

CHAPTER FIVE

5. SYNTHETIC STUDY: SOIL MOISTURE MODEL PROXSIM

The first step towards estimating the temporal variation and spatial distribution of soil moisture profiles, was the establishment of a procedure for estimating the temporal variation of the soil moisture profile in a one-dimensional soil column. Current generation remote sensing observations of soil moisture content generally have a temporal resolution in excess of 1 month, depending on satellite orbit. This necessitated application of the water balance approach (section 3.4.4), for estimation of soil moisture profiles between satellite overpasses. Hence, this chapter presents the soil moisture model that was used in the synthetic study of Chapter 6, for establishing the soil moisture profile estimation algorithm.

5.1 SOIL MOISTURE AND TEMPERATURE PROFILE ESTIMATION

Microwave remote sensing observations are a function of the soil dielectric properties in a thin near-surface layer. Thus to be useful for updating model forecasts of the soil moisture profile, the soil's near-surface dielectric profile (Chapter 4) must be related to the near-surface volumetric soil moisture content. Chapter 2 has shown that this relationship is heavily dependent on the soil temperature (section 2.2). In addition, passive microwave remote sensing observations are dependent on both the soil temperature and soil dielectric constant (section 2.4.4). As diurnal variations in near-surface soil temperature on the order of 30°C to 40°C are common, it is necessary to have an estimate of the near-surface soil temperature that corresponds with the time of microwave remote sensing observation.

While some microwave remote sensing platforms also make thermal infrared observations, those measurements only give the surface skin temperature, which must be related to the soil temperature over the near-surface soil layer

observed by the microwave remote sensor. Furthermore, thermal infra-red data are only available on cloud free days and thus may not be available for all microwave measurements of near-surface soil moisture content. Hence, it is necessary to model the soil temperature profile in addition to the soil moisture profile, if microwave observations are to be of use in estimating the near-surface soil moisture content within an operational setting. Thus the synthetic study in Chapter 6 estimates both soil moisture and temperature profiles, by assimilating observations of near-surface soil moisture content and soil surface temperature.

5.2 ONE-DIMENSIONAL SOIL MOISTURE AND HEAT TRANSFER MODEL

In developing models for the coupled flow of soil moisture and heat, numerous simplifying assumptions are made as a result of the complexity of soils. However, soils do not generally conform to the usual assumptions, with soils being anisotropic, non-uniform, non-isothermal and sometimes water repellent. In addition, they contain entrapped air as isolated bubbles, and the gas phase may not, in some circumstances, be at constant pressure, let alone atmospheric. Fissures, cracks and worm holes are also common features of soil profiles, and soil deformation may occur from swelling (Klute, 1973).

The coupled flow of heat and moisture in a vertical soil column occurs in both vapour and liquid phases. The relative magnitudes of vapour versus liquid moisture fluxes and the effects of temperature versus hydraulic gradients are not well defined (Klute, 1973). While some (eg. Cary and Taylor, 1967) have considered temperature effects very important over a wide range of soil wetness, others (eg. Philip, 1957) have indicated that thermally driven moisture flow from evaporative drying is only important when the soil is very dry. Klute (1973) has suggested that at depths greater than about 20 cm the thermal effects can be safely ignored.

In a theoretical and experimental study of soil moisture flow in the near-surface layer, Rose (1968a,b) found that liquid moisture flux arising soil from temperature gradients was relatively unimportant. Vapour phase moisture flux, on the other hand, was comparable in magnitude to that in the liquid phase and became increasingly important with the advancing stages of drying. Kimball *et al.*

(1976) concluded, based on a comparison of field measured and calculated soil heat fluxes, that both soil moisture and heat fluxes can be predicted better by ignoring thermally induced vapour movement at high and low soil moisture contents. But at intermediate soil moisture contents, soil moisture flux prediction is better if thermally induced vapour flux is included (Kimball *et al.*, 1976).

The vapour phase is mainly critical in modelling the thermal regime, due to the relatively large magnitude of heat exchange during phase change. For moisture flux, however, the vapour term is orders of magnitude smaller than the liquid term and can be neglected (Entekhabi *et al.*, 1994). In representing the heat and moisture transfer in the following model development, we only consider the liquid phase, as modelling of the soil temperature profile is only of secondary importance. This means that the coupling between the heat and moisture equations is solely through the heat capacity of the soil and through the influence of moisture on thermal conductivity.

