.5(Z_{j+1} - Z_{j-1})(Z_j - Z_{j-1})(Z_{j+1} - Z_j)}{\left\{\begin{array}{l}\left(Z_{j+1} - Z_j\right)\left[\exp\left(-\gamma Z_{j-1}\right) - \exp\left(-\gamma Z_j\right)\right] \\ \quad - \left(Z_j - Z_{j-1}\right)\left[\exp\left(-\gamma Z_j\right) - \exp\left(-\gamma Z_{j+1}\right)\right]\end{array}\right\}} \tag{4.7}$$

The attenuation coefficient γ is the inverse of a propagation depth, and therefore depends on the dominant forcing frequency at the depth $Z_{G,j}$ for which α_j is calculated. Since the dominant forcing frequencies are either daily or annual, we have calculated α_j using either $\gamma = 1/Z_{G,day}$ or $\gamma = 1/Z_{G,year}$ (see Equation (4.2)), depending on whether $Z_{G,j}$ is closer to the daily or the annual propagation depth.

We have found that adequate representations of analytic solutions to the heat diffusion equation are obtained from this scheme with $m = 4$, with layer depths $Z_{G,j} = 0.06$, 0.2, 0.6 and 2.0 m, independent of soil type and moisture content. The enhancement factors are calculated using daily propagation depth to define γ at 0.06 and 0.2 m, and the annual propagation depth at 0.6 m. This gives $\alpha_1 = 1.186$ (at 0.06 m), $\alpha_2 = 1.476$ (at 0.2 m), $\alpha_3 = 1.169$ (at 0.6 m). Note that α_4 is not required because of the assumption that the flux is zero at the bottom boundary. These choices are used in SCAM.

4.2 Soil Water Fluxes

To find the evolution of the soil moisture contents ($\eta_j, j = 1,\ldots,m$) in m layers of a soil column, it is necessary to know (a) the soil water fluxes at the boundaries of the soil column; and (b) how the η_j evolve under the influence of water fluxes across the soil column boundaries and the internal redistribution of water in the column. These two topics are dealt with here and in Section 4.3, respectively.

The soil hydrology depends critically on the soil hydraulic properties, principally the hydraulic conductivity $K(\eta)$ and soil water diffusivity $D(\eta)$. These can be specified using one of several available parameterisations. Here we use the functions of Campbell (1974). Our soil type classification is that of Clapp and Hornberger (1978) and Cosby *et al.* (1984), which consists of 11 soil types with specifications for each type of the parameters entering the Campbell soil hydraulic functions. Details of the soil hydraulic functions are in Appendix A.

The soil water fluxes required are:

(a) fluxes at the surface and bottom boundaries of the soil column, including the soil evaporation rate q_{Es}, the Hortonian surface runoff q_{Hrun}, the infiltration rate q_{inf}, the deep drainage rate q_{drain};

(b) sink water fluxes out of each layer, including the plant transpiration rate q_{Ev} and the Dunne-Black runoff rate for each layer $q_{DBrun,j}$.

Specifications of soil evaporation q_{Es} and plant transpiration q_{Ev} have already been given. Equations (3.17) to (3.19) define q_{Es}, and Equation (3.33) defines q_{Ev} [in terms of the latent heat fluxes f_{Ej} for each canopy layer, so $q_{Ev} = (f_{E1}+\ldots+f_{En})/(\rho\lambda)$]. Below, we give two alternative schemes for estimating the infiltration flux (q_{inf}): a "threshold" scheme (Section 4.2.1) and an event-based scheme (Section 4.2.2). Deep drainage (q_{drain}) is covered in Section 4.2.3 and the runoff fluxes (q_{Hrun} and $q_{DBrun,j}$) are described in Section 4.2.4.

