

The Soil-Plant-Atmosphere model

Manual, version 1.3, September 2005

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Changes to version 1.1.
New note on the ι parameter in “Running the model”.

Change to version 1.2.
Update photosynthetic equations – references to internal rather than mesophyll concentrations.

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Introduction

The **Soil-Plant-Atmosphere** model (SPA, Williams *et al.* 1996) is a process-based model that simulates ecosystem photosynthesis and water balance at fine temporal and spatial scales (30 minute time-step, ten canopy and twenty soil layers). The scale of parametrization (leaf-level) and prediction (canopy level) have been designed to allow the model to diagnose eddy flux data, and to provide a tool for scaling up leaf level processes to canopy and landscape scales (Williams *et al.* 2001c).

The model is written in FORTRAN 90. The code is divided among several files, each associated with a particular component of the overall model. This means that the core files can be shared among users, who should only have to alter the input/output file and the main program file in order to customise the model for their own uses.

In this document we will describe the underlying ecological and physical principles that govern the construction of SPA. We will also work through and describe the subroutines and functions that make up the code. We will describe the input and output files – how to create drivers, alter parameters, and interpret model products.

Ecological and Physical Fundamentals

Radiative Transfer

The model employs a detailed radiative transfer scheme that determines the time-varying transmittance, reflectance and absorption of long wave, near infra-red and direct and diffuse photosynthetically active radiation (PAR) by canopy layers and the soil surface. Absorption of PAR in each canopy layer is determined by Beer-Lambert's Law, and is partitioned between sunlit and shaded foliage fractions.

The model requires, as inputs, measured PAR above the canopy at each time step. Short wave radiation can be estimated from PAR or vice versa. If the data are available, then the model can be driven with measured proportions of direct and diffuse PAR for each time step. If these data are not available, then the ratio of diffuse to direct radiation is estimated using an empirical formula (Erbs *et al.* 1982). Solar geometry (i.e. solar declination) is determined from the day, the hour and the latitude of the simulation.

Canopy interaction with radiation is determined by the area and distribution of foliage. At its simplest the canopy is described by the vertical patterns of leaf area density (the amount of leaf area in each canopy layer, the sum of which gives the leaf area index, or LAI). The model assumes no foliage clumping, a spherical leaf angle distribution, and no interaction of radiation with non-photosynthetic tissues. There is a clumping parameter ('*clump*') which can be adjusted if relevant data are available, and the leaf angle parameter ('*spherical*', G in the equation below) can also be adjusted manually.

We assume a spherical leaf angle distribution (Russell *et al.* 1989), so the proportion (P) of radiation incident on the top a layer that passes through without striking a leaf is given by

$$P = \exp(-GL_i/\sin\beta)$$

where G is 0.5 for a spherical leaf angle distribution, L_i is the leaf area ($\text{m}^2 \text{m}^{-2}$) in canopy layer i , and β is the elevation of the radiation source (which varies with latitude and time of day for beam radiation (Jones 1992); for diffuse radiation it is held constant at 30°).

Radiation not intercepted in a layer is incident on the layer below (for downward radiation) or the layer above (for upward radiation). Radiation that strikes leaves in a layer is either absorbed, reflected or transmitted. Reflectivity and transmissivity of leaves and soils are estimated from empirical data (Baldocchi & Harley 1995). After the first downward pass, there is an upward pass through the canopy to determine the fate of the reflected radiation. Any beam radiation that is reflected or transmitted is converted to diffuse radiation. This whole process is repeated two or three times until all radiation has been absorbed by leaves or soil, or reflected back to the sky. Both PAR and NIR regimes are calculated in a similar fashion, but separately, because leaf optical properties in relation to these wavebands differ markedly.

In 1998 the model was modified to introduce a revised radiation subroutine that calculates sun-lit and shaded fractions of the foliage in each canopy layer (Norman 1981) for the PAR routines only. Sun-lit foliage fractions are lit by both incident direct and diffuse PAR, while the shaded fractions receive only diffuse PAR. For each canopy layer the model calculates absorbed radiation separately for the sun-lit and shaded fractions.

Sunlit leaf area (L_s) is determined by

$$L_s = (1 - e^{-kL})/k$$

Where $k = G/(\sin\beta)$. The sunlit fraction of each layer receives the full amount of the direct beam radiation incident at the top of the canopy, plus the attenuated diffuse radiation that penetrates to that layer.

Radiative transfer of NIR follows the same principles as for PAR, but there are different reflectance/transmittance constants, and no separation of sunlit and shaded leaf fractions.

For long wave energy balance, down-welling long wave radiation is either provided directly from data, or we estimate it under clear skies (Φ_{Ld}) from an empirical relation (Jones 1992)

$$\Phi_{Ld} \approx \sigma (T_a - 20)^4$$

The upward emittance of long wave radiation of the canopy layers (Φ_l , W m^{-2}) is estimated by

$$\Phi_{lu} \approx \sigma \epsilon T_a^4 (1 - \exp(-kL_i))$$

where T_a is air temperature (K) of the canopy layer, which approximates leaf temperature, k is the extinction coefficient (0.5, as for diffuse radiation), and L_i is leaf area in the canopy layer ($\text{m}^2 \text{m}^{-2}$). The final term scales emittance according to reabsorptance within the same layer (Amthor *et al.* 1994). The downward emittance of longwave radiation is set equal to the upward emittance. The fate of longwave radiation is determined in a similar manner to short-wave radiation. The sum of PAR (derived from PPFD), NIR and longwave radiation absorbed (Φ_{la}) determines the net isothermal radiation (Φ_{ni} ; W m^{-2}) for each canopy layer. Long wave

emissions from foliage are estimated by assuming leaves are at ambient temperatures. Thus the radiation model is not currently coupled directly to the leaf energy balance model in the leaf level process routines. Such a coupling would increase the model accuracy, but at a large computational cost, and likely would only make a small change to current predictions.

Boundary layer conductance

The multilayer approach requires that we estimate the variation of boundary layer characteristics of leaves within the canopy. Windspeeds, and thus boundary layer conductances, decline within the canopy (Roberts *et al.* 1990). We use an exponential wind relationship (Cionco 1985) to approximate the windspeed at different heights within the canopy;

$$u(h) = u_z \exp(\alpha (h/h_z - 1))$$

where u_z is measured windspeed above the canopy at height h_z (m), $u(h)$ is windspeed at height h (m) within the canopy, and α is the canopy flow index. We use a value of 4.0 for α , from Cionco (1978) for maple-fir forest.

Within each canopy layer, we approximate the thickness of the boundary layer of a leaf (δ ; m) using a relationship from Nobel (1983);

$$\delta = 0.004 \sqrt{\frac{l_l}{u(h)}}$$

where l_l is the characteristic dimension of the leaf (m). For a default value, we use 0.08m, a representative measure of the size of *Quercus/Acer* leaves.

One-sided leaf boundary layer conductance to water vapour (g_b ; m s^{-1}) varies with the diffusion coefficient of water vapour in air (D_{wv} ; $\text{m}^2 \text{s}^{-1}$) and the thickness of the boundary layer (δ),

$$g_b = D_{wv}/\delta.$$

Boundary layer conductance to heat (g_H ; m s^{-1}) is calculated in a similar manner, using thermal diffusivity (D_H ; $\text{m}^2 \text{s}^{-1}$), and the factor 2 accounting for transfer from both leaf surfaces,

$$g_H = 2D_H/\delta.$$

Plant and leaf ecophysiology

The SPA model employs some well tested theoretical representations of eco-physiological processes, such as the Farquhar model of leaf-level photosynthesis (Farquhar & von Caemmerer 1982), and the Penman-Monteith equation to determine leaf-level transpiration. These two processes are linked by a novel model of stomatal conductance that optimizes daily carbon (C) gain per unit leaf nitrogen (N), within the limitations of canopy water storage and soil-to-canopy water transport. The maximum flux rate of water through vegetation is determined by the difference between soil water potential and the minimum sustainable leaf water potential, and by the hydraulic resistance of the soil-root-leaf pathway. Stomata adjust to equalise evaporative losses with the maximum hydraulic supply, minimising the risk of cavitation.