More comprehensive models accounting for simultaneous heat and moisture transport could be used. However, it would not change the results of the synthetic study in Chapter 6, as the same model was used to produce the simulated data and to process these data. However, the complexity of such models, the difficulty to obtain proper soil parameters for vapour flux, and the lack of knowledge about their spatial variability would probably make illusory the increase of the accuracy expected by using such comprehensive models in the application we are dealing with. In the same way, hysteresis on the unsaturated hydraulic conductivity relationship has been neglected. Such a simplified model based on Richards equation and neglecting hysteresis has been shown to simulate with reasonable accuracy the time evolution of soil moisture profiles in field conditions (Bernard *et al.*, 1981).

The following sections describe the soil moisture and heat transfer model PROXSIM1D (**PRO**file **eXplicit SIM**ulation in **1 Dimension**), which was used for the one-dimensional synthetic study of soil moisture and temperature profile estimation in Chapter 6. This model uses an explicit finite difference approximation to a simplified version of the soil moisture and heat transfer

equations given by Philip and de Vries (1957) and de Vries (1958). A complete listing of the computer code is given on the CD-ROM accompanying this thesis.

5.2.1 MOISTURE EQUATION

The conservation of water mass in a porous medium is expressed by the continuity equation for one-dimensional simultaneous saturated-unsaturated flow as

$$\frac{\partial S_{\theta}}{\partial t} = -\nabla q_m \quad (5.1),$$

where S_{θ} is the mass of water storage per unit bulk volume and q_m is the total mass flux of water. S_{θ} may be expressed as (Bear, 1979)

$$S_{\theta} = \rho_l (\theta_l + \theta_v) = \rho_l \theta \quad (5.2a)$$

or

$$S_{\theta} = \rho_l \phi S_w \quad (5.2b),$$

where ρ_l is the density of liquid water, θ_l is the volumetric liquid water content, θ_v is the volumetric water vapour content, ϕ is the soil porosity and S_w is the water saturation equal to θ/ϕ .

Differentiating (5.2b) with respect to time yields

$$\begin{aligned} \frac{\partial S_{\theta}}{\partial t} &= S_w \frac{\partial(\rho_l \phi)}{\partial t} + \rho_l \phi \frac{\partial S_w}{\partial t} \\ &= S_w \left(\rho_l \frac{\partial \phi}{\partial t} + \phi \frac{\partial \rho_l}{\partial t} \right) + \rho_l \phi \frac{\partial S_w}{\partial t} \\ &= S_w \left(\rho_l \frac{\partial \phi}{\partial \psi} + \phi \frac{\partial \rho_l}{\partial \psi} \right) \frac{\partial \psi}{\partial t} + \rho_l \phi \frac{\partial S_w}{\partial t} \end{aligned} \quad (5.3),$$

where ψ is the soil water matric potential, otherwise known as the capillary potential. The matric potential is equal to the work needed to bring a unit mass of

water from a unit mass of soil against the force of attraction between the soil and water (Sasamori, 1970).

Substitution of the coefficient of compressibility for water given by (Bear, 1979)

$$\beta = \frac{1}{\rho_l} \frac{\partial \rho_l}{\partial \psi} \quad (5.4a)$$

and the coefficient of compressibility of the soil solid matrix given by (Bear, 1979)

$$\alpha = \frac{1}{1-\phi} \frac{\partial \phi}{\partial \psi} \quad (5.4b),$$

into (5.3) allows simplification to the relationship (Bear, 1979)

$$\begin{aligned} \frac{\partial S_\theta}{\partial t} &= \rho_l \left\{ S_w [\alpha(1-\phi) + \beta\phi] \frac{\partial \psi}{\partial t} + \frac{\partial \theta}{\partial t} \right\} \\ &= \rho_l \left\{ S_w S_{0\psi} \frac{\partial \psi}{\partial t} + \frac{\partial \theta}{\partial t} \right\} \end{aligned} \quad (5.5a),$$

where $S_{0\psi}$ is the specific storativity with respect to soil matric potential

$$S_{0\psi} = \alpha(1-\phi) + \beta\phi \quad (5.5b).$$

Following Philip and de Vries (1957) and de Vries (1958), the equations for liquid and vapour flux densities may be written as

$$\frac{q_l}{\rho_l} = -D_{\psi l} \nabla(\psi + z) - D_{Tl} \nabla T \quad (5.6a)$$

$$\frac{q_v}{\rho_l} = -D_{\psi v} \nabla \psi - D_{Tv} \nabla T \quad (5.6b)$$

for elevation z positive upwards. The dependent variables are the soil water matric potential ψ and the soil temperature T . The transport coefficients are the isothermal liquid hydraulic conductivity D_{ψ_l} , the thermal liquid diffusivity D_{T_l} , the isothermal vapour conductivity D_{ψ_v} and the thermal vapour diffusivity D_{T_v} . Combination of (5.6a) and (5.6b) leads to the total moisture flux density

$$\frac{q_m}{\rho_l} = \frac{q_l}{\rho_l} + \frac{q_v}{\rho_l} = -D_{\psi} \nabla \psi - D_T \nabla T - D_{\psi_l} \quad (5.7),$$

where the transport coefficients are the isothermal moisture conductivity $D_{\psi} = D_{\psi_l} + D_{\psi_v}$ and the thermal moisture diffusivity $D_T = D_{T_l} + D_{T_v}$.