4.2.1 "Threshold" Infiltration

This infiltration parameterisation follows Mahrt and Pan (1984). The infiltration rate is limited by a maximal rate at which ponding (or runoff) occurs. Below ponding, the infiltration rate is equal to the rainfall rate reaching the soil (after accounting for canopy interception):

$$q_{inf} = \min(q_{pres}, q_{pond}) \tag{4.8}$$

The ponded infiltration rate is estimated from Darcy's law as

$$q_{pond} = K(\eta_{sat}) + D(\eta_{sat})\frac{\eta_{sat}-\eta_1}{Z_{W1}/2} \tag{4.9}$$

where $K(\eta)$ and $D(\eta)$ are the soil hydraulic conductivity and soil moisture diffusivity. The hydraulic conductivity at saturation $K(\eta_{sat})$ is equivalent with K_{sat}, the saturation hydraulic conductivity. The gradient of soil moisture is calculated from the surface to the midpoint of the first layer ($Z_{W1}/2$).

4.2.2 Event-Based Infiltration

This infiltration parameterisation is based on the Philip (1957b) equation for saturated-surface or ponded infiltration into a soil of uniform initial moisture content:

$$I_{pond}(t) = \int_0^t q_{pond}(t)\,dt = St^{1/2} + At; \quad q_{pond}(t) = \frac{St^{-1/2}}{2} + A \tag{4.10}$$

where q_{pond} is the ponded infiltration rate, I_{pond} is the cumulative ponded infiltration since the beginning of the rainfall event, S is the sorptivity (m $s^{-1/2}$), and A is a constant with the dimension of velocity related to K_{sat}. For most soil types $A \approx K_{sat}/2$, and although this is not an exact equality (Philip 1988), we assume $A = K_{sat}/2$. The sorptivity S is given by

$$S = S_{ref}\left[\frac{\eta_{sat} - \eta_{init}}{\eta_{sat} - \eta_{dry}}\right]^{1/2} \tag{4.11}$$

where η_{init} is the uniform soil moisture at the onset of the rainfall event and S_{ref} the reference sorptivity for initially dry soils. Equation (4.10) is a short-time approximation, replaced at long times by $q_{inf} = q_{pond} \rightarrow K_{sat}$.

Application of Equation (4.10) requires recognition of the fact that, at the beginning of a rainfall event, the soil surface is not initially saturated. This can be accounted for by using the "time compression analysis" of Salvucci and Entekhabi (1994) for discrete rainfall events, which Cook *et al.* (1997) have extended to calculate infiltration over time steps significantly smaller than entire rainfall events. This is an event-based scheme in which times are measured from the start of a rainfall event (t=0). The condition for resetting and triggering the event timer is the commencement of rainfall after a sufficiently long period of no rain (so that frequent intermittent showers constitute a single rainfall event). The rain-free time interval necessary to reset the event timer, and define a new rainfall event, is defined as the gravitational time constant t_g of the soil,

$$t_g = \left(\frac{S_{ref}}{K_{sat}}\right)^{1/2} \tag{4.12}$$

where S_{ref} is the reference (maximal) sorptivity (m $s^{-1/2}$).

The time-compression method is based on the following chain of reasoning. First, the time to ponding (t_p) is defined as the time at which the soil surface becomes saturated and runoff commences. At times less than t_p, infiltration equals rainfall incident on the soil ($q_{inf} = q_{pres}$), while for times greater than t_p, $q_{inf} < q_{pres}$. For steady rainfall, the time to ponding satisfies $I(t_p) = t_p q_{pres}$, where $I(t)$ is the actual cumulative infiltration (the integral of $q_{inf}(t)$ from 0 to t). The infiltration equation (4.10) does not apply when $t < t_p$, because the soil surface is not saturated.