The principle behind stomatal dynamics is that C assimilation is maximised within the limitations of the hydraulic system, so stomatal resistance is adjusted to balance atmospheric demand for water with rates of water uptake and supply from soils. Atmospheric demand is governed by the vapour pressure difference between leaf internal air spaces and the atmosphere, and vapour phase exchange (E) is determined using the Penman-Monteith equation. Water loss ($= E$) is linked to changes in leaf water potential (Ψ_l), according to the water potential gradient between leaf and soil, liquid-phase hydraulic resistances (both in the rhizosphere, R_s , plant stems, R_p , and roots, R_r) and the capacitance (C) of the pathway that links soil to leaf. Stomatal resistance is varied to maintain evapotranspiration (E) at the rate that keeps Ψ_l from falling below a critical threshold value (Ψ_{lmin}), below which potentially dangerous cavitation of the hydraulic system may occur. Thus, once $\Psi_l = \Psi_{lmin}$, E is set so that $d\Psi_l/dt = 0$, where

$$\frac{d\Psi_l}{dt} = \frac{\Psi_s - \rho_w gh - E(R_s + R_r + R_p) - \Psi_l}{C(R_s + R_r + R_p)}$$

The gravitational component of leaf water potential is determined by the density of water (ρ_w), acceleration due to gravity (g), and the height above the reference plane (h), set to the soil surface.

Plant hydraulics

We assume that the plant resistance per unit leaf area to flow of water along the xylem to a layer in the canopy (R_p ; $\text{MPa s m}^2 \text{mmol}^{-1}$) increases with the height (h ; m) of each layer above the ground;

$$R_p = \frac{h}{G_p}$$

where G_p is the canopy hydraulic conductivity ($\text{mmol s}^{-1} \text{m}^{-1} \text{MPa}^{-1}$). The layers higher in the canopy are subject to the greatest resistance to xylem water supply (Hellkvist *et al.* 1974). In some plants there is evidence that resistance is not strongly related to path length (it may be that the resistance is concentrated at nodes in the conductive network, for example). In such a case, it may be better to specify a constant plant resistance for each canopy layer. There is a switch in the model ('CONDUCTIVITY') to select either option. More details are given in the operating instructions.

The following equations can be used to describe the relationship between steady-state flow and water potential between the soil and the roots, between the roots and the leaves, and for the whole plant system;

$$J_p = \frac{\Psi_s - \Psi_r}{R_b} = \frac{\Psi_r - \Psi_l - hd}{R_a} = \frac{\Psi_s - \Psi_l - hd}{R_b + R_a}$$

where J_p is water flux ($\text{mmol m}^{-2} \text{s}^{-1}$), Ψ_l is leaf water potential (MPa), d is gravitational head of pressure (MPa m^{-1}), and the denominators contain belowground and aboveground resistances to water transport ($\text{MPa s m}^2 \text{mmol}^{-1}$).

The water in the xylem can rupture under the extreme tensions that occur naturally - there is often a threshold water potential for such cavitation (Jones 1992). The onset of xylem cavitation can lead to a rapid and catastrophic decline in stem hydraulic conductivity by inducing further

cavitations (Tyree & Sperry 1989). Jones and Sutherland (1991) have shown that the maintenance of a maximally efficient conducting system requires that stomata close as evaporative demand rises to prevent shoot water potentials falling below the threshold value (Ψ_{min}).

The relationship between J_p and the water potential drop is not unique; initially water is drawn from stores within plant tissues, so that liquid flow lags behind the evaporative demand (Landsberg *et al.* 1976; Schulze *et al.* 1985). This hysteresis can be modelled by incorporating capacitors into the circuit analogue (Jones 1978). The capacitance (C , $\text{mmol MPa}^{-1} \text{m}^{-2}$) of any part of the system is defined as the ratio of the change in tissue water content (W , mmol m^{-2}) to the change in water potential (Ψ);

$$C = \frac{dW}{d\Psi}$$

As shown above, the flow through the plant to the leaves (J_p ; $\text{mmol m}^{-2} \text{s}^{-1}$) can be written;

$$J_p = (\Psi_s - \Psi_l - hd)/(R_a + R_b)$$

The rate of change of layer water content (dW_l/dt) is given by the difference between the flow of water into the layer and that lost by evaporation;

$$dW_l/dt = J_p - E$$

Thus,

$$dW_l/dt = (\Psi_s - \Psi_l - hd)/(R_a + R_b) - E$$

Assuming constant capacitance, the first order differential equation describing leaf water potential is;

$$\frac{d\Psi_l}{dt} = \frac{\Psi_s - hd - E(R_a + R_b) - \Psi_l}{C(R_a + R_b)}$$

Calibration of the belowground resistances is described below (Root distribution and water uptake).

Leaf level processes

For each canopy layer, once every half-hour an iterative procedure is used to determine the maximum stomatal conductance (g_s) and the assimilation rate associated with this conductance. We use a bisection routine to calculate the stomatal conductance very rapidly, but in essence the procedure is hypothesized to work in the following manner:

Starting from a very low g_s :

1. Increment g_s .
2. Determine leaf temperature (T_l , °C) resulting from the leaf energy balance at this g_s using a steady-state approximation (Jones 1992).

$$T_l - T_a = \frac{r_{\text{HR}}(r_{\text{aW}} + r_{\text{lW}})\gamma\Phi_{\text{ni}}}{\rho_p[\gamma(r_{\text{aW}} + r_{\text{lW}}) + S_{\text{rHR}}]} - \frac{r_{\text{HR}}\delta\epsilon}{[\gamma(r_{\text{aW}} + r_{\text{lW}}) + S_{\text{rHR}}]}$$

where T_a (°C) is air temperature in the canopy layer, Φ_{ni} is net isothermal radiation (KW m^{-2}), r are leaf resistances (m s^{-1} ; subscripts: r_{HR} parallel heat and radiative transfer (Jones 1992); r_w water; r_a boundary layer; r_l leaf), γ is the psychrometer constant (KPa K^{-1}), S is the rate of change of saturation vapour pressure with temperature (KPa K^{-1} , assumed constant between T_l and T_a), δe is vapour pressure deficit (Pa), ρ is air density (g m^{-3}), and c_p is the specific heat capacity of air ($\text{KJ g}^{-1} \text{K}^{-1}$).

3. Determine biochemical parameters for Farquhar & Von Caemmerer (Farquhar & von Caemmerer 1982) equations. These photosynthetic parameters are dependent on foliar N concentrations (Field & Mooney 1986) and leaf temperature. Photosynthesis is limited by the minimum of the ribulose biphosphate carboxylation rate and the rate of ribulose biphosphate (RuBP) regeneration. We determine the maximum rates of these two processes.

Maximum Carboxylation Capacity (V_{cmax})

$$V_{cmax} = N \tau_{tc} \kappa_c$$

where N is leaf nitrogen content (g m^{-2}), and τ_{tc} is a temperature coefficient (described below), and κ_c is the catalytic rate coefficient, determined from A/Ci curve data.

Maximum electron transport rate (J_{max})

$$J_{max} = N \tau_{tj} \kappa_j$$

where τ_{tj} is a temperature coefficient.

The temperature dependencies of J_{max} (τ_{tj}) and V_{cmax} (τ_{tc}) are described using response curves (Rastetter *et al.* 1991) fitted to the polynomial relationships of McMurtrie *et al.* (1992), but with temperature optima set to 30°C to reflect those of temperate deciduous vegetation.

Biochemical Constants

The values and temperature dependencies of K_c and K_o , the Michaelis-Menten constants for enzyme catalytic activity for CO_2 and O_2 respectively are taken from Kirschbaum and Farquhar (1984) and McMurtrie *et al.* (1992). I^* , the CO_2 compensation point in the absence of non-photorespiratory respiration, is derived from measurements of V_{cmax} , amongst other parameters. We approximate woody plant I^* by $36.5 \mu\text{mol mol}^{-1}$ at 25°C (Epron *et al.* 1995), using an Arrhenius relationship for temperature sensitivity (McMurtrie *et al.* 1992).

4. Determine the internal CO₂ concentration (C_i) that satisfies both diffusion and metabolic uptake;

a) *Diffusion model*;

$$A = g_t (C_a - C_i)$$

where C_a is ambient air CO₂ concentration, A is assimilation rate ($\mu\text{mol m}^{-2} \text{s}^{-1}$) and g_t is total CO₂ conductance ($\text{mol m}^{-2} \text{s}^{-1}$), determined from stomatal (g_s) and leaf boundary layer (g_b), all m s^{-1} , to CO₂;

$$g_t = \frac{P / RT_1}{1.65 / g_s + 1.37 / g_b}$$

where P is atmospheric pressure (Pa), R is the gas constant ($\text{Pa m}^3 \text{mol}^{-1} \text{K}^{-1}$) and T_1 is leaf temperature (K).

