CHAPTER 3. PROGRAM STRUCTURE AND NUMERICAL SOLUTIONS

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3.1 Introduction

This section details the logical flow, and numerical solution methods for the four balances solved in WAVES: water, energy, carbon, and solute. All models that perform balances of quantities follow the same pattern: the amount present at the end of a time-step is equal to the amount present at the beginning of the time-step, plus the amount added, minus the amount removed; WAVES is no different in this regard. The water, carbon, and solute balances use the method mentioned, while the energy balance only partitions the amount of energy received, and we assume there is no carry-over from one day to the next. The amount at the start and end of the time-step is effectively zero.

3.2 Energy Balance

The energy balance equations and theory are discussed in Chapter 2, but the important steps, theories, and assumptions are repeated here for completeness with the three other balance descriptions.

3.2.1 Radiation

The energy balance of any point can be described by:

$$R_n = P_s + \lambda E + H + A_h + G + S \tag{3.1}$$

where R_n is net radiation, P_s is energy absorbed for photosynthesis, λE is energy used for evapotranspiration, H is sensible heat, A_h is advected energy from or to the surroundings, G is energy that heats the soil, and S is energy that is stored. All these terms are in units of W m^{-2}. The variable R_n can also be expressed as:

$$R_n = R_{sd} - R_{su} + R_{ld} - R_{lu} \tag{3.2}$$

where R_{sd} is the downward shortwave radiation, R_{su} is the upward shortwave radiation, R_{ld} is the downward longwave radiation, and R_{lu} is the upward longwave radiation. All these terms are in units of W m^{-2}.

The energy balance assumptions in WAVES are that:

- the temperature of the soil, canopy, and air is the same, and equal to the average of the maximum and minimum daily temperature,
- differences in upward longwave radiation from the different surfaces is a function of emissivity alone,
- on the daily time-step, all storage and heating terms are negligible,
- in a one-dimensional model, lateral energy transfers cannot be estimated or used,
- leaf angles are randomly distributed and do not reflect energy within the canopy, so that the canopy may be treated as translucent absorbing layer (the so-called 'big leaf model').

Applying the appropriate assumptions to (3.1) leaves us with:

$$R_n = \lambda E + H \tag{3.3}$$

Such an equation looks relatively easy to work with. However, in general the two largest terms are R_n and λE (Monteith and Unsworth 1990), so H can be estimated by difference. In practice within WAVES, H has no significance to the water, carbon, or solute balance, so only R_n and λE are modelled explicitly.

WAVES expects as input daily downward shortwave radiation, which is easy to measure or estimate. To complete the terms in Equation (3.2) we need estimates of longwave radiation. Following Brutsaert (1982), we have:

$$R_{ld} = \varepsilon_a \sigma T_a^4 \tag{3.4}$$

$$R_{lu} = \varepsilon_s \sigma T_a^4 \tag{3.5}$$

$$\varepsilon_a = 1.24 \left(\frac{e_a}{T_a} \right)^{1/7} \tag{3.6}$$

where ε_a is the atmospheric emissivity, ε_s is the surface emissivity (this ranges from 0.95 to 0.99 for surfaces like snow, open water, soil, and plant canopies, so in WAVES it is a constant set at

0.97), σ is the Stefan–Boltzman constant (5.67×10^{-8} W m^{-2} K^{-4}), T_a is the average of daily maximum and minimum air temperature (Kelvin), and e_a is vapour pressure (millibars) based on T_a.

Net longwave radiation, that is $R_{ld} - R_{lu}$, is in general a negative quantity. In the cascading energy balance WAVES performs, *i.e*. one layer at a time, longwave losses must be subtracted from each layer, not as a bulk cost to the total available energy. For a vegetation layer, the energy balance components are:

$$R_{sin} = R_{sd}(1 - exp(k\ LAI)) \tag{3.7}$$

$$R_{snet} = R_{sin}(1 - \alpha) \tag{3.8}$$

$$R_{lnet} = (R_{ld} - R_{lu})\frac{R_{sin}}{R_{sd}} \tag{3.9}$$

$$R_{net} = R_{snet} + R_{lnet} \tag{3.10}$$

where R_{sd} is the downward shortwave radiation that reaches the soil or canopy surface (for the first canopy it is incoming solar radiation, for the next canopy it is the shortwave radiation that passes through the first canopy, *etc*), k is the light extinction coefficient of the canopy, *LAI* is the leaf area index of the vegetation canopy (m^2 leaf m^{-2} ground), α is surface albedo, R_{sin} is the shortwave radiation that is potentially available to the canopy, R_{snet} is the net shortwave radiation after reflection from the canopy, R_{lnet} is the net longwave radiation of the canopy (these wavelengths are not affected by albedo), and R_{net} is the net available total radiation to the canopy.

These equations can be cascaded through a series of canopies, by repeating the calculations with that radiation passing through the canopy as R_{sd} for the next lower canopy. At the soil surface there is no canopy to filter and absorb radiation, so in (3.7) $R_{sin} = R_{sd}$. Other than that, these equations hold for the soil energy balance also.

3.2.2 Vapour Pressure Deficit

Just as the amount of radiation cascades down through a series of canopies, so the vapour pressure deficit under a canopy is, in general, less than above the canopy. Jarvis and McNaughton (1986) proposed a method of estimating how to quantify this decrease, through use of a coefficient describing how well coupled the atmosphere is to the air within and below the canopy. The method for the omega coefficient is as follows:

$$D_i = \Omega_c D_{eq} + (1 - \Omega_c) D_a \tag{3.11}$$

where D_i is the within and below canopy vapour pressure deficit (millibars), D_a is the above canopy vapour pressure deficit (millibars), D_{eq} is the equilibrium vapour pressure deficit (millibars), and Ω_c is the atmospheric coupling coefficient, defined by:

$$D_{eq} = \frac{\gamma \varepsilon R_{nv} r_c}{c_p(\varepsilon + 1)} \tag{3.12}$$

$$\Omega_c = \frac{\varepsilon + 1}{\varepsilon + 1 + r_c/r_a} \tag{3.13}$$

where $\varepsilon = \Delta/\gamma$, Δ is the slope of the saturated vapour pressure *v.* temperature curve (millibar K^{-1}), γ is the psychrometric constant, r_c is bulk canopy resistance (s m^{-1}), c_p is the specific heat of air at constant pressure (W kg^{-1} K^{-1} s), and r_a is bulk aerodynamic resistance (s m^{-1}).

Just as radiation cascades downward, using the amount of radiation passing through the next highest canopy as the starting energy, the vapour pressure deficit is progressively reduced moving down toward the ground. The vapour pressure deficit in the climate file will affect the upper canopy, the lower canopy will use a reduced vapour pressure deficit, and the soil below will use yet another vapour pressure deficit.

3.2.3 Aerodynamic and Canopy Resistance

The Soil Surface

For the soil, aerodynamic and canopy (read as surface) resistance for evaporation are extremely simplified. The aerodynamic resistance (r_a) is set to a constant of 100 s m^{-1}. The values of roughness length for soil reported in Brutsaert (1982) are from 0.001 to 0.01 m, and assuming a constant wind speed of 2 m s^{-1} at 2 m this translates to a resistance of 85 to 172 s m^{-1}.

The surface resistance is a function of four possible variables; (1) the wetness of the surface soil, (2) the depth of any drying front, (3) the amount of litter, and (4) whether the site is flooded. When the soil is not air-dry at the surface, r_s is set to zero. When the soil is air-dry at the surface, then the depth of drying front is calculated from the soil water potentials solved by the water-balance module (see section 3.3). The surface resistance is then set according to Choudhury and Monteith (1988):

$$r_s = \frac{\tau \ell}{\rho D_v} \tag{3.14}$$

where τ is the tortuosity factor (constant set to 2), ℓ is tortuous path-length equal to the depth of drying front (m), ρ is soil porosity, and D_m is the molecular diffusion coefficient for water vapour in air (constant set to 2.5 x 10^{-5} m^2 s^{-1}). If there is plant litter on the soil surface, then the path-length ℓ is increased by:

$$\ell = \ell + \frac{C_{lit}}{20} \tag{3.15}$$

where C_{lit} is the weight of litter (kg m^{-2}).

If the soil is flooded, *i.e.* has standing water with a positive soil water potential at the surface node, $r_s = 0$ and $r_a = 80$ s m^{-1}.

The Plant Canopy

The aerodynamic resistance of each plant canopy in WAVES is treated as a constant. This is for several reasons related to the exposition in section 2 from (2.36) to (2.42). The first is that we do not always have windspeed available as input data. Second, and more importantly, we do not know the roughness length of the vegetation, or how that varies in time. For example, it may be adequate to express the height of a grass or crop as a fraction of the leaf area index, but this would clearly not work for trees. In that case, a relationship based on accumulated stem mass might be good, but only up to certain ages. In any event, these data and relationships are so rarely available, that a constant value for r_a is the only practical alternative. For very rough canopies, such as closed canopy forests, the surface is very rough and a small constant resistance is a good approximation, $r_a = 10$ s m^{-1} (Monteith 1981). For smoother surfaces, such as grass and crops, a higher resistance is required, but the value is likely to be less constant over the whole growing season, $r_a = 30$ s m^{-1}.