Next, the time to ponding is estimated by assuming that the actual cumulative infiltration up to the ponding time is equal to the ponded (saturated-surface) cumulative infiltration up to the time at which $q_{pond}(t) = q_{pres}$. This time, denoted t_c, is the time prior to

which the *ponded* infiltration rate exceeds the rainfall rate (see Figure 4.1). From Equation (4.10), t_c is given by

$$t_c = \left[\frac{S}{2q_{pres} - K_{sat}}\right]^2 \tag{4.13}$$

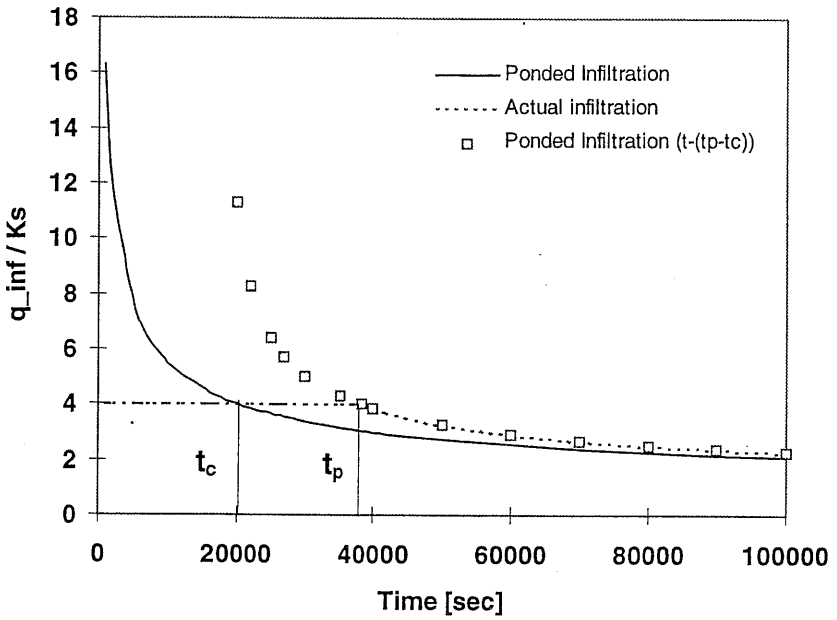

Figure 4.1: Time compression analysis for infiltration with a constant rainfall rate.

It follows that the estimate of the ponding time is given from

$$I(t_p) = t_p q_{pres} = I_{pond}(t_c) = St_c^{1/2} + t_c K_{sat}/2 \tag{4.14}$$

so the ponding time is:

$$t_p = \frac{St_c^{1/2} + t_c K_{sat}/2}{q_{pres}} \tag{4.15}$$

Finally, the actual infiltration rate at times $t > t_p$ is assumed to follow the ponded infiltration curve once the ponding time has elapsed, as shown in Figure 4.1. Therefore, this curve is displaced on the time axis by $(t_p - t_c)$. It follows that, for $t > t_p$,

$$q_{inf} = \max\left[\left(\frac{S}{2(t - t_p + t_c)^{1/2}} + \frac{K_{sat}}{2}\right), K_{sat}\right] \tag{4.16}$$

The first term in the maximum is the Philip equation for ponded infiltration, with a displaced time axis, while the second accounts for the fact that the Philip equation is an approximation which breaks down at large times.

4.2.3 Deep Drainage

Deep drainage is the water flux through the bottom boundary, $Z=Z_{W,m}$ for an m-layer scheme. It is estimated (accounting for gravitational water movement only and ignoring capillarity) by:

$$q_{drain} = f_{drain} K(\eta_m) \tag{4.17}$$

where $K(\eta_m)$ is the soil hydraulic conductivity of the layer adjacent to the bottom boundary, and f_{drain} is a parameter between 0 and 1 which determines whether the bottom boundary is free-draining ($f_{drain} = 1$), zero-flux ($f_{drain} = 0$) or intermediate ($0 < f_{drain} < 1$, representing a semi-impermeable soil below the bottom boundary).