The existence of a limitation to CO₂ assimilation by internal resistances to CO₂ transfer has been shown in several woody plant species. However, for simplicity, we assume that g_i is very large ($=1.0$) and thus insignificant. To assume otherwise (as we did in early publications) means that calibrating V_{cmax} and J_{max} from A/C_i curves becomes far more complex. This simplification of g_i is not really satisfactory, and the issue of finding a way to deal with a realistic mesophyll conductance is important.

b) *Metabolic model*;

We determine the Rubisco limited carboxylation rate (W_c , $\mu\text{mol m}^{-2} \text{s}^{-1}$) as (Farquhar *et al.* 1982)

$$W_c = \frac{V_{\text{cmax}} C_i}{C_i + K_c (1 + O_c / K_o)}$$

where C_i is internal CO₂ concentration, O_c is the oxygen concentration at the same site ($210 \text{ mmol mol}^{-1}$), and the other parameters are described in (3), above.

The RuBP regeneration-limited carboxylation rate is described by

$$W_j = \frac{J C_i}{4.5 C_i + 10 \Gamma_*}$$

where J is the potential rate of electron transport, which is a function of J_{max} and absorbed photosynthetic photon flux density (Q ; $\mu\text{mol m}^{-2} \text{s}^{-1}$), satisfying the relationship (McMurtrie *et al.* 1992),

$$\theta J^2 - (\alpha_i Q + J_{\text{max}}) J + \alpha_i Q J_{\text{max}} = 0$$

in which α_i and θ are the initial slope and the curvature of the quantum response of the electron transport slope (Farquhar & Wong 1984).

We determine the actual rate of carboxylation by

$$V_c = \min (W_c, W_j)$$

and the photosynthetic rate (A , $\mu\text{mol m}^{-2} \text{s}^{-1}$) by

$$A = V_c(1 - \Gamma^*/C_c) - R_d$$

where R_d is respiration rate ($\mu\text{mol m}^{-2} \text{s}^{-1}$). R_d is parametrised from leaf level data, and is a function of leaf temperature and foliar N.

5. Calculate evapotranspiration rate ($\text{mmol m}^{-2} \text{s}^{-1}$) at this g_s with the Penman-Monteith equation,

$$E = c \frac{\varepsilon \Phi_n / \lambda + g_b \delta c_w}{1 + \varepsilon + g_b / g_s}$$

where g_b is leaf boundary layer conductance (m s^{-1}), λ is the latent heat of vaporisation (KJ g^{-1}), δc_w is atmospheric water deficit (g m^{-3}), c converts from $\text{g m}^{-2} \text{s}^{-1}$ to $\text{mmol m}^{-2} \text{s}^{-1}$, ε is the ratio of latent heat content increase to sensible heat content increase (unitless), and Φ_n is net radiation (KWm^{-2}), approximated by (Jones 1992),

$$\Phi_n \approx \Phi_{ni} - 4\varepsilon\sigma T_a^3(T_l - T_a)$$

where ε is emissivity, σ is the Stefan-Boltzmann constant and the temperatures are in K.

6. Calculate the change in Ψ_l after one time step of evapotranspiration at the specified g_s ;

$$\frac{d\Psi_l}{dt} = \frac{\Psi_s - \rho_w gh - E(R_s + R_r + R_p) - \Psi_l}{C(R_s + R_r + R_p)}$$

7. Return to step 1 (for a further increment of g_s), unless either;

- a) previous g_s increment failed to raise assimilation appreciably. After an initial rapid increase, the response of A to g_s becomes asymptotic, and the carbon gain per unit water loss declines. We argue that plants use their *water store* conservatively; it is more efficient to limit g_s when water deficits are low (morning), so that stored water can be utilised later to buffer the impacts of high afternoon water deficits (Cowan 1977). For this reason, optimal g_s is fixed when an increment in g_s ($\sim 1 \text{ mmol m}^{-2} \text{s}^{-1}$) fails to increase A by more than $1-\iota$ (the threshold parameter ι). ι was initially selected to give maximum conductances of $300 \text{ mmol m}^{-2} \text{s}^{-1}$ (Weber & Gates 1990).
- b) Ψ_l has reached its specified cavitation limit. The water supply system is now operating at its maximum rate. Any further increase in g_s would take the xylem beyond its threshold for cavitation, and result in a catastrophic failure in water supply.

It is this iterative procedure of setting stomatal conductance, especially as relates to step 7, that sets our canopy model apart from similar models. Embedded in this procedure is our underlying hypothesis that stomatal variation operates to minimise water stress, by effectively

using stored water in terms of C gained per unit water loss over the course of a day, and by preventing xylem cavitation.

Soil energy and water balance

The model contains a detailed representation of soil hydrology and thermal dynamics. From the estimated transmission of radiation through the canopy, we determine the down-welling radiation at the soil surface. We then solve the surface energy balance by estimating the soil surface temperature, and partition net radiation into sensible, latent and ground heat fluxes. The soil is divided into 10 layers of varying thickness, each of a given organic matter and mineral content. The flux of heat through the soil profile is determined on the basis of the ground heat flux, the thermal gradient between soil layers, the soil thermal conductivity and thermal heat content of each layer. The thermal parameters are dependent on soil organic matter and mineral fractions and soil water content, and phase transitions between liquid water and ice. The field capacity of each layer is determined according to soil texture and soil water retention curves. Heat is redistributed through the soil profile according to water movement, and from patterns of freezing and thawing we determine the ice content of each soil layer daily. Root water uptake is explicitly linked with soil water potential and soil hydraulic conductivity, as determined from soil water retention curves, through the plant hydraulic model outlined above. Roots are distributed through the upper soil layers and water is withdrawn from the layers with greatest moisture content. Precipitation inputs to soils are calculated after canopy interception, drainage and evaporation from the canopy water store, and infiltration through the soil surface. A snow sub-model tracks the dynamics of the snow-pack and its effects on soil temperature.

Soil surface energy balance

The canopy radiative transfer scheme determines the down-welling radiation at the soil surface. We use this to solve the surface energy balance, by using a bisection method to find the soil surface temperature (T_{sur}) that balances net radiation (Q_{net} , determined from down-welling radiation and long-wave losses from the soil surface) with sensible (Q_{h}), latent (Q_{e}) and ground heat fluxes (Q_{c}), following the approach of Hinzman et al. (1998):

$$Q_{\text{h}} + Q_{\text{e}} + Q_{\text{net}} + Q_{\text{c}} = 0 \quad (\text{W m}^{-2}),$$

Calculation of the various components is described in the appendix. For calculation of soil evaporation (Q_{e}), the model keeps track of multiple wetted layers that can develop with successive drying and wetting, merging layers that overlap. We found that without this detailed accounting, comparisons of predicted soil evaporation against measured fluxes were very poor during summer, when heavy storms alternate with periods of very low atmospheric humidity.

Sensible heat fluxes are determined from the temperature gradient between the soil surface (T_{s} , K) and the air above (T_{a} , K), and the specific heat capacity (c_{p} , J kg⁻¹ K⁻¹), density (ρ_{a} , kg m⁻³), and heat conductance (g_{AH} , m s⁻¹) of air,

$$Q_{\text{h}} = c_{\text{p}} \rho_{\text{a}} g_{\text{AH}} (T_{\text{a}} - T_{\text{sur}})$$

Latent heat flux is estimated from the latent heat of vaporisation (λ , J kg⁻¹), vapour boundary layer conductance (g_{AW} , m s⁻¹), soil conductance to water vapour transfer (g_{ws} , m s⁻¹), atmospheric pressure (P_{a} , Pa), and the gradient of vapour pressure (e) between the soil air spaces (e_{s} , Pa) and the air above (e_{a} , Pa)

$$Q_e = \lambda \rho_a \frac{0.622}{P_a} \frac{(e_a - e_s)}{(1/g_{AW} + 1/g_{ws})}$$