Canopy or surface resistance is the mechanism for coupling environmental stresses back to transpiration. In Ball *et al.* (1987) type conductance models, canopy conductance (the reciprocal of canopy resistance) is a function of the assimilation of carbon. In section 3.5 there is a detailed description of how daily assimilation is calculated, and so here we will assume this value is available, and proceed with the estimation of canopy conductance. First the conductance to CO_2 is calculated by:

$$g_c = 0.0005 LAI\, k + \frac{g_1 A}{0.9[CO_2]DL(1 + D_a / 3.5)} \tag{3.16}$$

where g_c is the conductance to CO_2 (m s^{-1}), g_1 is the slope of the assimilation versus conductance line, A is the actual assimilation (kg C m^{-2}), [CO_2] is the atmospheric CO_2 concentration (constant set to 1.8324 x 10^{-4} kg C m^{-3}), and DL is the day length (in seconds). Next, the conductance to water vapour is estimated by:

$$g_w = g_c\left(1 + \frac{\chi_w}{sm_c \chi_l \chi_t}\right)1.6 \tag{3.17}$$

where g_w is the conductance to water vapour (m s^{-1}), χ_w is the relative availability of water, χ_l is the relative availability of light, χ_t is the relative favourability of temperature, sm_c is the ratio of stomatal to mesophyll conductance (constant equal to 0.2 for C_3 vegetation and 0.8 for C_4 vegetation), and 1.6 is the ratio of the diffusion rates of CO_2 and H_2O vapour.

The result from (3.17) is limited to the maximum value obtained when A is at the maximum assimilation rate, and the three availability scalars χ_w, χ_l, and χ_t are equal to 1.0. Canopy resistance for estimating transpiration is the reciprocal of conductance from (3.17).

3.2.4 Transpiration and Evaporation

With all the necessary quantities defined and calculated, we can estimate the daily transpiration and evaporation rates. WAVES uses the Penman–Monteith combination equation:

$$\lambda E = \frac{\Delta R_n + \rho c_p \Delta_a / r_a}{\Delta + \gamma(1 + r_c / r_a)} \tag{3.18}$$

where E could be for any vegetation layer or the soil surface (m d^{-1}), using the appropriate value for R_n, D_a, r_c, and r_a. The constant c_p is set to 1010, and constants are applied to (3.18) give the estimated rate in m d^{-1}. The following empirical functions are used to determine the parameters for equations (3.1) to (3.18). Saturation vapour pressure e_a, psychrometric constant γ, slope of saturation vapour pressure curve Δ, density of air ρ, and latent heat of vapourisation λ, are calculated by:

$$e_a = 6.1078 \exp\left(\frac{17.269 T_a}{T_a + 237.16}\right) \tag{3.19}$$

$$\gamma = 0.646 + 0.0006 T_a \tag{3.20}$$

$$\Delta = e_a(T_a + 0.5) - e_a(T_a - 0.5) \tag{3.21}$$

$$\rho = 1.292 - 0.00428 T_a \tag{3.22}$$

$$\lambda = 2501000 - 2400 T_a \tag{3.23}$$

where T_a is the average of daily maximum and minimum air temperature in degrees Celsius, and in (3.21) a value of saturation vapour pressure at more than, and less than, daily air temperature by one-half of a degree is determined from (3.19).

The transpiration from (3.18) is then distributed within the root zone according to the following function:

$$rw_i = E \frac{rp_i \left(1 - \frac{\Psi_i + \eta \Pi_i}{\Psi_{wilt}} \right)}{SRP} \tag{3.24}$$

where rw_i is the root-water demand at depth *node i* (m d^{-1}), rp_i is the proportion of total root mass at *node i*, Ψ_i is the water matric potential (m) at *node i*, Π_i is the osmotic potential (m) due to solutes at *node i*, η is the salt sensitivity factor of the vegetation, Ψ_{wilt} is the wilting point of the vegetation (m), and SRP is the sum of the numerator over all nodes. The result from (3.24) can be further reduced if there is not enough water at any particular node while solving the water movement equations.

3.2.5 Computational Flow

The sequence of steps to run a single day time-step is as follows:

- adjust incoming shortwave direct and diffuse radiation for slope and aspect
- calculate downward and upward longwave radiation
- calculate root-water experience by adding matric and osmotic potential at each depth node with roots; sum this for whole profile for water availability, and sum this multiplied by proportion of roots at each node for distributing transpiration
- calculate net radiation of each vegetation canopy layer
- calculate net radiation of soil surface
- calculate rainfall interception for each canopy layer (see section 3.5) and reduce available radiation by the amount of energy required to vapourise that water
- CALL plant growth routine, which calculates actual assimilation
- calculate constants required for estimating evapotranspiration, including soil surface resistance and plant canopy conductance

- calculate transpiration from each vegetation canopy layer, reducing vapour pressure deficit below each one
- calculate soil surface evaporation
- distribute transpiration down profile; where roots compete for water at a node with less water available than required, reduce demand at that node proportionally.

3.3 Water Balance

WAVES does the water balance in a specific order, with relevant assumptions for use of a one-day time-step, and the rate of change of processes. The different types of fluxes, and order in which they are calculated in, are shown in Fig. 3.1.

The solution for soil water movement, water sources, and sinks, is all handled within the solution of Richards' equation (Richards 1931). The soil-water gradients provide the internal driving forces, while ponded and free infiltration, evaporation, plant transpiration, lateral fluxes, drainage, and groundwater exchange are all simple sources and sinks within the soil profile. Some of these are coupled into the iterative solution, such as the depth of a watertable, and some rates are constant, such as plant extraction rates over the day.

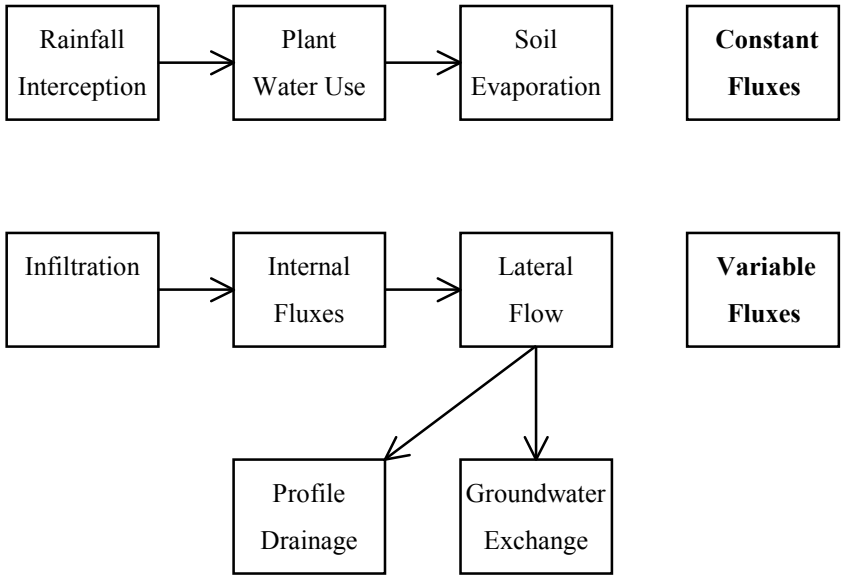

Fig. 3.1: WAVES Water Balance Flux Components. *Constant Fluxes* are calculated once at the beginning of the time-step and do not change during solution. *Variable Fluxes* are updated each iteration of the water movement solution until they are consistent with the calculated water contents.

3.3.1 Theory

The assumptions used in WAVES for water-balance modelling are that:

- the soil is rigid, *i.e.* it does not shrink or swell
- the soil is isothermal, *i.e.* the air temperature is the same as the soil temperature and this has no feedback onto the soil properties
- the soil is non-hysteretic, *i.e.* single-valued functions describe the relationships between water content and potential, and water content and hydraulic conductivity
- all soil-water flow is through the matrix, *i.e.* macropores, pipes, preferred pathways, and bypass flows are not modelled explicitly
- soil air flow is ignored
- solute in the water is conservative, *i.e.* it is not adsorbed by the matrix, and does not feed back onto the soil properties
- soil properties do not change with time or climate, *i.e.* the surface does not form a seal (reducing hydraulic conductivity) or compact (reducing hydraulic conductivity and water holding capacity), or possess other features that change soil properties, *e.g.* sodicity or acidity
- rainfall intensity is constant for the duration of the event, and similarly, soil evaporation and plant transpiration rates are constant for the non-raining duration of the time-step.