4.2.4 Runoff

Surface runoff can be generated by two major mechanisms: *infiltration excess runoff*, or Hortonian overland flow, and *saturation excess runoff*, or Dunne and Black overland flow (Freeze, 1974). The Hortonian mechanism gives rise to runoff from patches (elementary areas within a catchment) where soils become saturated at the surface as a result of a downward water flux from above. This occurs when rainfall intensity exceeds infiltration capacity. The elementary areas where this occurs are controlled by the distribution of soil types. Dunne and Black overland flow is generated by rainfall on areas where the soil is already saturated by saturation from below. This mechanism of surface runoff generation occurs primarily on the lower slopes of hills and along valley bottoms adjacent to stream channels. The two mechanisms can occur concurrently, and merge into one another in a given catchment. The predominance of one mechanism over the other depends on the controls (soil type and initial water content) existing at a given point.

Hortonian runoff occurs when the precipitation rate incident on the soil, q_{pres}, exceeds the infiltration rate q_{inf} given by either the threshold scheme (Section 4.2.1) or the event-based scheme (Section 4.2.2). The consequent runoff rate is simply

$$q_{Hrun} = q_{pres} - q_{inf} \tag{4.18}$$

Dunne-Black runoff occurs when part of the soil column becomes saturated and can absorb no more water, even if the net incoming water flux is very small. Numerically, this is handled by a two-stage process at each time step: first, the soil moisture distribution at the end of the time step (time $t+\Delta t$) is calculated using any choice of schemes in Sections 4.2 and 4.3. Let the result of this calculation be $\eta_j'(t+\Delta t)$. Since there is no constraint against oversaturation, it is possible that $\eta_j'(t+\Delta t)$ exceeds η_{sat} in any layer. The second step is to dispose of the excess soil moisture $\eta_j'-\eta_{sat}$ by Dunne-Black runoff, so that

$$q_{DBrun,j} = \frac{Z_j - Z_{j-1}}{\Delta t} \max(\eta_j' - \eta_{sat}, 0) ; \qquad \eta_j = \min(\eta_j', \eta_{sat}) \tag{4.19}$$

If j=1 (the top soil layer), then this runoff necessarily occurs as overland flow. For deeper layers the runoff from layer j may accumulate in layer j-1 as the soil saturates from below. However, for simplicity we treat Dunne-Black runoff from all layers as being a direct loss from the soil column. Physically, this happens if deeper layers intersect the surface near stream beds.

In the force-restore scheme for soil water storage (Section 4.3.2), the Dunne-Black runoff term only appears in the equation for the bulk layer (layer 2), because the first and second layers overlap and saturation occurs from below.

4.3 Soil Water Storage

The evolution of the soil moisture stores (η_j) is described by two alternative methods, both based on two soil layers ($m = 2$) with depths Z_{W1} (shallow) and Z_{W2} (deep) and average moisture contents η_1 and η_2, respectively. The methods are a finite-difference scheme following Mahrt and Pan (1984) (Section 4.3.1) and a force-restore scheme following Noilhan and Planton (1989) (Section 4.3.2).

4.3.1 Soil Water Storage with Mahrt-Pan 2-Layer Finite Differences

This method is based on a scheme proposed by Mahrt and Pan (1984). The layers do not overlap, so layer 1 extends from depth 0 to Z_{W1} and layer 2 from Z_{W1} to Z_{W2}. Layer depths are preset at Z_{W1} = 0.05 m, and Z_{W2} equal to the active soil depth. The governing equations are

$$\begin{aligned} Z_{W1}\frac{d\eta_1}{dt} &= q_{inf} - q_{Es} - \alpha_1 q_{Ev} - q_{dif} - q_{grav} - q_{DBrun,1} \\ (Z_{W2}-Z_{W1})\frac{d\eta_2}{dt} &= q_{dif} + q_{grav} - (1-\alpha_1) q_{Ev} - q_{drain} - q_{DBrun,2} \end{aligned} \tag{4.20}$$