The vapor pressure in the soil air spaces (e_s , Pa) is determined from the saturation vapour pressure (e_{sat} , Pa) in the air spaces of the surface layer, the soil water potential (ψ_s , Pa) of the surface layer, the partial molal volume of water (V_w , m³ mol⁻¹), and the gas constant (\mathfrak{R} , Pa m³ mol⁻¹ K⁻¹);

$$e_s = e_{sat} \exp\left(\frac{\psi_s \bar{V}_w}{\mathfrak{R} T_s}\right)$$

Following Choudhury and Monteith (1988), g_{ws} is dependent on the diffusion coefficient of water vapour in air (D_w , m² s⁻¹), the tortuosity (τ) and porosity (ζ) of the soil surface layers (determined by the physical structure of the soil matrix), and the thickness of the dry soil at the surface (l_t). Total porosity is determined by the soil texture (sand and clay content) using Saxton equations. Thus,

$$g_{ws} = \zeta D_w / (\tau l_t)$$

We assume that the distance from the soil surface to the top of the wetted soil layer (which is equal to l_t) is increased by soil evaporation, and reduced by dew formation and precipitation (I , mm), while the total water content of the surface layer is also altered by root water uptake and gravitational drainage. We calculate the magnitude of wetting or drying (Δl , mm)

$$\Delta l = -(\Delta t Q_e / \lambda + I) / \theta_f$$

where θ_f is the field capacity and Δt is the time-step length (s). Drying ($\Delta l > 0$) increases the distance to the top of the wetted soil (l_t),

$$\text{If } \Delta l > 0, l_t = l_t + \Delta l$$

Wetting can have two effects. If the wetting depth Δl is less than the thickness of the current surface dry layer, then a new wet layer (here denoted *) is formed, extending from close to the surface ($l_{t*} = l_{min}$, the minimum wetting depth) to a depth l_{b*} ,

$$\text{If } \Delta l < l_t, l_{t*} = l_{min}, l_{b*} = \Delta l$$

thus sandwiching a dry layer, extending from l_{b*} to l_t between two wet layers.

Alternatively, the wetting recharges the current wet layer, filling it first to the surface, with remaining water extending its depth, l_b

$$\text{If } \Delta l > l_t, l_t = l_{min}, l_b = l_b + (l_t - \Delta l)$$

The distance from the soil surface to the topmost wetted layer determines l_t for the soil evaporation equation.

Atmospheric conductance to heat and water vapour are assumed equal and are dependent on wind-speed (u_z , m s⁻¹, where z is measurement height), the von Karman constant (0.41), and mean surface roughness (z_o , m), here set at 13% of canopy height,

$$g_{AH} = g_{AW} = \frac{u_z k^2}{[\ln(z/z_o)]^2}$$

Soil heat and water transport

The soil is divided into layers of constant thickness, of a given organic matter and mineral content. The flux of heat through the soil profile is determined on the basis of the ground heat flux, Q_h , the thermal gradient between soil layers, the soil thermal conductivity (k) and thermal heat content of each layer (c_v , the soil volumetric heat capacity), by the Fourier heat conduction equation

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\frac{k}{c_v} \frac{\partial T}{\partial z} \right),$$

The thermal parameters are dependent on soil organic matter and mineral fractions and soil water content (Hillel 1980), and phase transitions between liquid water and ice (Waelbroeck 1993). The Fourier equation is solved implicitly by the Crank-Nicholson scheme (Farlow 1993).

The porosity and soil water retention curves of each layer are estimated according to empirical relationships with soil texture (Saxton *et al.* 1986). Changes to layer water content are regulated by precipitation and evaporation (surface layer only), abstraction by roots (rooted layers only), and gravitational drainage. Heavy snowfall is uncommon at the study site, and there is no detailed snow model; below freezing, precipitation is stored and only added to the upper soil layer when temperatures rise above freezing. Infiltration rates are assumed to be greater than precipitation rates, and surface runoff occurs only when the water content of the surface layer exceeds porosity. Gravitational drainage occurs when water content is above a set fraction of porosity; the rate of drainage is set directly by the soil hydraulic conductivity (m s^{-1}), another function of texture and water content (Saxton *et al.* 1986). The discharge from the soil profile is determined as the flux of water crossing the lower boundary of the soil profile via gravitational drainage. Heat is redistributed through the soil profile according to water movement. From patterns of freezing and thawing, the ice content of each soil layer is determined by linear interpolation.

Root distribution and water uptake

Plant root distribution is determined by total fine root biomass (F_{total} , g m^{-2}), maximum root biomass per unit volume (F_{max} , g m^{-3}) which is assumed to occur at the soil surface, and depth of rooting (D_{max} , m). Assuming an exponential decay in root length with depth, root biomass per unit volume (F , g m^{-3}) at any depth is given by:

$$F = F_{\text{max}} e^{-\kappa D}$$

where coefficient κ is linked to the other parameters by:

$$F_{\text{total}} = F_{\text{max}} \int_0^{D_{\text{max}}} e^{-\kappa D} dD$$

This equation can be rearranged and κ determined numerically.

Below-ground hydraulic resistance (R_b , $\text{MPa s m}^2 \text{mmol}^{-1}$) has a soil component (R_s) and a root component (R_r). The soil component is dependent on soil conductivity (G_{soil} , $\text{mmol m}^{-1} \text{s}^{-1} \text{MPa}^{-1}$, a function of soil water content and texture), fine root radius (r_r , m), root length per unit soil volume (l_R , determined from biomass and radius), depth of the soil layer (D , m) and mean distance between roots (r_s , m, $(1/(\pi l_R))^{0.5}$) (Newman 1969)

$$R_s = \frac{\ln(r_s / r_r)}{2\pi R_D G_{\text{soil}}}$$

Root hydraulic resistance for each rooted soil layer declines linearly with increasing root biomass according to root resistivity R_r^* (MPa s g mmol⁻¹)

$$R_r = R_r^*/(FD)$$

The relative contribution of roots in each soil layer to total root activity is determined from the maximum potential water uptake (E_{max}) of each soil layer. According to eqn. (1), once the minimum leaf water potential has been reached, the sustainable flux rate is determined by the difference between soil water potential (Ψ_s) and minimum sustainable leaf water potential (Ψ_{min}), and hydraulic resistance of soil and roots in each soil layer ($R_b = R_s + R_r$);

$$E_{\text{max}} = \frac{\Psi_s - \Psi_{\text{min}}}{R_b}$$

From the estimate of E_{max} for each of the l soils layers with roots, we determine a weighted soil water potential (Ψ_{sw}),

$$\Psi_{\text{sw}} = \frac{\sum_{i=1}^l (\Psi_{si} E_{\text{max}i})}{\sum_{i=1}^l (E_{\text{max}i})}$$

For each canopy layer i , the total root and soil hydraulic resistance (R_{bi}) is determined by assuming that each such layer is connected to each soil layer; i.e., the roots in each soil layer supply a fraction of the water to each canopy layer. We assume that the fraction of roots in each root layer supplying each canopy layer is the same as the ratio of leaf area in the canopy layer (L_i) to total leaf area (L_{tot})

$$R_{bi} = \frac{1}{\sum_{j=1}^l \left(\frac{R_{bj} L_{\text{tot}}}{L_i} \right)}$$

The total amount of water extracted by roots from the soil in each time-step is determined by eqn. (1) and is split between rooted layers according to the weighting $E_{\text{max}i}/\Sigma (E_{\text{max}})$.

Interception and evaporation on canopy surfaces

Precipitation inputs to soils are calculated after canopy interception, drainage and evaporation from the canopy water store, following the approach of Rutter et al. (1975). The canopy is regarded as having a surface storage capacity S that is charged by rainfall and discharged by evaporation and drainage. The through-fall parameter determines what fraction of precipitation reaches the soil surface directly; the remainder is added to the canopy store. When the amount of water on the canopy equals or exceeds S , then evaporation (E) is determined by the Penman Monteith equation, with stomatal resistance set to zero. When storage s is less than capacity S , then evaporation occurs at a rate $s/S \cdot E$. The rate of drainage from the canopy (d , mm hr⁻¹) is given by

$$d = \exp(a + b s)$$

where a and b are empirically derived constants. A Runge-Kutta integrator (Press *et al.* 1986) determines the total drainage and evaporation during each model time-step (30 minutes).