Therefore, substitution of (5.5a) and (5.7) into the continuity equation given by (5.1) yields the following relationship for one-dimensional saturated-unsaturated flow through porous media, assuming that $\nabla \rho_l$ is zero

$$S_w S_{0\psi} \frac{\partial \psi}{\partial t} + \frac{\partial \theta}{\partial t} = \nabla [D_{\psi} \nabla \psi + D_T \nabla T + D_{\psi_l}] \quad (5.8).$$

In modelling only unsaturated flow, the $S_w S_{0\psi}$ term is generally neglected, yielding

$$\frac{\partial \theta}{\partial t} = \nabla [D_{\psi} \nabla \psi + D_T \nabla T + D_{\psi_l}] \quad (5.9),$$

which is the mixed form of the governing equation for flow of soil moisture in both the liquid and vapour phases under both moisture and temperature gradients. In order to satisfy the required form of the linear state space forecasting equation of the Kalman-filter (3.1), the moisture equation must be in either the θ -based or ψ -based form. By inclusion of the soil capillary capacity factor $C_{\psi} = \partial \theta / \partial \psi$, the soil moisture equation can be transformed to either a θ -based form or a ψ -based form. One important advantage of the θ -based form of the governing equation is that the mass balance of the system is guaranteed, regardless of discretisation and time step size, with only its distribution throughout the profile being affected

(Milly, 1985). However, the θ -based form cannot be used to model multi-layered soils. The reason for this is that the soils hydraulic potential must be continuous across the interface between each layer, while the soils moisture content can vary. Furthermore, it facilitates modelling of soil systems that are locally saturated (Milly, 1985). Thus, it is desirable to write the governing equation for flow of soil moisture in the ψ -based form as

$$C_{\psi} \frac{\partial \psi}{\partial t} = \nabla [D_{\psi} \nabla \psi + D_T \nabla T + D_{\psi l}] \quad (5.10).$$

By neglecting the vapour flux and considering a purely isothermal situation, (5.10) reduces to

$$C_{\psi} \frac{\partial \psi}{\partial t} = \nabla [D_{\psi l} \nabla \psi + D_{\psi l}] \quad (5.11),$$

which is the ψ -based form of the Richards equation for liquid moisture transport under capillary action only (Richards, 1931), and can be derived from the Buckingham-Darcy equation directly. The Buckingham-Darcy equation for flow through porous media is given by

$$\frac{q_l}{\rho_l} = -D_{\psi l} \nabla (\psi + z) \quad (5.12),$$

for z positive upwards.

As it is possible for a water table to develop in the soil column being modelled, the governing equation for simultaneous saturated-unsaturated flow that will be considered is

$$(S_w S_{0\psi} + C_{\psi}) \frac{\partial \psi}{\partial t} = \nabla [D_{\psi l} \nabla \psi + D_{\psi l}] \quad (5.13),$$

which neglects the vapour flux and considers a purely isothermal situation.

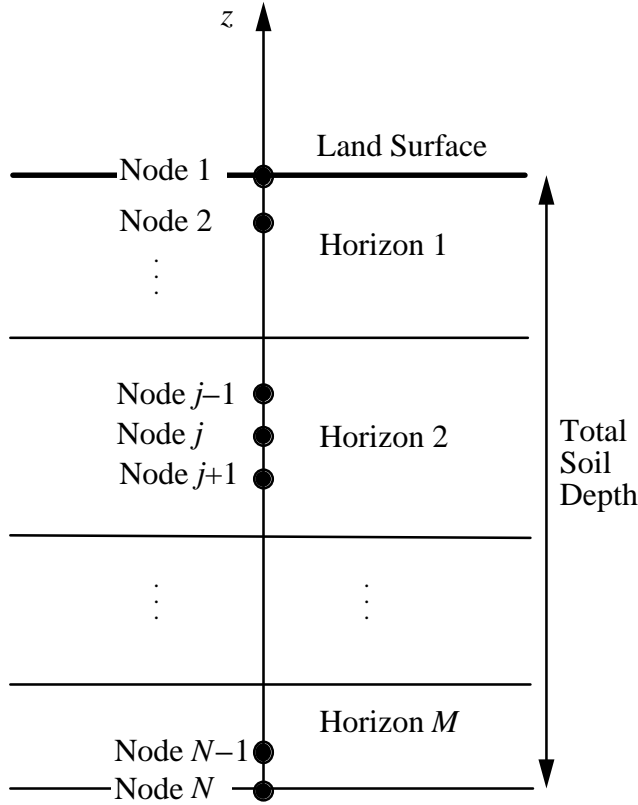


Figure 5.1: Discretisation and coordinate system for the one-dimensional finite difference model.