The last point requires some explanation. WAVES will use a one-day time-step for days when there is no rain, or when the rain lasts for the entire day. When only part of the day experiences rain, the duration of the rainfall will infer an intensity. Since high rainfall intensity can cause surface saturation and runoff, this is an important process to represent. Thus, on a day when rain lasts for only part of the day, a time-step is processed for the duration of the rain, then a second time-step is processed for the remainder of the day. During any of these time-steps, with rainfall or evaporation, the flux crossing the surface soil boundary and the leaf boundary, is assumed to be constant for the entire time-step. Diurnal fluctuations in rates are not modelled, only the average rate for the time-step. This is an appropriate compromise to maintain the largest time-step, *i.e.* a full day, while modelling the most important short-duration processes, *i.e.* runoff and saturation from high-intensity rainfall.

To solve a soil water mass balance, we must provide a framework that allows the important fluxes and feedbacks to be incorporated directly, and without special conditions. Because WAVES is a one-dimensional model concerned with the interactions between water, plant roots,

and salt, it is desirable to keep track of the vertical distribution the these quantities within the soil. Accordingly, the WAVES water balance is based around solution of Richards' equation (Richards 1931). This starts with a statement of mass balance:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} \tag{3.25}$$

where θ is water content ($L^3\ L^{-3}$), q is water flux ($L\ T^{-1}$), t is time (T), and z is depth positive downwards (L). Looking at the left-hand side (LHS) of (3.25), we see the change in water content with time (water storage at the end of the time-step minus water storage at the start of the time-step), and the right-hand side (RHS) of (3.25) says the change in flux with depth (water flux out of the bottom of the soil column minus water flux into the top of the soil column). The negative sign on RHS is because depth is positive downwards, and so the sign of flux matters. This is a direct statement of mass balance that matches exactly with the description in the Introduction.

Richards combined (3.25) with Darcy's Law for unsaturated conditions:

$$q = K\left(1 - \frac{\partial \psi}{\partial z}\right) \tag{3.26}$$

where K is hydraulic conductivity ($L\ T^{-1}$), and ψ is water potential (L), and derived:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial z}\left(K\left(1 - \frac{\partial \psi}{\partial z}\right)\right) \tag{3.27}$$

This is the classical 'mixed form' of Richards' equation. It is called a 'mixed form' because the dependent variable on the LHS is θ and on the RHS is ψ. Equation (3.26) has three equivalent forms that have been used in the RHS of (3.25):

$$q = K - K\frac{\partial \psi}{\partial z} = K - D\frac{\partial \theta}{\partial z} = K - \frac{\partial U}{\partial z} \tag{3.28}$$

where D is soil water diffusivity ($L^2\ T^{-1}$), and U is the Kirchhoff transform variable ($L^2\ T^{-1}$) (see for example Gardner 1958) defined by:

$$U = \int_{-\infty}^{\psi} K\, d\psi = \int_{0}^{q} D\, d\theta \tag{3.29}$$

The LHS of (3.25) has similar equivalent forms to (3.28):

$$\frac{\partial \theta}{\partial t} = C \frac{\partial \psi}{\partial t} = \frac{1}{D} \frac{\partial U}{\partial t} \tag{3.30}$$

where C is differential moisture capacity (L^{-1}) defined as $\partial\theta/\partial\psi$.

Richards (1931) stated that the solution of (3.27) was unique while the functions between variables, *i.e.* K and ψ as functions of θ, or K and θ as functions of ψ, remained monotonic throughout the entire range of application, and he placed no restrictions of the variables used in (3.28). Using different combinations of (3.28) and (3.30), Richards' equation can be described in one or more dependent variables. While each of the forms in (3.30) is analytically equivalent, when described in difference form for numerical solutions, they are not equivalent, and cause mass balance errors. Only the θ-based form of the LHS can explicitly conserve mass. Given that our primary concern here is to accurately keep track of all water, we must use θ on the LHS.

Analytic solutions of (3.27) up to the point of saturation and in uniform soils have traditionally used the θ-based form, commonly known as the Fokker–Planck equation, with θ in the LHS and RHS (*e.g.* Broadbridge and White 1988). Traditionally the ψ-based form has been used where the soil becomes saturated, or layers are required, but this form cannot conserve mass except with very small time and space steps. Haverkamp *et al.* (1977) used the U-based form of (3.27) for their numerical experiments, but this form is cumbersome and also cannot conserve mass.

Brutsaert (1971) used (3.27) for saturated and layered soils, thus proving that the traditional ψ-based form was not required for these purposes. The major step forward was to not use a Picard-type solution methods requiring a single dependent variable in the equation, but a Newton–Raphson solution scheme (see for example Shoop 1979). This allowed the equation to be formulated in any way, as long as a derivative with respect to a single dependent variable existed for each independent variable. In the general case of saturated and layered (or gradational) soils, the only continuous variable is ψ, and Brutsaert used this as the dependent variable of the solution.

Redinger *et al.* (1984) and Ross and Bristow (1990) used U on the RHS to reduce the apparent non-linearity of the flux term, while using a Newton–Raphson solution. Ross (1990) compared different transforms of ψ on the RHS, and found that a speed difference up to a factor of 200 could be achieved by using the different forms. Further, he found that different forms yielded different accuracy, compared to a detailed solution, for the same spatial discretisation. Given all forms of (3.28) are analytically equivalent and do not cause mass balance errors, the results of Ross (1990) were a function of the soil hydraulic properties used in the experiment.

In WAVES the form of Richards' equation used is:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial z}\left(K - \frac{\partial U}{\partial z} \right) + S(\psi) \tag{3.31}$$

where S represents all source and sink terms, *e.g.* root water extraction, and may be a function of the water potential at a node, *e.g.* water potential on a soil boundary specifies the depth of a water table that may be a lateral flowing sink term.

There are several reasons for using (3.31). Firstly, we do not know what soil hydraulic model the user will use. Equation (3.31) is the form that Ross (1990) found was fastest to run with a particular soil model. Since WAVES does not impose any particular soil model on the user, this will be the best equation for the soil model used by Ross. Secondly, the Newton–Raphson solution scheme requires derivatives of each term with respect to the dependent variable, in this case ψ. The derivative of U is K, and therefore we will not need extra information for derivatives of other variables. Finally, we want to minimise the number of arithmetic operations involved. With fewer variables in the equation we must reduce the absolute number of operations required.

3.3.2 Numerical Solution

Differential Equations

Equation (1) can be represented in finite-difference form at a depth node i, over time-step j to $j+1$, with arbitrary temporal weighting and central spatial weighting as:

$$F_i = \alpha(q_{i+0.5}^{j+1} - q_{i-0.5}^{j+1}) + (1-\alpha)(q_{i+0.5}^{j} - q_{i-0.5}^{j}) + e_i + S_i = 0 \tag{3.32}$$

where

$$q_{i+0.5}^{j} = K_{i+0.5}^{j} - \frac{U_{i+1}^{j} - U_{i}^{j}}{Dz_{fi}} \tag{3.33}$$

$$K_{i+0.5}^{j} = \sqrt{K_i^j K_{i+1}^j} \tag{3.34}$$

$$e_i = \left(\theta_i^{j+1} - \theta_i^j\right)\frac{Dz_{ci}}{Dt_j} \tag{3.35}$$

z_c refers to a central difference, z_f refers to a forward difference, and S_i is any combination or source and sink terms that may or may not be functions of soil water potential. Equation (3.34) is a geometric mean of the conductivity. In finite-element solution schemes, linear or arithmetic

averages are required due to the solution formulation. Using a finite-difference solution, there is no restriction on the form of flux, or even how the average is taken or the variables used to describe it. As long as they are consistent between iterations there is no numerical problems created. The geometric mean causes 'average' values to be lower, which we think is more physically realistic than the arithmetic average, or an upstream or downstream weighting.

At the top and bottom boundary, the equations are modified because a central difference does not exist at these points. At the surface node, nominally *node zero*, we have:

$$F_0 = \alpha\left(q_{0.5}^{j+1} - q_0^{j+1}\right) + (1-\alpha)\left(q_{0.5}^{j} - q_0^{j}\right) + e_0 = 0 \tag{3.36}$$

$$e_0 = \left(\theta_0^{j+1} - \theta_0^{j}\right)\frac{\Delta z_{f0}}{2\Delta t_0} \tag{3.37}$$

Note that there are no extra source or sink terms at *node zero*. At the bottom node, nominally *node n*, we have

$$F_0 = \alpha\left(q_n^{j+1} - q_{n-0.5}^{j+1}\right) + (1-\alpha)\left(q_n^{j} - q_{n-0.5}^{j}\right) + e_n + S_n = 0 \tag{3.38}$$

$$e_0 = \left(\theta_n^{j+1} - \theta_n^{j}\right)\frac{\Delta z_{fn-1}}{2\Delta t_j} \tag{3.39}$$

Let us consider the value of α, which sets the temporal weighting of the solution. When $\alpha = 1$ it is a fully implicit equation that requires an iterative solution, does not use information from the previous time-step to get solution fluxes, and has few restrictions on time and space step size. When $\alpha = 0.5$ it is a Crank–Nicolson type, or central weighted, equation that requires an iterative solution, uses the last time-steps results as well as current estimates of the solution to proceed to an answer, and has some restrictions on time and space step size. When $\alpha = 0$ it is a fully explicit equation that does not require iteration, uses only the result from the current time-step to get a solution, makes guesses at the fluxes and boundary conditions (since you can't go back!), but has great restrictions on the allowable size of space and time-steps.