Snow pack

The snow pack model is that described by Lynch-Stieglitz (1994). The snow pack is modelled with three snow layers. Heat and mass (water) flow within the pack are physically modelled. Radiation conditions determine the surface energy fluxes, and heat flow within the pack is governed by linear diffusion. Each layer is characterized by a volumetric water-holding capacity. As such, melt-water generated in a layer will remain in the layer if the liquid water content of the layer is less than the layer holding capacity. Otherwise, it will flow down to a lower layer where it will either refreeze in the layer, remain in the layer in the liquid state, or pass through. Finally, two independent processes govern densification of the pack. A simple parameterisation is used to describe mechanical compaction, or compaction due to the weight of the overburden, and a separate densification is accomplished via the melting-refreezing process. All the equation and parameters of the model physics are given in Lynch-Stieglitz (1994). The snow pack model is important because in winter the snow pack acts like a giant insulating blanket, preventing the escape of heat from the warm soil to the cold atmosphere, or conversely, to damp out the cold wintertime temperature signal well before it reaches the ground. The low thermal conductivity of snow, about an order of magnitude lower than that of the soil, makes snow an especially good insulator. As such, the snow cover results in much warmer wintertime ground temperatures.

Model Subroutines (SR) and Functions

All_declarations.f90

This file contains the bulk of the modules that define the key variables that are shared among the model subroutines. All the variables are described in the accompanying spreadsheet: SPA model variables.xls.

Scale declarations.f90

These declarations are separated from the bulk of the others because they define the size of the soil ('layer', 'core') and canopy ('numl') profiles, and the time resolution ('steps').

Canopy.f90

SUBROUTINE DAY

This SR controls the daily runs of SPA leaf-level and soil processes. For each time step, the SR first calls SR Soilday, which initiates the calculation of soil surface energy balance, precipitation inputs to the soil surface, soil heat and water transfer (with water abstractions from roots calculated in the previous time step) and snow pack dynamics. The SR returns a new weighted soil water potential that will be used to determine the availability of soil moisture for plant uptake.

The SR then cycles through each canopy layer. The specific hydraulic conditions and leaf water potential are loaded into new variables out of storage locations. Then determines if there

is any sunlit foliage in this layer and this time step. If so, the nitrogen content of the sunlit portion is determined, as is the PAR and total short wave radiation incident on the sunlit leaves. Temperature, water deficit and boundary layer conductance for the time and location are pulled out of storage, or calculated from input. In cases where information on air temperature and humidity is not available through the canopy, the model assumes that above canopy conditions apply at all canopy layers.

The SR then calls SR ASSIMILATE, part of the Leaf.f90 files (see below). Once control is returned to the calling SR, time totals of photosynthesis, respiration, transpiration are updated, and PAR absorption is cross-checked. The leaf water potential of the sunlit leaves is stored.

Then the process is repeated for the shaded fraction of the foliage. Of course, variables are re-initialised (the leaf water potential from the start of the time step is reset, for example). The incident PAR and radiation are of course different, and so on.

Once the shaded leaves have been simulated, a final, total canopy layer leaf water potential is calculated as an area-weighted fraction of the predicted sunlit and shaded LWPs.

SUBROUTINE SET_LEAF

This SR sets the Farquhar parameters (V_{cmax} and J_{max}) and hydraulic parameters (r_{plant} and r_{soil}) for the sunlit and shaded fractions of each canopy layer.

Setting these parameters depends on how they have been calibrated.

Farquhar parameters (FP): FPs are derived from A/Ci curves (best case) or literature values (Wullschleger 1993). The FPs are used to generate parameters that relate each FP to the nitrogen (N) content of the leaf layer, according to the equations given above (see Leaf level processes). This means that in this SR, the FPs are regenerated for each layer according to the equations

$$vcm = kappac * nit / la$$

$$vjm = kappaj * nit / la$$

$kappac$ and $kappaj$ have units $\mu\text{mol g}^{-1} \text{N s}^{-1}$, nit has units g N layer^{-1} , la has units m^{-2} leaf area layer^{-1} . vcm and vjm have units $\mu\text{mol m}^{-2} \text{s}^{-1}$.

Determining the correct temperature responses is critical. The calibration spreadsheet includes a temperature response worksheet showing the nature of the temperature responses functions. Currently, you must first correct your FPs to give an estimate of their values at 30°C, which we assume is the optimal temperature. So, if the data were collected at 25°C, then they must be divided by the 25°C multipliers for V_{cmax} and J_{max} , which are 0.95 and 0.94 respectively. You can adjust the temperature response functions as you wish in FUNCTION STOMATA – for instance for arctic vegetation you may want to set lower optima.

Hydraulic parameters (HP): The default assumption is that plant conductivity is a constant, and thus that stem conductance is determined by the path length (see the first equation in Plant hydraulics). The default situation has been set by $conductivity=1$, a variable in module VEG. The g_{plant} parameter that is set in the parameter file is, in this case, defined as plant stem conductivity.

However, some stems may be better describe as having a similar conductance to all canopy layers (perhaps it is the number of nodes in the vascular pathway that sets the resistance).

To set conductance equal in all layers, manually set *conductivity*=0 in SR INIT. The *gplant* parameter that is set in the parameter file is, in this case, defined instead as plant stem conductance.

Leaf.f90

SUBROUTINE ASSIMILATE.

This SR determines leaf level fixation of C, dark respiration, evapotranspiration, and leaf temperature. It makes a number of calls to other SR and functions.

FUNCTION CDIFF

Determines the difference between metabolic assimilation and CO₂ diffusion at a given internal CO₂ concentration (*C_i*). Called by RF STOMATA to determine *C_i* that ensures equal metabolic assimilation and CO₂ diffusion. Units = μmol m⁻² s⁻¹

FUNCTION STOMDIFF

Determines whether a stomatal conductance value meets either an efficiency criterion or balances water supply with water losses. The function calculates leaf state vector at the given *g_s* and then again at a very slightly lower value. The efficiency test asks whether there has been an appreciable decrease in productivity for the small decrease in *g_s*. The *iota* parameter determines the threshold for this test, which really sets the maximum stomatal conductance, and stops very large values of *g_s* occurring in the early morning. The water supply test examines whether the leaf water potential has reached its minimum value, set by the min LWP parameter. Units not relevant.

FUNCTION STOMATA

Determines the stable *C_i* for a given *g_s*. First calculates leaf temperature, leaf net radiation, leaf evapotranspiration, temperature modifications to the Farquhar parameters, and leaf respiration rate. The function then uses a bisection routine (ZBRENT) to find the stable *C_i* value for a specified *g_s*, temperature, absorbed PAR etc. From this the routine then calculates C uptake from diffusion and metabolism (which are equal of course, in the steady state here calculated). Then calculates the change in LWP. Units = μmol mol⁻¹

SUBROUTINE DELTAPOTENTIAL

Calculates the change in leaf water potential using a Runge-Kutta integrator.

SUBROUTINE LWP

This routine is called by SR DELTAPOTENTIAL, and defines the differential equation describing change in leaf water potential (*y*) given supply & demand:

$$dydt(1)=secs*(psis-(head*ht)-1000.*la*et*(rplant+rsoil)-y(1))/(layer_capac*(rplant+rsoil))$$

FUNCTION FARQUHAR

Determines the metabolic carboxylation rate, given the Farquhar parameters at the specified leaf temperature and internal CO₂ concentration. Units = $\mu\text{mol m}^{-2} \text{s}^{-1}$

FUNCTION DIFFUSION

Determines the diffusion limited assimilation rate. Units = $\mu\text{mol m}^{-2} \text{s}^{-1}$

FUNCTION EVAP

Determines evapotranspiration rate ($\text{g m}^{-2} \text{s}^{-1}$) from q (kW m^{-2}), tt ($^{\circ}\text{C}$), $wdef$ (g m^{-3}) and gbb and gs (m s^{-1}), using the Penman-Montieth equation. Units = $\text{g m}^{-2} \text{s}^{-1}$

FUNCTION LEAFTEMP

Determines leaf temperature from a steady-state energy balance approximation. Units = $^{\circ}\text{C}$.

FUNCTION ARRHENIOUS

Determines Arrhenious relationship, a temperature response function. Units are determined by the input data.

FUNCTION TEMPMET

Another temperature response function. Units are determined by the input data.

Light.f90**SUBROUTINE SOLAR**

This SR determines the attenuation, absorption, transmittance and reflectance of short wave and long wave radiation between sky, canopy and soil surface. The SR is run before any of the ecophysiological routines, and is relatively uncoupled from the ecology. This SR determines the absorbed radiation of each canopy layer and the soil surface, and these estimates are then used to drive many other functions in **leaf.f90** and **soil functions.f90**.

SUBROUTINE ATTENUATE_PAR

Calculates PAR attenuation, taking account of sunlit and shaded parts of the canopy.