where $q_{Es} = f_{Es}/\rho_w\lambda$ is the soil evaporative flux; $q_{Ev} = f_{Ev}/\rho_w\lambda$ the transpired evaporative flux via roots (with ρ_w the density of liquid water); q_{dif} is the downward diffusive moisture flux by capillary action; q_{grav} is the downward gravitational moisture flux; q_{drain} the deep drainage flux through $Z = Z_{W2}$; and $q_{DBrun,\,j}$ is the Dunne-Black or saturation excess runoff from layer j (described in Section 4.3.3). The vegetative evaporation is partitioned between layers 1 and 2 by the ratio of the total available water in each layer, so the fraction from the upper layer is

$$\alpha_1 = \frac{(\eta_1 - \eta_{dry})Z_{W1}}{(\eta_1 - \eta_{dry})Z_{W1} + (\eta_2 - \eta_{dry})(Z_{W2} - Z_{W1})} \tag{4.21}$$

and the fraction from the lower layer is $1-\alpha_1$. The inter-layer diffusive and gravitational fluxes, q_{dif} and q_{grav}, are evaluated using K and D values at the larger of the two moisture contents, $\eta_* = \max(\eta_1, \eta_2)$:

$$\begin{aligned} q_{dif} &= D(\eta_*)(\eta_1 - \eta_2)/(Z_{W2}/2) \\ q_{grav} &= K(\eta_*) \end{aligned} \tag{4.22}$$

Thus, the diffusive flux from layer 1 to layer 2 is approximated by a crude finite difference (similar to the finite difference used for the infiltration flux in Section 4.2.1). This scheme is not modified from the Mahrt and Pan (1984) proposal, except for the inclusion of the vegetative evaporation q_{Ev} and the saturation excess runoff flux $q_{DBrun,\,j}$.

4.3.2 Soil Water Storage by Noilhan-Planton Force-Restore Method

We use the force-restore scheme of Noilhan and Planton (1989), a revision of the scheme for soil moisture suggested by Deardorff (1978). The layers now overlap, so layer 1 extends from 0 to Z_{W1} and layer 2 from 0 to Z_{W2}. Layer depths are $Z_{W1} = 0.1$ m, and Z_{W2} equal to the active soil depth. Similar to the force-restore method for heat (Section 4.1.1), this scheme solves for the surface moisture content η_0 (not the layer 1 average) and the bulk moisture content η_2 averaged over the interval (0, Z_{W2}). The governing equations are of the same form as the force-restore equations (4.3) for heat:

$$\begin{aligned} \frac{d\eta_0}{dt} &= c_{\eta 1}\frac{q_{inf}-q_{Es}}{Z_{W1}} + c_{\eta 2}\frac{\eta_{eq}-\eta_0}{t_{day}} \\ \frac{d\eta_2}{dt} &= \frac{q_{inf} - q_{Es} - q_{Ev} - q_{drain} - q_{DBrun,2}}{Z_{W2}} \end{aligned} \tag{4.23}$$

where the q fluxes are given in Section 4.2, and η_{eq} is the "equilibrium" bulk soil moisture at which gravitational and capillary forces are in balance. Note that the Dunne-Black runoff term appears only in the equation for the bulk soil moisture η_2, because of the use of overlapping layers (see Section 4.3.3). Each of η_{eq}, $c_{\eta 1}$ and $c_{\eta 2}$ is a function of soil moisture, determined empirically by Noilhan and Planton (1989) by matching predictions from this scheme with those from a multilayer soil moisture model based on Richards' equation. The results were fitted by:

$$\begin{aligned} c_{\eta 1} &= c_{1sat}(\eta_{sat}/\eta_0)^{(b/2)+1} \\ c_{\eta 2} &= \min\left(\frac{c_{2ref}\,\eta_2}{\eta_{sat}-\eta_2}, 14\right) \end{aligned} \tag{4.24}$$

$$\eta_{eq}/\eta_{sat} = \eta_2/\eta_{sat} - a(\eta_2/\eta_{sat})^p\left[1-(\eta_2/\eta_{sat})^{8p}\right] \tag{4.25}$$

where a, p, c_{1sat} and c_{2sat} are specified for each of the 11 soil types of Clapp and Hornberger (1978). The limit of 14 on $c_{\eta 2}$ follows Figure 3 of Noilhan and Planton (1989). Note that, unlike the force-restore method for heat (for which the coefficients c_{T1} and c_{T2} have an analytical basis), the coefficients $c_{\eta 1}$ and $c_{\eta 2}$ are purely empirical and the force-restore method for moisture is accordingly less well-founded.