WAVES is designed to be a daily time-step hydrologic model, running with arbitrary soil types and climate, and practical to run on a PC, so we therefore cannot be restricted by using $\alpha = 0$. Using $\alpha = 0.5$ presents some conceptual problems, especially with boundary fluxes. The flux passing the surface node from time *j* to *j+1* is, from (3.36):

$$q_s = \alpha q^{j+1} + (1-\alpha) q^j \tag{3.40}$$

so with $\alpha = 0.5$ we have the flux at the end of the last time-step contributing to flux for this time-step. Consider a daily evaporation flux of 10 mm day^{-1}, dropping at a rate of 1 mm day^{-1} until it reaches 1 mm day^{-1}. The actual flux, q_s, passing the surface is 10, 9, 8, 7, 6, 5, 4, 3, 2, 1, 1, 1 mm day^{-1}, etc. The q^j on the other hand would be 10, 10, 8, 8, 6, 6, 4, 4, 2, 2, 0, 2, 0 mm day^{-1}, etc. With a less smooth drop off, such as the q_s halving each day, e.g. 16, 8, 4, 2, 1, 1, 1 mm day^{-1}, you can generate absurd values of q^j such as 16, 16, 0, 8, –4, 6, –4 mm day^{-1}, etc. The values of q^j generated for alternating days of rain and evaporation are similarly absurd. This leaves $\alpha = 1$ as the most useful compromise. From (3.40) we have the daily surface flux as a constant for the whole time-step, and perfectly defined. The number of terms, and therefore the number of operations, amount of storage, and derivatives required, in (3.36) and (3.38), will be minimised.

There are similar conceptual concerns with inferring the flux across a boundary with a constant potential. When there is a constant potential at the surface node, there is no change in water content at that node. From (3.38), with $S_0 = e_0 = 0$, we have:

$$F_0 = \alpha\left(q_{0.5}^{j+1} - q_0^{j+1}\right) + (1-\alpha)\left(q_{0.5}^{j} - q_0^{j}\right) = 0 \tag{3.41}$$

If $\alpha = 1$, then the solution to (3.41) is that $q_0 = q_{0.5}$, with $\alpha = 0$ we have a guessed solution based on last time-steps conditions, and with any other weighting we have a mixture of terms that will contain the surface fluxes described with flux boundary conditions. These arguments clearly point out that $\alpha = 1$ is the only practical temporal weighting. The other benefits in terms of maximising the solution convergence space, minimising the amount of storage and operations required, and reducing code size and scope for coding errors, are bonuses on this pragmatic decision.

The spatial weighting is much less important than the temporal weighting, since we must retain all the detail in the vertical regardless of the solution. Ross (1990) and Ross and Bristow (1990) did make some comments on the use of upstream weighting, but this may have had more to do with the soil hydraulic functions than the actual solution technique. In any event, WAVES uses a central spatial weighting in solution of (3.31).

Matrix Solution

The Newton–Raphson solution solves a matrix of the form:

$$-[F]=\left[\frac{\partial F}{\partial \psi}\right][\Delta\psi] \tag{3.42}$$

where $[F]$ is a 1 × N matrix describing how well mass is balanced at each depth node based on current estimates of $[\psi]$ (see Equations (3.32) – (3.39)), $[\partial F/\partial\psi]$ is a tridiagonal N × N matrix of the derivatives of Equations (3.32), (3.36), and (3.38), and $[\Delta\psi]$ is a 1 × N matrix to be solved for that are the corrections to $[\psi]$ to make all $[F]$ approach zero. Estimates of $[\psi]$ are updated by:

$$[\psi_{new}]=[\psi_{old}]-[\Delta\psi] \tag{3.43}$$

This procedure allows re-calculation of $[F]$ with $[\psi_{new}]$ and iteration until the solution converges. This criterion for convergence can be done on the basis of either mass balance (the $[F]$ matrix), or required changes to the dependent variable (the $[\psi]$ matrix). Given that we may have a range in ψ from millimetres to hundreds of metres and both positive and negative values, a consistent criterion for a change in ψ is difficult. However, being primarily concerned with mass balance, $[F]$ gives a direct estimate of how well balance is achieved at each node, and provides a very convenient convergence criterion. In WAVES, the solution is deemed to have converged when:

$$|F_i| \le 10^{-10} \tag{3.44}$$

Theoretically, and in practice, this allows mass to be balanced to within 10^{-10} of the largest water balance component, usually rainfall or evaporation. Other important considerations are the size of changes to $[\psi]$, and an oscillating solution. Using a tangent method, such as Newton–Raphson, where very small gradients exist, a very large change in the value of ψ at a node can result. To prevent this from causing further problems, a bi-directional limit is set:

$$\Delta\psi_i < 0.8|\psi_i| + k, \ \ for\ all\ \psi_i < 0 \tag{3.45}$$

where k is a suitable finite number, set to 0.1 m. Points to note about this limit are as follows.

Ross and Bristow (1990) used a limit that only stopped a node becoming wetter too quickly, *i.e.* essentially (3.45) without taking absolute values and if the change is to make the node wetter, but numerical experiments quickly found this to be unsuitable for the continual wetting and drying cycles modelled with WAVES.

A finite offset value is required in (3.45) to allow a node to reach saturation, otherwise it would asymptotically approach saturation and never reach it, and converge the solution.

The factor 0.8 is apparently arbitrary, but stops a node from becoming saturated in a single iteration. Again numerical experiments quickly showed the worth of this.

The value of ψ_i only needs to be negative, since above saturation the behaviour of ψ is linear and therefore does not require constraint with a gradient method, even when the node is becoming drier, i.e. $\Delta\psi_i$ is towards the unsaturated.

The second criterion for changes in $[\psi]$ is to minimise the effects of an oscillating solution. Where successive iterations indicate a change in the sign of the correction to ψ_i, the size of the correction is halved. This avoids the classical oscillation a constant amount above and below the actual solution.

Solution of the matrix equation (3.42) requires assemblage of $[\partial F/\partial\psi]$. The contents of this matrix are the derivatives of (3.32), (3.36), and (3.38) with respect to ψ at each depth *node i*. As stated, this is a tridiagonal matrix and is subject to extremely efficient solution. The components of $[\partial F/\partial\psi]$ at *node zero* are:

$$\frac{\partial F_0}{\partial \psi_0} = \frac{K'_0}{2}\sqrt{\frac{K_1}{K_0}} + \frac{K_0}{\Delta z_{f0}} + \frac{\theta'_0\,\Delta z_{f0}}{2\Delta t_j} \tag{3.46}$$

$$\frac{\partial F_0}{\partial \psi_1} = \frac{K'_1}{2}\sqrt{\frac{K_1}{K_0}} - \frac{K_1}{\Delta z_{f0}} \tag{3.47}$$

where K_i is unsaturated hydraulic conductivity, K' is the derivative of K with respect to ψ, and θ' is the derivative of θ with respect to ψ. The components of $[\partial F/\partial\psi]$ at *node i* are:

$$\frac{\partial F_i}{\partial \psi_{i-1}} = \frac{K'_{i-1}}{2}\sqrt{\frac{K_i}{K_{i-1}}} - \frac{K_{i-1}}{\Delta z_{fi-1}} \tag{3.48}$$

$$\frac{\partial F_i}{\partial \psi_i} = \frac{K'}{2}\left(\sqrt{\frac{K_{i+1}}{K_i}} - \sqrt{\frac{K_{i-1}}{K_i}}\right) + K_i\left(\frac{1}{\Delta z_{fi-1}} - \frac{1}{\Delta z_{fi}}\right) + \frac{\theta_i'\Delta z_{ci}}{\Delta t_j} \tag{3.49}$$

$$\frac{\partial F_i}{\partial \psi_{i+1}} = \frac{K'_{i+1}}{2}\sqrt{\frac{K_i}{K_{i+1}}} - \frac{K_{i+1}}{\Delta z_{fi}} \tag{3.50}$$

The components of $[\partial F/\partial\psi]$ at *node n* are:

$$\frac{\partial F_n}{\partial \psi_{n-1}} = \frac{K'_{n-1}}{2}\sqrt{\frac{K_n}{K_{n-1}}} - \frac{K_{n-1}}{\Delta z_{fn-1}} \tag{3.51}$$

$$\frac{\partial F_n}{\partial \psi_n} = \frac{K'_n}{2}\sqrt{\frac{K_{n-1}}{K_n}} + \frac{K_n}{\Delta z_{fn-1}} + \frac{\theta'_n \Delta z_{fn-1}}{2\Delta t_j} \tag{3.52}$$

Source and Sink Terms

All sink terms are added or subtracted from (3.32), (3.36), or (3.38) as required. If these terms are constant, such as evaporation or rainfall rate, or root water extraction rate, then they have a zero derivative with respect to ψ, and therefore do not appear in any of the derivative terms. An example of a sink term that is a function of ψ at a node is lateral flux. A watertable that develops on a soil layer boundary *node i* will generate a lateral flux, defined by Darcy's law for saturated conditions:

$$q_\ell = \psi_i K_s m \tag{3.53}$$

where q_ℓ is the lateral flux (m^3 d^{-1}), ψ_i is the positive water potential at *node i* (m), K_s is the saturated hydraulic conductivity of the soil layer (m d^{-1}), and m is the slope of the land surface (m m^{-1})*. Equation (3.53) would be added to (3.32) or (3.38) as required. The derivative term is:

$$\frac{dq_\ell}{d\psi_i} = K_s m \tag{3.54}$$

This term is added to (3.49) or (3.52) as appropriate. Equation (3.53) is recalculated each iteration with an updated value of ψ_i.