SUBROUTINE ATTENUATE_NIR

Calculates NIR attenuation

SUBROUTINE LONGWAVE

Determines long wave radiation transfer.

FUNCTION FRACDIFF

Determines actual:potential radiation ratio for the day, from total potential daily PAR, and then uses a relationship from Erbs et al (1982) to estimate fraction of incoming radiation that is diffuse.

Soil functions.f90

A critical issue to understand is how we link the characteristics and dynamics of soil layers to those of canopy layers. The canopy and leaf routines treat each canopy layer as biologically independent. **However, we assume that each canopy layer has roots located in each and every one of the rooted soil layers.** (It would be possible to modify the model so that canopy layers have roots in different layers, for instance to restrict understorey plants to shallower soil layers. But such modifications have not yet been carried out.)

For each canopy layer, we assume there is a single resistivity and soil water potential that applies to each. The amount of leaf area in each canopy layer determines the actual belowground resistance (that is, soil and root resistance). The relevant calculations are in SR WATERUPTAKELAYER.

SUBROUTINE SOILDAY runs all the non-biological water and energy balance routines for the canopy (interception, dripage, evaporation of rain) and the soil (snow pack dynamics, infiltration, surface energy balance, drainage). The SR also couples the biological water demand to soil water status. For simplicity, soil water status at the start of the time step is used to set limits on plant water abstraction. Only at the end of the time step is water status is updated for total abstraction

SR SOILDAY starts by loading the specific time step drivers into new variables. Then it calls routines to determine the soil hydraulic characteristics, based on soil conditions (SR SOILFC and SR SWPSOILR). Next, it checks if it is snowing or if there is snow on the ground. If so, then it calls the SR SNOWRUN. For simplicity we assume that the canopy does not intercept any snowfall. If it is not snowing, we run FN ZBRENT to calculate the soil surface energy balance and we call SR CANOPY_BALANCE to simulate interception of rainfall, and subsequent dripping and evaporation.

The SR then call SR WATERUPTAKELAYER to calculate from which of soil layers the water abstraction by plants occurs. For each soil layer, water gains and losses are then accumulated in SR WATERFLUXES. Thermal corrections due to water movement are calculated and water fluxes are actually implemented in SR WATERTHERMAL.

SR CRANK_NICHOLSON is the solver for the partial differential equations describing heat flow through the soil profile. SR THAWDEPTH determines the distribution of frozen and liquid water and ice fractions in each soil layer.

The remainder of SR SOILDAY sets up some unit conversions, and then calculates some check sums. The SR compares the change in total water storage in the soil profile (*delw*), with the sum of all the fluxes into and out of the profile (*fluxsum*). If mass is conserved, then these two numbers should be the same, and thus the difference between them (*checkdiff*) should be zero.

SUBROUTINE WATERUPTAKELAYER

This SR determines from which layer is water withdrawn. It does this by roughly estimating a maximum rate of water supply from each of the rooted soil layers, using soil water potential and hydraulic resistance of each layer. Actual water uptake from each layer is determined by using the estimated value as a weighting factor. The weighting factors are also used to generate a weighted soil water potential, which is the value used in calculating the actual water uptake to

each canopy layer. For each canopy layer, we calculate a single resistivity; the amount of leaf area in each canopy layer determines the actual belowground resistance.

SUBROUTINE CRANK_NICHOLSON

This is a finite difference PDE solver for soil temperature profile.

SUBROUTINE SOIL_BALANCE

This routine calls the Runge-Kunte ODE integrator to estimate soil gravitational drainage. The SR makes sure that only liquid water, not ice, drains out of any layer, and also determines how much space there is in the layer below for water to drain into.

SUBROUTINE SOILSTOR

Called by the ODE integrator, this SR contains the equations that determine gravitational water drainage. Gravitational drainage only occurs if the liquid water content exceeds a set fraction of total porosity. The fraction is set by the variable *draincheck*. Soil porosity is determined in SR SOILFC.

SUBROUTINE CANOPY_BALANCE

This SR calls the ODE integrator to determine the drainage and evaporation of water from leaf surfaces, and the amount of water reaching the soil surface.

SUBROUTINE CANSTOR(time,y,dydt)

Called by the ODE integrator, this SR contains the equations that determine canopy water storage and evaporation, and water reaching soil surface.

REAL FUNCTION WETEVAP()

This FN determines the rate of evaporation from wetted surfaces. Units = mm per time step.

SUBROUTINE THAWDEPTH

This routine determines layer ice fraction, and depth of thaw

REAL FUNCTION THERMCOND

Determines the thermal conductivity of soil based on clay, sand, organic, water and ice content. Units = $W m^{-1} K^{-1}$

REAL FUNCTION HEATCAP

Determines the volumetric heat capacity of soil (equations from (Waelbroeck 1993)), and incorporates the impacts of freeze/thaw on energy fluxes. Units = $J m^{-3} K^{-1}$

REAL FUNCTION ENERGY

Determines the surface soil energy balance, by finding the temperature that balances all the energy exchanges across the soil surface – latent and sensible heat, short and longwave radiation, and soil heat flux. Units = $W m^{-2}$

REAL FUNCTION EXCO

Estimates the heat or vapour exchange coefficient/boundary layer conductance ($m s^{-1}$). Currently assumes a neutral buoyancy. Could be improved with calculations of atmospheric stability. Units = $m s^{-1}$

REAL FUNCTION QEFLUX

Calculations latent energy loss from soil surface based on moisture gradient and a series of resistors – atmospheric boundary layer and soil pore space.

SUBROUTINE WATERTHERMAL

This SR redistributes heat according to water movement in the soil. Heat gain and loss for each soil layer is adjusted according to heat of water gained and water lost.

SUBROUTINE WATERFLUXES

Calculates the gains and losses of water from each soil layer. These calculations include calling WETTLINGLAYERS to determine the distribution of water in the top layer. Water losses are determined by evaporation from the top layer, dew fall in the top layer, root water abstraction from rooted layers (calculated from *totet*, the total transpiration), and gravitational drainage, calculated in SR SOIL_BALANCE. The SR also calls INFILTRATE to determine water additions through precipitation and snowmelt.

SUBROUTINE INFILTRATE

This SR takes *surface_watermm* and distributes it among top soil layers, starting from the top and working down. We assume total infiltration in time step – that the presence of roots and absence of soil disturbance ensures this. If the entire soil profile is saturated, then any excess water is regarded as overland flow and is lost from the system as runoff.

SUBROUTINE WETTINGLAYERS

This SR tracks surface wetting and drying in the top soil layer. Thus, it determines the thickness of uppermost dry layer and thus latent energy losses from the soil to the atmosphere. We track the dynamics of multiple wet and dry mini-layers within the top soil layer (see Soil surface energy balance).

SUBROUTINE ROOT_ALLOCATION

This SR determines root mass density (g m^{-3}) in each soil layer. Input parameters are root mass density in the surface layer (*surfbiomass*), total root mass in the soil profile (*rootbiomass*), and depth of rooting (*rootl*). We assume that maximum biomass is at the surface, and there is an exponential decline in root biomass with depth.

FUNCTION DECLINEROOT.

The FN calculates the coefficient for exponential decline with depth. Units=N/A

SUBROUTINE SNOWRUN

This SR calculates the dynamics of any snowpack. Snow falls if precipitation occurs at temperatures below freezing. The routine calculates the change the snow height and weight arising from new snowfall.

If there is no existing snow when snow falls, then the new snow is distributed among three snow layers in the ratio 25:50:25 below a height threshold. If snow is higher than the threshold, then increasing proportions of the snow are allocated to the lower snow layers. Snow height in the upper snow layer is not allowed to exceed 0.05 m.

If there is existing snow and new snow falls, snow height and weight is incremented. Then gravitational packing is invoked to alter snow density, heat content, and thermal conductivity.

Next the SR calculates melting in the snowpack. Calculations are only undertaken if snow height exceeds 0.006 m – if snow is thinner than this we assume that it melts away. This section

of the routine contains a simple time step calculator, that adjusts the number of computations according to rates of change in the snow pack. The SR calls SR SNOWCALC (see below) to determine the energy dynamics in the snowpack over the full time step. The SR then calls SNOWCALC again for another time step, and compares the first and second estimates of snow heat content for similarity to test for stable behaviour. If the predictions are stable, then the first set are used to update the snow pack energy balance.