4.4 Comparisons of Component Schemes Under Idealised Forcing

We have presented alternative schemes for soil evaporation (Section 3.2), soil heat storage (Section 4.1), infiltration (Section 4.2) and soil water storage (Section 4.3). It is clearly necessary to assess the relative performance of these alternatives. A thorough investigation of relative performance is a major task, requiring a full investigation of the parameter space of

soil type, soil depth and atmospheric conditions. This is not attempted here. We only present a few sample comparisons for one soil type (sandy clay loam) and a particular set of idealised meteorological conditions, consisting of steady temperature (20 °C), humidity (7.3 g/kg), wind speed (2 m s^1) and downward longwave radiation (329 W m^2), and half-sine wave downward shortwave radiation (peak 1000 W m^2, 12 hours daylight). Precipitation and initial soil moisture vary from test to test. The "default" scheme choices are: "beta" soil evaporation (Equation (3.18)), 4-layer diffusion soil heat storage (Section 4.1.2), event-based infiltration (Section 4.2.2) and force-restore soil moisture (Section 4.3.2). These are used throughout except as a particular scheme is changed for comparison.

4.4.1 Soil Evaporation Schemes

Figure 4.2 shows a simple comparison of the "alpha" and "beta" schemes for soil evaporation (Equations 3.17, 3.18). The comparison is initialised with saturated soil and examines the drying behaviour of a sandy clay loam under the idealised meteorology without precipitation. The agreement between the two schemes for these conditions is fair. Sensible and latent heat fluxes agree apart from a tendency for the "beta" scheme to evaporate more in the first 10 days of drydown from saturation, leading to a drier top soil layer at later times. Qualitatively similar behaviour is observed for other different soil types.

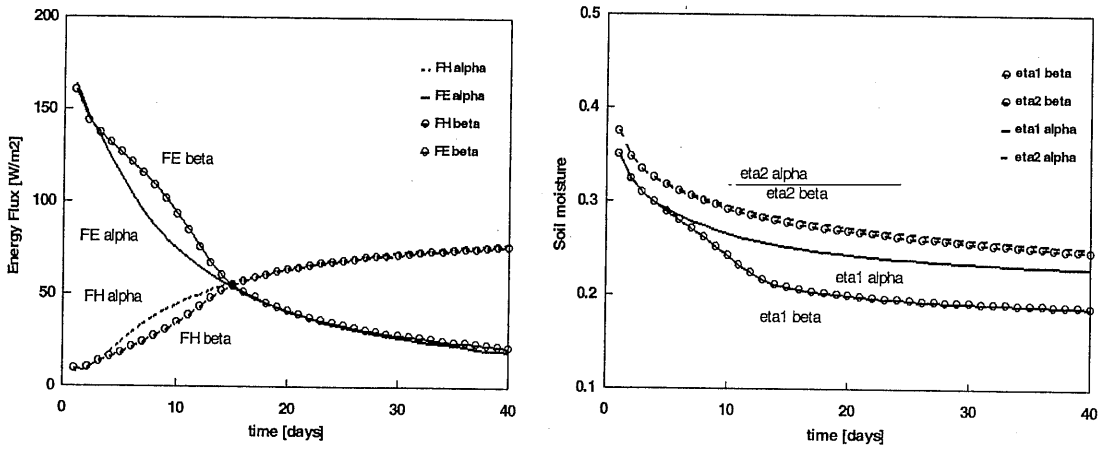

Figure 4.2: Comparison of predictions of "alpha" (lines) and "beta" (circles) soil evaporation schemes for drydown of initially saturated soil (sandy clay loam) under conditions specified in text. (a) Daily evaporation and sensible heat flux; (b) soil moistures.