Soil Layers

With layered soils, there are special considerations. At a soil layer boundary, the only continuous quantities are soil water potential and soil water flux. We plan to calculate water content changes using variables other than ψ, so we must take into account that two values of these variables exist at the layer boundary. Since flux terms are defined between nodes, they require no special treat-

* Darcy's law of saturated flux consists of a conductivity, depth, slope, and width. Conductivity is taken from the soil hydraulic properties, depth of flow is the soil water potential at the layer boundary, slope is a constant for the soil profile specified by the user, and for dimensional consistency, the lateral flux flows across a unit width of soil.

ment. However, the e_i terms in (3.36) and (3.38) are defined at nodes, and do require special formulation and derivatives. At a *node i* straddling a boundary, e_i is defined by:

$$e_i = ((\theta_{up}^{j+1} - \theta_{up}^{j})\Delta z_{fi-1} + (\theta_{lo}^{j+1} - \theta_{lo}^{j})\Delta z_{fi})\frac{1}{2\Delta t_f} \qquad (3.55)$$

where θ_{up} refers to the soil layer above the boundary, and θ_{lo} refers to the soil layer below the boundary. Similarly, the derivative term in (3.49) and (3.52) will contain a mixture of derivatives.

Boundary Conditions

There are two possible boundary conditions at the top and bottom of the soil column: constant flux and constant water potential. At the surface, a constant flux condition would occur with non-ponded infiltration or energy-limited (stage 1) evaporation, and a constant potential condition would occur with ponded infiltration or soil-limited (stage 2) evaporation. WAVES allows a range of different options for surface ponded water: all ponded water becomes runoff, water is allowed to pond as if the area were flooded, or a flood depth is imposed. All of these options are handled transparently.

A constant flux boundary condition is set when rainfall or evaporation occurs with an unsaturated surface soil. This is done by prescribing the rate of rainfall or evaporation as q_0^{j+1} in Equation (3.36). If evaporation causes the surface node to become drier than the air-dry water potential of the soil, or rainfall causes the surface node to become saturated, then the time-step is re-run with a potential boundary condition. This will cause a mass balance problem, because the potential at the surface is imposed for the entire time-step. To avoid this, a triangle of water equal to the difference between the current water content and that at the constant potential for the top depth node must be added or removed, and placed in the accounting for water passing the surface node, *i.e.* $(\theta_{pot} - \theta_{old}) / 2 \times \Delta z_{f0}$.

If the surface dries out due to evaporation, the time-step is re-run and the flux passing the surface boundary is $q_{0.5}^{j+1}$, from (3.41) with $\alpha = 1$, plus the triangle of mass removed. When the surface node becomes saturated, forcing a constant flux would cause compression of water in the soil profile, and very large water potentials. The apparent rainfall flux is therefore reduced by the amount of water that is ponded, thus:

$$q_0 = q_{rain} - \frac{\psi_0}{\Delta t_{rain}} \qquad (3.56)$$

where q_0 is the flux that appears in (3.36), q_{rain} is the rainfall rate, and ψ_0 is the estimated water potential at *node zero* equivalent to the depth of ponded water, and Δt_{rain} is the duration of the rainfall. Because (3.56) is a function of the potential at *node zero*, a derivative equal to $-1/\Delta t_{rain}$ will appear in (3.46). If water is allowed to pond, then after convergence the program continues. If ponded water is runoff, then the time-step is re-run using a constant potential condition of $\psi_0 = 0$, and the runoff becomes the rainfall minus the infiltration ($q_{0.5}^{j+1}$) minus the triangle of mass added.

At the base of the soil column there is only a single boundary condition: constant flux. This flux however, may interact with a user imposed groundwater level. In the simplest case, the soil column is allowed to drain at a rate determined by the conductivity of the boundary node and a throttle value β ranging from 0 to 1. If $\beta = 0$, there is no drainage out of the soil column, and a watertable may develop. If $\beta = 1$ there is gravity drainage assuming a unit gradient, at a rate equal to the unsaturated hydraulic conductivity of the boundary node. When $0 < \beta < 1$, we have a throttled condition which assumes a gradient less than free drainage, due conceptually to a semi-infinite block of lower conductivity material below the modelled soil profile. In general the drainage flux is:

$$q_d = \beta K_n \tag{3.57}$$

where q_d is the drainage rate, and K_n is the unsaturated hydraulic conductivity at *node n*. This term appears in (3.38), and it has a derivative term:

$$\frac{dq_d}{d\psi_n} = \beta K'_n \tag{3.58}$$

which appears in (3.52). This flux is always a sink term, *i.e.* it is water lost to the soil column, and is always recalculated between iterations.

The other condition that may exist at the base of the soil column is a groundwater interaction term. In this coupling, the user specifies the depth of an external regional groundwater table, and this level may be changed daily through the weather file. This regional level interacts with any local water table through the following flux:

$$q_g = \varepsilon (d_{gw} - z_n + \psi_n) \tag{3.59}$$

where q_g is the rate of drainage from the local to regional groundwater table, d_{gw} is the depth to regional groundwater, z_n is the depth of the soil column, ψ_n is the water potential at *node n*,

equivalent to the depth of water table in the soil column, and ε is a coupling coefficient related to the rate of bore recession after a rise. Again, this term appears in (3.38) and has a derivative term:

$$\frac{dq_g}{d\psi_n} = \varepsilon \tag{3.60}$$

which appears in (3.52). When the regional groundwater table is deeper than the local water table, q_g is positive and can be thought of as drainage from the soil column. When the local water table is deeper than the regional water table, q_g is negative and represents filling of the soil depleted by evapotranspiration. The value of q_g from (3.59) is restricted so that its magnitude, whether positive or negative, never exceeds the saturated hydraulic conductivity of the bottom soil layer. Under these conditions, no derivative exists because the value is no longer a function of potential, and (3.60) is not required.

The quantity ε deserves some description. In a system where the regional groundwater table strongly controls local levels, because of high conductivity and good hydraulic connection, or in a lysimeter where groundwater levels are controlled externally, ε has a value close to 1.0, meaning that for every millimetre of water extracted, the regional groundwater can supply one in return. In this system the local water table is at the same depth as the regional groundwater table. As water table recessions become slower, the value of ε decreases. If $\varepsilon = 0.001$, for example, then for every 1.0 metre of head difference between the local and regional water table, 1.0 millimetre of water per day would be able to be exchanged, conductivity restrictions notwithstanding. So if vegetation were able to evaporate 1 mm day^{-1} more than rainfall, then the local water table would be 1.0 m below the regional groundwater table on average. The value of ε should theoretically be based on the ratio of the hydraulic conductivities of the soil and aquifer systems.

3.3.3 Computational Flow

The sequence of steps to run a single day time-step is as follows:

- determine whether all rainfall can be intercepted → no rainfall time-step required
- calculate available water and total osmotic plus matric potential at each depth node
- if first call for this time-step, CALL energy-balance, which calculates net rainfall
- determine surface boundary condition

**** re-entry point for failed solution, or need to set new boundary condition ****

- get values of soil water functions for state of last time-step
- set first estimate of solution to state of last time-step
- LOOP
    - get values of soil water functions for current solution estimate

- calculate coefficients and derivatives for matrix solution
- incorporate source and sink terms into matrices, i.e. transpiration, watertables, groundwater interaction or drainage.
- solve matrix equation
- check for solution convergence
- modify estimates of solution, restricting large changes and oscillation
- check for failed solution, and re-enter if necessary
- check for change in boundary conditions, and re-enter if necessary
- accumulate all solved mass balance components.

This sequence is repeated if both rainfall and surface evaporation occur on the same day. Evaporation and transpiration fluxes, and stresses, are not recalculated in this case.