If there are indications of instability, then the time step is halved. If the time step is already very small, no further halving is done.

SUBROUTINE SNOWCALC

This SR first calculates the evaporation and sublimation of snow from the top snow layer, and the flux of heat between the snowpack (snow layer 3) and soil surface layer (soil layer 1). Then the energy balance of each snow layer is resolved, providing an estimation of snow layer temperature. If there is an excess of heat, the SR melts a fraction of the snow layer; if heat content is low, then a fraction of meltwater is refrozen. After melting, the SR adjusts snow density and snow height and determines the flux of water out of the layer.

Soil and air.f90

SUBROUTINE BOUNDARY

Determines the boundary layer conductance for each leaf canopy layer. See Boundary layer conductance above.

SUBROUTINE SOILFC

Determines the porosity (i.e. maximum water content in soil by volume fraction) and soil hydraulic conductivity of soil. Inputs are water content by volume fraction, and the fraction of soil matter comprised of sand and clay. We use the algorithms of Saxton et al. (1986) to make these calculations.

SUBROUTINE SWPSOILR

Determines the soil water potential (SWP) and the soil-root resistance in each soil layer. SWP is determined from the algorithms of Saxton et al. (1986), soil sand and clay content, and soil water content. Soil-root resistance is determined from soil radial resistance (flow from bulk soil to root surface) and root radial resistance (flow along the root to the base of the plant stem). Soil radial resistance is dependent on soil hydraulic conductivity and root surface area. Soil axial resistance is dependent on root resistivity and root mass.

FUNCTION SOILCOND

Determines the soil hydraulic conductivity for use in the soil drainage integrator. Again this uses the equations from Saxton et al. (1986). Units= m s^{-1}

RUNGE_KUTTA.f90

This is an integrator for ordinary differential equations. We use the RUNGE_KUTTA to track the dynamic behaviour of various model state variables, such a leaf water potential, and water stored on leaf surfaces. The RUNGE_KUTTA finds the time step that ensures dynamics are

smooth and that the relevant feedbacks are properly incorporated. For a full description see Press et al. (1986).

ZBRENT.f90

This is a bisection routine. When ZBRENT is called, we provide a reference to a particular function and also two values which bound the arguments for the function of interest. ZBRENT finds a root of the function (i.e. the point where the function equals zero), that lies between the two bounds. For a full description see Press et al. (1986).

IO.f90

The Input-Output file is generally modified to fit the particular model application, although there are some basic requirements and in most cases the code is very similar.

SUBROUTINE INIT

This SR opens up a series of files, for model parameterization, forcing, and output. Using data from the vegetation and soil parameterization files, the SR calls others to structure the vegetation aboveground (SR CANOPY) and belowground (SR ROOT_ALLOCATION).

SUBROUTINE IO_DAILY

This SR reads climate data and vegetation data each day to provide model drivers (radiation, air temperature, precipitation) and changes in vegetation structure (e.g. total LAI and total root biomass).

SUBROUTINE DATOUT

This SR generates model output.

FUNCTION DAYINT

This function is a simple integrator, using the trapezium rule to calculate daily summations of various data provided at finer timescales.

SUBROUTINE GAPFIX

This SR locates data gaps in time series and used linear interpolation to fill these gaps (only 1 or 2 missing data can be dealt with).

Main.f90

This contains the **program** file, the opening code of the model. The program file calls SR INIT to initiate input/output. It then steps into the daily loop to being reading in daily drivers (SR IO_DAILY) and calculating the physical environment (SR SOLAR and SR BOUNDARY). Next SR DAY is called to initiate the simulation of C and water fluxes. Once these are complete, the SR DATOUT is called to generate output, and the code loops onto the next day.

Running the model

The model is readily applied to different ecosystems as there are relatively few parameters to be changed. The most critical are LAI and foliar N (accounting for phenological changes), plant hydraulic conductance, minimum leaf water potential, rooting depth, and soil texture.

Parameter files

There are two parameter files, one mostly concerned with vegetation parameters, called 'demo veg.csv' (Table 1), and the other with soil, called 'demo soils.csv'. (Table 2). The 'demo' part of each name can of course be replaced with some site-specific name at your convenience, as long as you update the file names in SR INIT.

Some of the parameter settings are related to setting constants, while others define initial conditions.

Go to the excel spreadsheet 'SPA calibration worksheet.xls'.

First deal with the soil parameters. Describing how key parameters vary with depth is generally difficult:

1. *Rooting depth* is a particular problem as field studies rarely attempt to find this threshold and if pits are dug they are usually away from trees. Often we have to use the model to help us define the minimum rooting depth. If rooting depth is set too low we see a drought developing that is not supported by the data (sap flow, soil moisture, eddy flux). In such a case, extend the rooting depth and run again. A detailed set of soil moisture sensors at a series of depths can help to parametrize the root profile effectively.
2. *Root biomass*. At a minimum we must specify the root biomass density in the uppermost layer of the soil, and the total root biomass. We then assume that there is an exponential decline in root biomass with depth. The spreadsheet contains a solver that estimates how root biomass is distributed given these assumptions.

Next deal with the hydraulic parameters for the roots and stems. Read the detailed notes in the spreadsheet. You will need to enter a series of parameters; root density (i.e. the density of the root tissue itself), root radius, and the leaf area density and height of each canopy leaf layer. You must also specify whether stem conductance varies with length of stem (conductivity=1) or is invariant (conductivity=0). You then calibrate the two key hydraulic parameters – root resistivity and stem conductivity/conductance. You calibrate these parameters so that the estimated leaf specific conductivity matches an independent measure. The independent measure should come from either leaf level gas exchange and water potential measurements or (preferably) sap flow data.

Then move to the canopy parameters. There are two tables in this worksheet.

Table A. You need to enter the fraction of total foliar nitrogen in each canopy layer and the total foliar N.

Table B. This requires data from Aci curves (leaf level gas exchange data under a range of CO₂ concentrations). The data required are the estimated V_{cmax} and J_{max} from the relevant Aci curve, and the foliar N concentration of the leaves that were sampled.

Then move to the veg parameter file and soil parameter file worksheets and fill in the remaining blue cells. The tables below detail each of the parameters, their units, and some ranges of typical values. The *iota* parameter determines how much stomatal opening occurs during unstressed periods, usually early morning and late evening. Adjust this parameter if you find that modelled latent energy fluxes are too high or low in the early morning.

Table 1 Vegetation properties

Parameter	Explanation	Units	Typical values
(lafrac(i),i=1,numl)	Fraction of total leaf area in each canopy layer	Fraction	0–1
(nla(i),i=1,numl)	Fraction of total foliar nitrogen in each canopy layer	Fraction	0–1
(layerht(i),i=1,numl)	Height of each canopy layer	m	1–50
totla	Total LAI	m ² m ⁻²	0.1–10.0
totn	Total foliar N	gN m ⁻²	0.1–20.0
gplant	Stem conductivity or stem conductance	mmol m ⁻¹ s ⁻¹ MPa ⁻¹ mmol m ⁻² s ⁻¹ MPa ⁻¹	1–20 0.1–5.0
minlwp	Minimum leaf water potential	MPa	-2 – -4
iota	Stomatal efficiency	N/a	1.01-1.0007
capac	Leaf capacitance	mmol m ⁻² MPa ⁻¹	1,000–10,000
lat	Latitude	°N or °S	0–70
outt	Detailed layer by layer output?	0=no, 1=yes	0 or 1
dimen	Leaf characteristic dimension	m	0.01–0.2
rootresist	Root resistivity	MPa s g mmol ⁻¹ (biomass based)	10–500
towerht	Height of measurement tower	m	3–50
conductivity	Does conductance vary with stem length?	0=NO, 1=YES	0 or 1
kappac	Rate constant for V _{cmax}	μmol g ⁻¹ s ⁻¹	10–50
kappaj	Rate constant for J _{max}	μmol g ⁻¹ s ⁻¹	20–100

Table 2 Soil parameters

Parameter	Explanation	Units	Typical values
thickness(i),i=1,core	Thickness of soil layer	m	0.1–0.5
organicfrac(i),i=1,core	Organic fraction of each soil layer	Fraction	0.0–0.5
mineralfrac(i),i=1,core	Mineral fraction of each soil layer	Fraction	0.0–0.5
waterfrac(i),i=1,core	Initial water fraction of each soil layer	Fraction	0.0–0.5
soiltemp(i),i=1,core	Initial temperature of each soil layer	K	270–300
iceprop(i),i=1,core	Initial proportion of water in each layer in ice	Fraction	0-1
rootfrac(i),i=1,core	Fraction of total root biomass in each soil layer	Fraction	0-1
rootl	Number of rooted layer (starting from the top)	N/A	1–20
rootbiomass	Total root biomass	g biomass m ⁻² ground	100–2000
Sandpc	% sand in soil layers	%	10–50
claypc	% s clay in soil layers	%	10–50
rootrad	Fine root radius	m	0.0005
draincheck	Fraction of porosity above which gravitational drainage occurs	Fraction	0.5–0.7
snowweight	Initial total snow weight	Kg m ⁻²	0+
snowheight	Initial snow height	m	0+

Driver files

There are two key driver files

1. The first operates on a sub-daily timescale (usually 30 minute or 1 hour resolution, Table 3, called ‘demo met drivers.csv’) and it contains the meteorological drivers.
2. The other on a daily timescale (called ‘demo phenology.csv’) and contains the phenological drivers.