4.4.2 Soil Heat Storage Schemes

Figure 4.3 shows steady state solutions using the force-restore and 4-layer diffusion schemes for soil heat storage (Sections 4.1.1, 4.1.2). These were obtained from the idealised meteorology with no precipitation and initially dry soil (so that the system starts dry and remains dry). The layer depths for the force-restore scheme are 0.21 and 4.1 m, and for the 4-layer diffusion scheme are 0.06, 0.2, 0.6 and 1.6 m.The ground heat fluxes f_{G0} from the two schemes are very similar (and rather large because of the chosen conditions, which lead to a surface energy balance in which ground heat flux and net radiation are nearly equal and opposite). The surface (or top layer) soil temperature from the force-restore method is lower

than that from the 4-layer diffusion scheme. The deep soil temperatures of the two schemes agree well.

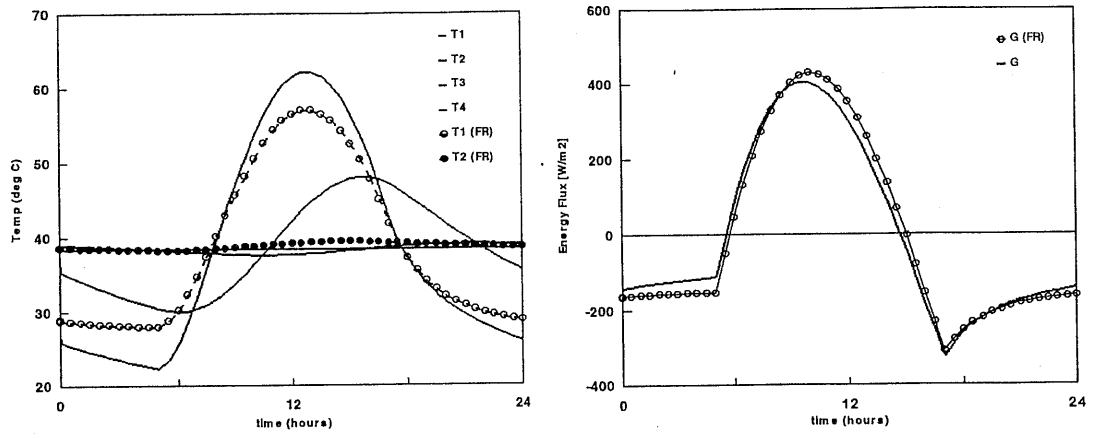

Figure 4.3: Comparison of predictions of force-restore scheme (circles) and 4-layer diffusion scheme (lines) for soil heat storage, under conditions specified in text. (a) Soil temperatures; (b) ground heat flux.

4.4.3 Infiltration Schemes

Figure 4.4 shows a comparison of the infiltration parameterisations (threshold, Section 4.2.1, and event-based, Section 4.2.2). This is performed with an extreme rainfall event (13 mm per half-hour time step) during the night to minimise the effect of evaporation. The soil is initially dry. For the soil type used (sandy clay loam), K_{sat} = 11.3 mm per half hour. The results from the two schemes are quite similar, the main difference being that the event based infiltration proceeds at the rainfall rate for a longer time. This is associated with the time to ponding, calculated by time compression analysis. After ponding occurs, the infiltration decreases as a function of time for the event based scheme. The infiltration for the threshold scheme is simply a choice between the rainfall rate and K_{sat} (depending on whether the soil surface is unsaturated or saturated). The runoff increases as a smooth function of time for event based infiltration, and as a step function for the finite-difference scheme. The runoff in the early stages is entirely infiltration-excess (Hortonian) and later has a saturation-excess (Dunne-Black) component which accounts for the increase in runoff after 28 hours.