3.3.4 Soil Hydraulic Functions

As stated at the end of section 3.3.1, we do not know what soil hydraulic model the user will want to use, so we place no restrictions on this. However, Short *et al.* (1995) provide a treatise on the use of the Broadbridge–White (BW) soil model in practical daily time-step modelling (Broadbridge and White 1988, White and Broadbridge 1988). They presented spaces where convergence was guaranteed with constant rate infiltration into very dry soil; one of the most numerically difficult problems. The strength of the BW soil model is that it links water potential, water content, and hydraulic conductivity by starting with a physically realistic representation of soil water diffusivity. Other important properties are that the functions between ψ, θ, and K are monotonic. With a solution scheme that depends on the gradients of these functions, not having zero or infinite slope is a great benefit; this is also physically realistic. It has been suggested that slope discontinuities are a problem for the Newton–Raphson solution scheme. However, a slope discontinuity apparently exists at every point on the soil tables used by WAVES without causing numerical problems. Brutsaert (1971) successfully used the Newton–Raphson solution scheme with only 10 points to describe the soil hydraulic curves. The issue of zero and infinite slopes in the curves is critical to the convergence of the solution, whereas slope discontinuities are almost irrelevant.

The BW soil model has five physically meaningful and measurable parameters, and can represent a wide range of soil moisture characteristics ranging from highly nonlinear, associated with uniform sands, to weakly non-linear, associated with well-structure forest soils. The space in which convergence of the solution is guaranteed for all rainfall rates into all soils described by the BW model, shown in Short *et al.* (1995), is where the spacing between depth nodes is no

greater than the characteristic length scale of the BW soil model. This condition is very practical, and for a model that must run for long times with dynamic climatic and vegetation stresses, the existence of this space is mandatory. Such spaces may exist for other soil hydraulic models but they are not available in general, so while another soil model, or a set of empirical equations fitting observations, may be used with WAVES, the stability and convergence of Richards' equation cannot be guaranteed.

3.4 Solute Balance

3.4.1 Generalised Equations

Solute Mass Balance

The solute balance in WAVES is concerned with conservative solutes only, and in particular common salt, sodium chloride (NaCl). This solute is assumed to not attach to the soil matrix, or affect soil hydraulic properties, or to removed by the plant roots or surface evaporation. Further we assume that the saturation concentration in water is never exceeded, thus avoiding problems with different solubilities of salts, precipitation of salt, and re-dissolving of salt. Under these conditions, we may write a mass balance equation for solute that is similar to that for water (3.31):

$$\frac{\partial (\theta \quad \varsigma)}{\partial t} = -\frac{\partial q_s}{dz} \quad + S(\varsigma) \tag{3.61}$$

where c_s is the concentration of salt (kg ℓ^{-1}), q_s is the flux of salt (m d^{-1} kg ℓ^{-1}, sometimes reduced to kg d^{-1}), and S is a source or sink term that may be a function of the salt concentration. With the salt transport in WAVES, we assume that the salt concentration does not affect the soil hydraulic properties, does not adsorb to the soil and transfer between the soil matrix and soil water, and is not removed from the soil by plants or evaporation. Under these conditions, the sink/source term can be omitted, and the soil property values and fluxes are constant for any concentration of solute.

In a similar way to water, we can write equations (3.32) to (3.35) for (3.61), thus:

$$G_i = q_{s,i+0.5}^{j+1} - q_{s,i-0.5}^{j+1} + h_i = 0 \tag{3.62}$$

where

$$q_{s,i+0.5} = q_{i+0.5} c_{s,i+0.5} - \theta_{i+0.5} D_{s,i+0.5} \frac{c_{s,i+1} - c_{s,i}}{\Delta z_{fi}} \tag{3.63}$$

$$h_i = (c_{s,i}^{j+1}\theta_i^{j+1} - c_{s,i}^{j}\theta_{s,i}^{j})\frac{\Delta z_{ci}}{\Delta t_f} \tag{3.64}$$

$$c_{s,i+0.5} = \frac{c_{s,i}\theta_i + c_{s,i+1}\theta_{i+1}}{\theta_i + \theta_{i+1}} \tag{3.65}$$

$$D_{s,i+0.5} = D_1\theta_{i+0.5}\tau + D_2\frac{|q_{i+0.5}|}{\theta_{i+0.5}} \tag{3.66}$$

where D_s is solute diffusivity ($m^2\ d^{-1}$), D_1 is diffusion coefficient in free water (constant set to 0.001 $m^2\ d^{-1}$), τ is an impedance factor (constant set to 0.5), and D_2 is dispersivity (constant set to 0.02 m). Equations (3.63) to (3.66) are formulated at *time j+1*, and this index has been omitted where possible for clarity.

Equations (3.62) and (3.64) are modified at the upper and lower boundary. At the surface *node 0*, we have:

$$G_0 = q_{s,0.5}^{j+1} - q_{s,0}^{j+1} + h_0 = 0 \tag{3.67}$$

$$h_0 = (c_{s,0}^{j+1}\theta_{s,0}^{j+1} - c_{s,0}^{j}\theta_0^{j})\frac{\Delta z_{f0}}{2\Delta t_j} \tag{3.68}$$

and at the bottom *node n*, we have:

$$G_n = q_{s,n}^{j+1} - q_{s,n-0.5}^{j+1} + h_n = 0 \tag{3.69}$$

$$h_n = (c_{s,n}^{j+1}\theta_n^{j+1} - c_{s,n}^{j}\theta_n^{j})\frac{\Delta z_{fn-1}}{2\Delta t_j} \tag{3.70}$$

With the water fluxes solved for, $q_{s,0}$ and $q_{s,n}$ are easily determined. If rainfall or irrigation has occurred, with or without a potential boundary condition, the surface flux of salt is the volume of water that infiltrated multiplied by the salt concentration in the rain or irrigation water. If evaporation has occurred, then there is no salt flux from the surface node. When a potential boundary condition is imposed at the surface however, the surface salt concentration must be adjusted to account for the change in water content at the surface; see section 3.3.2 *Boundary Conditions*. If there is drainage from the bottom node, then the flux out of the soil column is the drainage flux multiplied by the concentration of salt at the bottom node. Similarly if there is upflow from a

groundwater table then the flux of salt into the soil column is the inflow flux multiplied by the concentration of salt in the groundwater.

Matrix Derivative Terms

Equations (3.62) to (3.70) can be expressed in finite difference form, and have derivatives taken with respect to c_s at each node. At the surface *node 0* we have:

$$\frac{\partial G_0}{\partial c_{s,0}} = q_{0.5}\frac{\theta_0}{\theta_0 + \theta_1} + \frac{\theta_0 D_{s,0.5}}{\Delta z_{f0}} + \frac{\theta_0 \Delta z_{f0}}{2\Delta t_j} \tag{3.71}$$

$$\frac{\partial G_0}{\partial c_{s,1}} = q_{0.5}\frac{\theta_0}{\theta_0 + \theta_1} - \frac{\theta_{0.5} D_{s,0.5}}{\Delta z_{f0}} \tag{3.72}$$

At a general intermediate *node i* we have:

$$\frac{\partial G_i}{\partial c_{s,i-1}} = q_{i-0.5}\frac{\theta_{i-1}}{\theta_{i-1} + \theta_i} - \frac{\theta_{i-1} D_{s,i-0.5}}{\Delta z_{fi-1.0}} \tag{3.73}$$

$$\frac{\partial G_i}{\partial c_{s,i}} = q_{i+0.5}\frac{\theta_i}{\theta_i + \theta_{i+1}} + \frac{\theta_{i+0.5} D_{s,i+0.5}}{\Delta z_{fi}} - q_{i-0.5}\frac{\theta_i}{\theta_{i-1} + \theta_i} + \frac{\theta_{i-0.5} D_{s,i-0.5}}{\Delta z_{fi-1}} + \frac{\theta_i \Delta z_{ci}}{\Delta t_j} \tag{3.74}$$

$$\frac{\partial G_i}{\partial c_{s,i+1}} = q_{i+0.5}\frac{\theta_{i+1}}{\theta_i + \theta_{i+1}} - \frac{\theta_{i+1} D_{s,i+0.5}}{\Delta z_{fi}} \tag{3.75}$$

At the bottom *node n* we have:

$$\frac{\partial G_n}{\partial c_{s,n-1}} = q_{n-0.5}\frac{\theta_{n-1}}{\theta_{n-1} + \theta_n} - \frac{\theta_{n-0.5} D_{s,n-0.5}}{\Delta z_{fn-1}} \tag{3.76a}$$

$$\frac{\partial G_n}{\partial c_{s,n}} = q_{n-0.5}\frac{\theta_n}{\theta_{n-1} + \theta_n} + \frac{\theta_{n-0.5} D_{s,n-0.5}}{\Delta z_{fn-1}} + \frac{\theta_n \Delta z_{fn-1}}{2\Delta t_j} \tag{3.76b}$$

Inspection of the derivative terms (3.71) to (3.76b) reveals that c_s does not appear on the RHS of any of the equations. The system of equations is linear, and may therefore be solved in a single iteration with the Newton–Raphson gradient method. Even with other water-based processes included, the solution remains linear in salt concentration. Take for example lateral flows. Equation (3.53) describes a lateral flux q_ℓ as a function of water potential, conductivity and gradient.