Writing the parabolic partial differential equation of (5.13) in explicit finite difference form for node j and time step $n+1$ using the soil discretisation given in Figure 5.1, we obtain

$$\psi_j^{n+1} = \psi_j^n + \left(\frac{t^{n+1} - t^n}{S_{w_j}^n S_{0\psi_j}^n + C_{\psi_j}^n} \right) \left\{ \frac{1}{z_{j-1/2} - z_{j+1/2}} \left[D_{\psi^d_{j-1/2}} \left(\frac{\psi_{j-1} - \psi_j}{z_{j-1} - z_j} \right) - D_{\psi^d_{j+1/2}} \left(\frac{\psi_j - \psi_{j+1}}{z_j - z_{j+1}} \right) \right] + \left(\frac{D_{\psi^d_{j-1/2}} - D_{\psi^d_{j+1/2}}}{z_{j-1/2} - z_{j+1/2}} \right)^n \right\} \quad (5.14),$$

where

$$D_{\psi^d_{j-1/2}}^n = \frac{D_{\psi^d_{j-1}}^n + D_{\psi^d_j}^n}{2} \quad (5.15a)$$

$$D_{\psi_{j+1/2}}^n = \frac{D_{\psi_j}^n + D_{\psi_{j+1}}^n}{2} \quad (5.15b)$$

$$z_{j-1/2} - z_{j+1/2} = \frac{z_{j-1} - z_{j+1}}{2} \quad (5.15c),$$

and can be easily vectorised as

$$\{\psi_j\}^{n+1} = \left\{ \begin{array}{l} \left(\frac{(t^{n+1} - t^n)(D_{\psi_{j-1}}^n + D_{\psi_j}^n)}{(S_{w_j}^n S_{0\psi_j}^n + C_{\psi_j}^n)(z_{j-1} - z_{j+1})(z_{j-1} - z_j)} \right) \\ \left(1 - \frac{(t^{n+1} - t^n)}{(S_{w_j}^n S_{0\psi_j}^n + C_{\psi_j}^n)(z_{j-1} - z_{j+1})} \right) \\ \left[\frac{D_{\psi_{j-1}}^n + D_{\psi_j}^n}{z_{j-1} - z_j} + \frac{D_{\psi_j}^n + D_{\psi_{j+1}}^n}{z_j - z_{j+1}} \right] \\ \left(\frac{(t^{n+1} - t^n)(D_{\psi_j}^n + D_{\psi_{j+1}}^n)}{(S_{w_j}^n S_{0\psi_j}^n + C_{\psi_j}^n)(z_{j-1} - z_{j+1})(z_j - z_{j+1})} \right) \end{array} \right\}^T \left\{ \begin{array}{l} \psi_{j-1} \\ \psi_j \\ \psi_{j+1} \end{array} \right\}^n + \left\{ \left(\frac{t^{n+1} - t^n}{S_{w_j}^n S_{0\psi_j}^n + C_{\psi_j}^n} \right) \left(\frac{D_{\psi_{j-1}}^n - D_{\psi_{j+1}}^n}{z_{j-1} - z_{j+1}} \right) \right\} \quad (5.16).$$

Equation (5.16) requires knowledge of the matric potential and liquid hydraulic conductivity both above and below the node of interest. Hence, this equation cannot be used to solve for the matric potential at the top and bottom boundary of the one-dimensional soil column. In order to solve for the unsaturated flow of soil moisture in the soil column, boundary conditions must be applied. The simplest boundary conditions to apply are a fixed matric potential (Dirichlet boundary condition) at both the top and bottom of the soil column. However, a more realistic boundary condition, especially at the soil surface, is a modified flux (Neumann) boundary condition.