4.4.4 Soil Water Storage Schemes

Figure 4.5 compares the two soil water storage schemes (Mahrt-Pan 2-layer finite difference, Section 4.3.1, and Noilhan-Planton force-restore, Section 4.3.2), for a drying event from initially saturated sandy clay loam soil. The schemes are qualitatively similar, the main quantitative difference being that the soil moisture diffusion in the Mahrt-Pan finite difference scheme is more rapid than in the Noilhan-Planton force-restore scheme. In consequence, the Noilhan-Planton scheme exhibits more rapid drying out of the top layer, larger inter-layer differences, and lower soil evaporation during the first 20 days of simulation. Because the total time-integrated evaporation must equal the soil water initially present, the relative soil

evaporations would reverse at later times (longer than shown in this simulation) as the water retained in the Noilhan-Planton scheme slowly diffuses to the surface and evaporates.

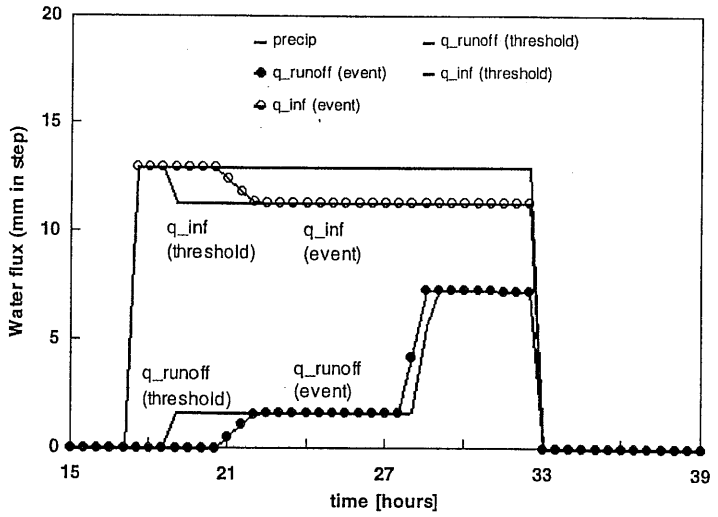

Figure 4.4: Comparison of infiltration and runoff during an extreme rainfall event (details in text) for the event-based infiltration scheme (circles) and the threshold scheme (lines).

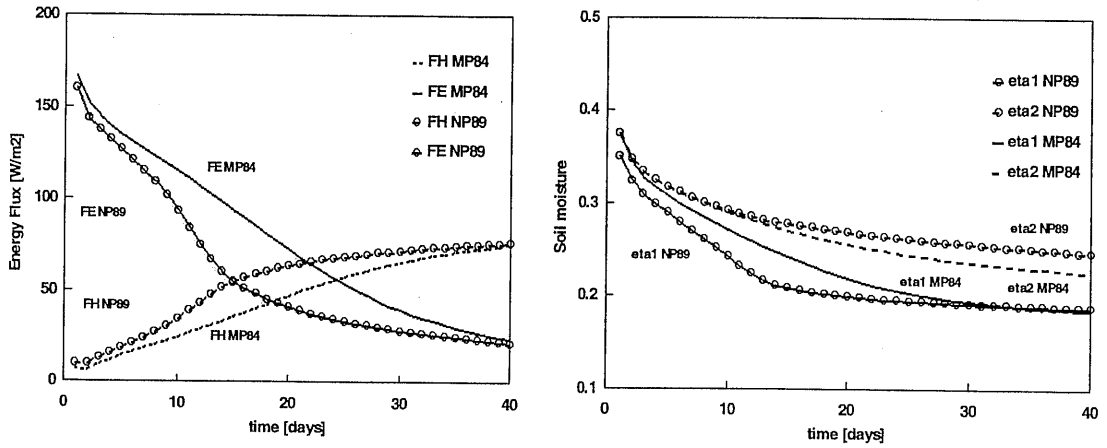

Figure 4.5: Comparison of (a) daily-averaged soil evaporation and sensible heat flux, and (b) soil moistures, for two soil moisture schemes: Mahrt-Pan 2-layer finite difference (lines) and Noilhan-Planton force-restore (circles).