The key meteorological drivers are listed in Table 3. The demo driver file shows how the drivers should be arranged to be input to the model. Generating gap-free meteorological drivers is a considerable effort for long time periods. But it is critical that this is done precisely. For instance, gaps in the wind speed column can cause model crashes that are quite hard to track down. If the model crashes suddenly on a certain day and time, the first thing to check are the meteorological drivers for that day to see if there is a gap.

Table 3 Meteorological drivers

Parameter	explanation	units
daytime	Decimal time	Days
temptop	Air temperature above canopy	°C
coa	Atmospheric CO ₂ concentration	μmol mol ⁻¹
windsp	Wind-speed	m s ⁻¹
swrad	Short-wave radiation	W m ⁻²
vpdtop	Vapour pressure deficit	kPa
partop	Photosynthetically active radiation	μmol m ⁻² s ⁻¹
ppt	precipitation	mm water equivalent

You should expect a close relationship between PAR and short-wave radiation. In fact, you can use one to estimate the other

PAR energy content = 4.6 μmol J⁻¹; ~50% of SWR is PAR

Therefore, we expect $2.3 \times \text{short wave radiation (W m}^{-2}\text{)} = \text{PAR (}\mu\text{mol m}^{-2} \text{s}^{-1}\text{)}$.

The daily phenological drivers are concerned with changes in key plant parameters- these are deemed to occur at daily or longer time scales. This version of SPA does not predict how plant structure changes over time, only plant function. So, you must prescribe any relevant changes.

The format of this driver file is flexible to some extent (see the demo for basic format), but at a minimum it should describe the variation in LAI, root biomass, and total foliar N over the time period of interest. If the time period is short, it may be that these parameters do not change significantly. In such a case the read statement can be commented out – the initial values for LAI ('totla'), root biomass ('rootbiomass'), and total foliar N ('totn') set in the vegetation parameter file will be used throughout the simulation.

Output files

Output files are all time series, at either daily or 60/30 minute time steps. The left most column of each file is always the time. Column headers help to identify the output variables – more details are given in Table 4 below. Output files are generated in the SR DATOUT, SOIL FUNCTIONS, SR LEAF, and SR CANOPY and SR LIGHT. The output files are formatted as 'comma separated values', so they are easily read in Microsoft excel and many graphical packages.

Table 4 Output files. Name of file, name of the subroutine (SR) from which the file is written, frequency of writing output, and details of the written variables. Some files (names in italics) are only written if a switch is set in a parameter file. For example, the switch ‘outt’ must be set to 1 in the vegetation parameter file if output is to be written to *energy.csv* and all the canopy layer files (*l1.csv* etc).

File name	Called in SR	Time step	Output
Daily.csv	DATOUT	daily	Daily GPP, water fluxes, hydraulic parameters
Drivers.csv	DATOUT	daily	Summarises meteorological and vegetation drivers
Hourly.csv	DATOUT	60 or 30 minutes	Photosynthesis, leaf respiration, evaporation and transpiration
<i>Energy.csv</i>	SOILDAY (‘outt’ switch)	60 or 30 minutes	Soil surface energy balance and soil surface temperature
Solar.csv	SOLAR	60 or 30 minutes	Radiation absorption in each leaf layer
Soilwater.csv	SOILFUNCTIONS	Daily (default) or 60 or 30 minutes (‘outt’ switch)	Water fraction in top 15 soil layers, weighted soil water potential
Upfrac.csv	SOILFUNCTIONS	Daily	Fraction of total plant water uptake removed from each of top 15 soil layers
Iceprop.csv	SOILFUNCTIONS	Daily (default) or 60 or 30 minutes (‘outt’ switch)	Ice proportion of water content in each of top 15 soil layers
<i>Parcheck.csv</i>	DATOUT (‘outt’ switch)	60 or 30 minutes	Checks that calculations in SOLAR match radiation assigned to each leaf in CANOPY
Soiltemp.csv	SOILFUNCTIONS	Daily (default) or 60 or 30 minutes (‘outt’ switch)	Soil temperature in each of top 15 soil layers
Waterfluxes.csv	DATOUT	Daily	Water fluxes, and water budget closure calculations
<i>Soilstatus.csv</i>	SOILDAY (‘outt’ switch)	60 or 30 minutes	Detailed water fluxes and water budget closure calculations
<i>l1.csv</i> (... <i>l10.csv</i>)	ASSIMILATE (‘outt’ switch)	60 or 30 minutes	Detailed leaf level diagnostics – stomatal conductance, photosynthesis, leaf water potential, absorbed radiation, temperature, for each canopy layer (numbered by file name)

The detailed descriptions of each output variable are in a spreadsheet, ‘output variables.xls’.

Common problems

The most common reason for the model to crash is an error in the driver files. Missing data or ‘-999’ values in the met drivers file will generally cause the model to explode. If the model is crashing at a certain time, check that time period in the driver file for problem data.

Model Applications

Because of its global applicability, the SPA model has been applied in ecosystems ranging from the 70°N to the 2°S. The SPA model has been extensively tested against independent eddy covariance data collected in temperate oak-maple forest at the Harvard Forest LTER site near

Petersham, Massachusetts (42.54°N, 72.18°W, elevation, 340m). Based on meteorological and stand data collected over more than 50 days in the summer of 1992, our predicted hourly CO₂ ($r^2=0.86$) and water ($r^2=0.87$) exchange rates are highly correlated with independent, whole-forest measurements made with the eddy correlation method (Wofsy *et al.* 1993; Williams *et al.* 1996). The model was also able to explain more than 90% of the variability in measured daily gross primary productivity at Harvard Forest (Williams *et al.* 1997). The SPA model has also been applied in tropical rain forests (Williams *et al.* 1998) to examine the seasonal patterns of C and LE exchange, in arctic tundra (Williams *et al.* 2000) to investigate spatial differences in C fluxes, and in ponderosa pine forests subject to seasonal water deficits (Williams *et al.* 2001b). The hydraulic hypothesis that controls stomatal conductance has been tested against sap flow data from ponderosa pine (Williams *et al.* 2001a). SPA has been used to elucidate biotic and climatic controls on water and carbon exchange in ponderosa pine stands of different ages (Schwarz *et al.* 2004). The snow model has been extensively tested in arctic tundra (Van Wijk *et al.* 2003).

History

SPA was constructed by Mathew Williams starting in 1994 during his post-doc at the Ecosystems Center of the Marine Biological Laboratory, under the supervision of Edward Rastetter. Ed provided a lot of encouragement and great assistance. During the period 1994-2000 Mat continued developing and applying the model, and introduced the more detailed below-ground components. Mat began a collaboration with Marc Stieglitz and Vic Engel during 1999-2000, and Vic worked on connecting SPA with Marc's TOPMODEL-like hydrological model – the new model, called SPLAT, is still under development with Vic (Engel *et al.* 2002). Mat moved to the University of Edinburgh in 2000. A student at Edinburgh, Rosie Fisher, applied the model in central Amazonia as the focus of her Master's Thesis, and is currently working with SPA in her PhD. Mat's post-doc, Mark van Wijk, then began using the model in 2001 and incorporated Marc Stieglitz's snow model into SPA. Interactions with other scientists have had an impact on the development of SPA – Bev Law, Dick Waring, Barbara Bond, Mike Ryan, Michael Goulden, Steve Wofsy, Gus Shaver, Yadvinder Malhi and many others.

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