When salt is also involved, some mass will be lost from the column via lateral transfers. Specifically, the flux is:

$$q_{\ell,s} = q_\ell \, c_{s,i} \tag{3.77}$$

where $q_{\ell,s}$ is the lateral salt flux at a node, q_ℓ is the lateral water flux from (3.53), and $c_{s,i}$ is the salt concentration at *node i* with a perched watertable. The derivative of (3.77) is:

$$\frac{\partial q_{\ell,s}}{\partial c_{s,i}} = q_\ell \tag{3.78}$$

which is not a function of salt concentration, and leaves the solution linear in c_s. Equation (3.77) is added to (3.62) or (3.69), and (3.78) is added to (3.74) or (3.76b).

Soil Layers

At soil layer boundaries, special consideration must be given to (3.64) and its derivative equation (3.74). At a soil layer boundary there are two parts to each of the mass components, yielding the following, where *node k* is the soil boundary, and the superscript 'a' is for the layer above and 'b' is for the layer below:

$$h_k = (c_{s,k}^{j+1}\theta_k^{a,j+1} - c_{s,k}^{j}\theta_k^{a,j})\frac{\Delta z_{fk-1}}{2\Delta t_j} + \left(c_{s,k}^{j+1}\theta_k^{b,j+1} - c_{s,k}^{j}\theta_k^{b,j}\right)\frac{\Delta z_{fk}}{2\Delta t_j} \tag{3.79}$$

$$\frac{\partial G_k}{\partial c_{s,k}} = \frac{\theta_k^{a,j+1}\Delta z_{fk-1} + \theta_k^{b,j+1}\Delta z_{fk}}{2\,\Delta t_j} \tag{3.80}$$

Calculation of (3.65) requires careful algebra also to ensure the integrity of the formulation and solution. If the solution fails to converge in a single iteration, then it is most likely that the equations have been derived or coded incorrectly.

3.4.2 Computational Flow

The sequence of steps to run a single day time-step is as follows:

*** allow soil water solution to converge to get state values and fluxes ***

- estimate values of soil hydraulic properties between nodes
- estimate values of solute diffusion and boundary solute fluxes
- set first estimate of solution to state of last time-step
- LOOP (once only!)

- calculate coefficients and derivatives for matrix solution
- incorporate source and sink terms into matrices, i.e. water tables, groundwater interaction or drainage.
- solve matrix equation
- check for solution convergence
- modify estimates of solution

- check for failed solution, indicating bad solution
- accumulate all solute mass balance components.

This sequence is repeated if both rainfall and surface evaporation occur on the same day. Because the solution is explicit (*i.e.* fixed coefficients requiring no iterations, there are theoretical restrictions on the size of time-steps given) we have fixed the depth nodes. These warnings are ignored in WAVES and, as a result, small negative values for solute concentration can occur with full solute transport but without a saline watertable. The presence of a watertable tends to smooth out fluxes, water contents, and sink terms, and provides a generally larger amount of solute that eliminates the negative values sometimes obtained.

3.5 Carbon Balance

3.5.1 Generalised Equations

The carbon balance is performed as part of calculation of evaporation and transpiration demand for a given day. These fluxes are calculated based on the soil conditions at the start of the day, and are not updated during the solution of the water flow equation. A portion of the energy balance, all of section 3.2.1, is first used to estimate the stresses on the vegetation, the carbon balance routine is called to calculate assimilation based on those stresses, and then evaporative demand is calculated using a conductance based on that assimilation rate. In this way a complete feedback between the atmosphere, soil and salt, and vegetation is made.

The WAVES plant growth model is a generic algorithm with rate-based equations and sound physical principles, however empiricism is used where appropriate. WAVES does not attempt to model discrete phenological growth stages, and does not fill grain in crops for a prediction of yield. WAVES further treats the plant as three buckets of carbon representing leaves, stems, and roots. Each of these is assumed to occupy the conceptual site fully. The leaves are evenly spread across each square metre, stem numbers are not determined but assumed to be again uniformly spread, and the roots totally explore the depths to which root carbon is allocated. This approach to plant growth modelling is a result of designing WAVES to be primarily a hydrological model

and leaf area index and root distribution are the primary variables interacting with the hydrologic cycle.

Gross Photosynthesis

The first step in growing our plant is to calculate the stresses on the plant. Within the transpiration subroutine the availability of water to the plant is calculated, in a similar way to (3.24).

$$\chi_w = \sum_{i=1}^{N} \frac{\left(1 - \frac{\psi_i + \eta \Pi_i}{\psi_{wilt}}\right) \Delta z_i}{z_{max}} \tag{3.81}$$

where χ_w is the relative availability of water, z_{max} is the depth of the deepest roots within the soil, and the sum is taken only over those depth nodes with roots present.

The osmotic potential due to salt is given by Metten (1966) as:

$$\Pi_i = 2 C_{s,i} R T_a \tag{3.82}$$

where $C_{s,i}$ is the molar concentration of salt at the depth *node i* (mol ℓ^{-1}) given by dividing $c_{s,i}$ (kg ℓ^{-1}) by the molar weight of salt in kilograms (0.0585 kg mol^{-1}), R is the universal gas constant (0.832 m ℓ K^{-1} mol^{-1}), and T_a is average daily temperature expressed in Kelvin. A factor of two appears because two ions contribute to osmotic potential, both Na^+ and Cl^-, and they are assumed to contribute equally.

Next the availability of light is calculated, along with the modifying effect of air temperature, thus:

$$\chi_l = \frac{R_n \, 4600}{2 \, DL \, L_{sat}} \tag{3.83}$$

$$\chi_t = exp[-\alpha_t (T_a - T_{opt})^2] \tag{3.84}$$

where R_n is the net radiation for the canopy of interest (kJ m^{-2} d^{-1}), 4600 is a units conversion factor, L_{sat} is the saturation light intensity (μmoles m^{-2} s^{-1}), the factor of two assumes that half of sunlight is photosynthetically active radiation, T_{opt} is the temperature at which maximum assimilation occurs, α_t is a factor so that $\chi_t = 0.5$ at the temperature when half of maximum assimilation occurs. The value of χ_ℓ is limited to lie between 0 and 1.

At this stage, the actual relative growth rate can be estimated using the integrated rate methodology of Wu *et al.* (1994) by:

$$g = \frac{1 + w_w + w_N}{\frac{1}{\chi_\ell \chi_t} + \frac{w_w}{\chi_w} + \frac{w_n}{\chi_N}} \tag{3.85}$$

where g is the actual relative growth rate, w_w is the weighting of water relative to light, w_N is the weighting of nutrients relative to light, and χ_N is the relative availability of nutrients. In WAVES full nutrient cycling and leaching calculations are not performed so χ_N is a constant set by the user.

Next gross production is calculated from Slavich *et al.* (1998):

$$A = A_{max} g(1 - exp(k\, LAI\,)) \frac{DL}{43200} \tag{3.86}$$

where A_{max} is the maximum production rate (kg C m^{-2} 12 hr^{-1}), and the scalar on the RHS is a correction for day lengths greater or less than 12 hours.

Respiration and Losses

There are two methods for estimating plant respiration. The first is to assume that it is some fixed or dynamic proportion of gross production (see, for example, Landsberg and Waring 1997), or to calculate it independently by invoking a rate equation based on the amount of material present; in WAVES we do the latter. The maintenance respiration loads for leaves, stems, and roots are calculated as follows:

$$L_{resp} = L_{rate}\, exp(0.085\, T_{min}) \left(1 - \frac{DL}{86400}\right) L_{car} \tag{3.87}$$

where L_{resp} is the dark respiration of the leaves (in units of kg C), L_{rate} is the leaf respiration rate (kg C kg C^{-1} d^{-1}), T_{min} is the minimum daily temperature, and L_{car} is the total amount of leaf carbon (kg C). The factor 0.085 in the exponential term doubles the respiration load for an 8 degree increase in temperature. This is termed dark respiration because the leaf is assumed to get all the sustenance it requires during the day as part of normal photosynthesis, and the maximum net production parameter A_{max} already accounts for this loss. This is also why the minimum

temperature, assumed to occur during the night, and the proportion of the day that is night is used in the calculation.

$$S_{resp} = S_{rate}\, exp(\, 0.085\, T_a\,)\, S_{car} \tag{3.88}$$

$$R_{resp} = R_{rate}\, exp(0.085 T_a\,)\, R_{car} \tag{3.89}$$

where S_{rate} is the stem respiration rate (kg C kg C^{-1} d^{-1}), S_{car} is the total amount of stem carbon (kg C, which may be zero if the plant has no woody stem), R_{rate} is the root respiration rate (kg C kg C^{-1} d^{-1}), and R_{car} is the total amount of root carbon (kg C). For all intents and purposes L_{resp}, S_{resp}, and R_{resp} are unknown, and are empirical fitting parameters.

Leaves and roots are subject to turnover also, where a fixed proportion of the carbon is lost each day, thus:

$$L_{loss} = M_{rate}\, L_{car} \tag{3.90}$$

$$R_{loss} = M_{rate}\, R_{car} \tag{3.91}$$

where M_{rate} is the mortality rate of leaves and roots, or fraction lost each day (d^{-1}).

Dynamic Partitioning

The losses in (3.87) to (3.91) are reconciled against the gross production after that production is partitioned to the available carbon pools. This is done on the basis of determining first how much is assigned to above-ground and below-ground. This is dictated by water availability and a maximum partitioning factor:

$$L_f = S_f = 0.1 + \beta\, \chi_w \tag{3.92}$$

$$R_f = 1 - L_f - S_f \tag{3.93}$$

where L_f is the fraction of production partitioned to leaves, S_f is the fraction of production partitioned to stems, β is the partitioning factor (between 0 and 0.4), and R_f is the fraction of production partitioned to roots. This model suggests that when water is not easily available, *i.e.* a low value of χ_w, more resources are placed below ground to find water, and when water is plentiful resources are put into growing canopy and above ground structures.

Now an updated value of the three carbon pools can be calculated by:

$$L_{car}^{new} = L_{car} + 0.65 L_f A - L_{resp} - L_{loss} \tag{3.94}$$

$$S_{car}^{new} = S_{car} + 0.65 S_f A - S_{resp} \tag{3.95}$$

$$R_{car}^{new} = R_{car} + 0.65 R_f A - R_{resp} - R_{loss} \tag{3.96}$$

where the 0.65 factor is a fixing efficiency of assimilate to actual material.

There are certain limits placed on the accumulation of carbon pools relative to one another, and in total. Leaf carbon will not be accumulated after 99% of light can be intercepted by the canopy, due to the marginal cost of maintaining extra leaf resources relative to the extra assimilation gained. If the plant has stems, then the stem carbon must be at least equal to the leaf carbon, to provide mechanical and hydraulic support to the leaf mass. Root carbon can only be accumulated to a maximum of twice the leaf carbon if no stems exist, and four times the leaf carbon if stems are present.

Considerations for Annual Vegetation

WAVES is simplistic with regard to perennial vegetation, so that when either leaf or root carbon is reduced to zero, the vegetation dies and does not regrow. Annual vegetation has a more predictable cycle of germination, growth, and death, and must be accounted for by the generic growth model. This is done by the addition of two parameters: the year-day of germination (1 to 365), and the lifespan of the plant in degree daylight hours.

WAVES must check for the day when the plant germinates, and initialise the leaf, stem, and root carbon pools. Annuals are assigned an amount of carbon such that the leaf area index is 0.1, a matching amount of carbon is given to stems (if they are present), and twice that amount to roots. The root carbon profile is assumed to be linear with depth at a density of 0.1 kg C m^{-3}.

On the day of germination, all resource availabilities are assumed to be at maximum for numerical purposes, and the counter for degree daylight hours is initialised to zero. The degree day hours are accumulated for each growing day by multiplying the average of maximum and minimum daily temperature by the number of sunlit hours in the day, with a minimum of 1 degree day hour for any one-day time-step. After an annual has been growing for its full lifetime, all production rates are assumed to be zero, and the respiration load is multiplied by 20 to cause the carbon pools to senesce. This last process representation is totally arbitrary, but avoids introducing extra parameters to better describe this part of the life cycle.

Estimates of yield can be made from knowledge of above-ground biomass and actual and potential transpiration, based on empirical curves (Charles-Edwards 1982). The simplest equation uses the Harvest Index:

$$Y = HI \cdot DM \tag{3.97}$$

where Y is grain yield (kg m^{-2}), HI is the harvest index, and DM is the total above ground dry matter produced (kg m^{-2}, in WAVES this is $2 \times L_{car}$). Values of HI can be found in literature, and commonly range from 0.2 to 0.5. Alternative yield estimates can be made by adding knowledge of transpiration (de Wit 1958), thus:

$$Y = Y_{max} m \cdot \frac{ET_{act}}{ET_{pot}} \tag{3.98}$$

where Y_{max} is maximum grain yield, m is an empirical constant, ET_{act} is actual transpiration (m), and ET_{pot} is average potential transpiration rate over the growing season (m). Within WAVES, the values of ET_{act} and ET_{pot} are stored and can be used for these calculations with a user-specified Y_{max} and m parameter.

Litter and Grazing

WAVES keeps track of a fourth carbon pool for ground litter. The effects of litter have already been described, for example in equation (3.15) for surface resistance to evaporation. The above-ground loss term in (3.90) is added to the ground litter pool, and is allowed to decompose over time. The decomposition rate is an empirical function of temperature and moisture at the soil surface:

$$d_\ell = \frac{\Theta_0 \chi_t}{10} \tag{3.99}$$

where d_ℓ is the proportion of litter decomposed, Θ_0 is the relative water content at the surface (0 is air-dry, and 1 is saturated), and the factor 10 indicates that 10% of the total litter may decompose each day under optimal rotting conditions.

Grazing can be imposed if plants are to be grown. Grazing pressure is indicated by specifying the number of stock equivalents (ewe and lamb pairs) per hectare, and the year-day that they are let on, and taken off. Each stock equivalent is assumed to consume 0.5 kg C d^{-1} ha^{-1}, and this amount is removed from the overstorey, understorey, and litter carbon pools in proportion to their sizes.

3.5.2 Root Growth

Roots are growth by a chaotic algorithm, with three very simple rules. The root zone is broken into the same node spacings as for the soil water dynamics modelling with Richards' equation (see section 3.3 *Water Balance*) and root carbon is assigned to each node. This root activity is assumed to occur in the region half-way to the next node up, and half-way to the next node down. Because of this, no root carbon is assigned to either the surface node at 0 m, or the bottom most node, at the base of the soil column.

The rules that cover root growth are as follows. Firstly, we must maintain a connected root system to the deepest node with roots; any net root carbon growth must first satisfy this need. Secondly, root growth occurs where there is the most water and oxygen available and an existing root mass. This is determined by a method similar to (3.81), thus:

$$FAV_i = \left(1 - \frac{\psi_i + \eta\Pi_i}{\psi_{wilt}}\right)\left(1 - \frac{z_i}{z_{max}}\right)\frac{R_{ci}}{R_{car}} \qquad (3.100)$$

where FAV_i is the favourability for root growth at *node i*, z_i is the depth of *node i*, and R_{ci} is the amount of root carbon at *node i*. The first term of the RHS represents the water availability, taking salt into account, the second term represents oxygen availability, *i.e*. the deeper below the ground the less oxygen diffuses down there, and the final term means that a greater investment will be made where roots already exist. The value of (3.100) is calculated at each node, summed, made into a relative value, and carbon is assigned to nodes on the basis of the favourability as a proportion of the root carbon to be assigned.

The final rule for root growth is that the plant wants to explore new areas. In practice, if the deepest roots are shallower than the maximum rooting depth of the plant, then the favourability of the next node is calculated as available for assignment of carbon.

The other housekeeping issues involved are (1) to maintain a maximum level of root carbon accumulation, (2) that root carbon respiration is subtracted on the basis of the proportion of total root carbon at each depth node, and (3) that roots will not grow in saturated soil.

3.5.3 Computational Flow

The sequence of steps to run a single day time-step is as follows:

(General Plant Growth)

- gather availability of water and root growth favourability from other routines
- calculate availability of light and modifying effect of temperature

- determine maximum allowable carbon accumulation levels
- calculate growth rate and gross assimilation
- check status of annual plants

  IF GERMINATION

  - set growth rate and assimilation to maximum
  - assign minimum carbon to plant carbon pools
  - distribute roots down soil profile

  ELSE

  - accumulate degree day hours of growing season
- calculate respiration loads

  IF PLANT IS SENESCING

  - set growth rate and assimilation to zero
  - increase respiration loads by factor of 20
- calculate dynamic allocation amounts
- calculate carbon pool mortality amounts
- update carbon pools for assimilation, respiration, and mortality
- update litter pool for leaf drop
- check status of grazing
  - calculate amount of carbon grazed
  - reduce leaf carbon and litter pools

(Dynamic Root Growth)

- gather favourability index and carbon allocation and respiration from other routines
- calculate distribution of potential losses due to respiration or saturated soil
- calculate distribution of potential growth according to general favourability
- update root carbon for all losses
- update root carbon at each depth to maintain minimum root carbon for connected root system
- update root carbon from remaining assimilation
- recalculate relative amount of carbon at each depth node.