If there is a volume flux boundary condition at the soil surface of Q_{top}^ψ (positive upward), then the Buckingham-Darcy equation for one-dimensional unsaturated flow can be written as

$$Q_{top}^{\psi} = -D_{\psi l} \nabla \psi - D_{\psi l} \quad (5.17).$$

Writing (5.17) in explicit finite difference form for the surface node (node 1) at time step $n+1$ (the superscript) and rearranging, we obtain

$$\psi_1^{n+1} = \psi_2^{n+1} - (z_1 - z_2) \left[\frac{Q_{top}^{\psi}}{D_{\psi l_1}^{n+1/2}} + 1 \right] \quad (5.18).$$

Substitution of (5.14) for ψ_2^{n+1} and vectorising yields

$$\{\psi_1\}^{n+1} = \left\{ \begin{array}{c} \frac{(t^{n+1} - t^n)(D_{\psi l_1}^n + D_{\psi l_2}^n)}{(S_{w_2}^n S_{0\psi_2}^n + C_{\psi_2}^n)(z_1 - z_3)(z_1 - z_2)} \\ \left(1 - \frac{(t^{n+1} - t^n)}{(S_{w_2}^n S_{0\psi_2}^n + C_{\psi_2}^n)(z_1 - z_3)} \right) \\ \left[\frac{D_{\psi l_1}^n + D_{\psi l_2}^n}{z_1 - z_2} + \frac{D_{\psi l_2}^n + D_{\psi l_3}^n}{z_2 - z_3} \right] \\ \frac{(t^{n+1} - t^n)(D_{\psi l_2}^n + D_{\psi l_3}^n)}{(S_{w_2}^n S_{0\psi_2}^n + C_{\psi_2}^n)(z_1 - z_3)(z_2 - z_3)} \\ + \left(\frac{t^{n+1} - t^n}{S_{w_2}^n S_{0\psi_2}^n + C_{\psi_2}^n} \right) \left(\frac{D_{\psi l_1}^n - D_{\psi l_3}^n}{z_1 - z_3} \right) \\ - (z_1 - z_2) \left[\frac{2Q_{top}^{\psi}}{D_{\psi l_1}^n + D_{\psi l_2}^n} + 1 \right] \end{array} \right\}^T \left\{ \begin{array}{c} \psi_1 \\ \psi_2 \\ \psi_3 \end{array} \right\}^n \quad (5.19).$$

Likewise, if there is a specified volume flux of Q_{bot}^{ψ} (positive upward) at the base of the soil column, then the Buckingham-Darcy equation for one-dimensional unsaturated flow can be written as

$$Q_{bot}^{\psi} = -D_{\psi l} \nabla \psi - D_{\psi l} \quad (5.20).$$

Writing (5.20) in explicit finite difference form for the bottom node (node N) at time step $n+1$ and rearranging, we obtain

$$\psi_N^{n+1} = \psi_{N-1}^{n+1} + (z_{N-1} - z_N) \left[\frac{Q_{bot}^\psi}{D_{\psi_{N-1/2}}^n} + 1 \right] \quad (5.21).$$

Substitution of (5.14) for ψ_{N-1}^{n+1} and vectorising yields

$$\{\psi_N\}^{n+1} = \left\{ \begin{array}{l} \frac{(t^{n+1} - t^n)(D_{\psi_{N-2}}^n + D_{\psi_{N-1}}^n)}{(S_{w_{N-1}}^n S_{0\psi_{N-1}}^n + C_{\psi_{N-1}}^n)(z_{N-2} - z_N)(z_{N-2} - z_{N-1})} \\ \left(1 - \frac{(t^{n+1} - t^n)}{(S_{w_{N-1}}^n S_{0\psi_{N-1}}^n + C_{\psi_{N-1}}^n)(z_{N-2} - z_N)} \right) \\ \cdot \left[\frac{D_{\psi_{N-2}}^n + D_{\psi_{N-1}}^n}{z_{N-2} - z_{N-1}} + \frac{D_{\psi_{N-1}}^n + D_{\psi_N}^n}{z_{N-1} - z_N} \right] \\ \frac{(t^{n+1} - t^n)(D_{\psi_{N-1}}^n + D_{\psi_N}^n)}{(S_{w_{N-1}}^n S_{0\psi_{N-1}}^n + C_{\psi_{N-1}}^n)(z_{N-2} - z_N)(z_{N-1} - z_N)} \end{array} \right\}^T \left\{ \begin{array}{l} \psi_{N-2} \\ \psi_{N-1} \\ \psi_N \end{array} \right\}^n + \left\{ \begin{array}{l} \left(\frac{t^{n+1} - t^n}{(S_{w_{N-1}}^n S_{0\psi_{N-1}}^n + C_{\psi_{N-1}}^n)} \right) \left(\frac{D_{\psi_{N-2}}^n - D_{\psi_N}^n}{z_{N-2} - z_N} \right) \\ + (z_{N-1} - z_N) \left[\frac{2Q_{bot}^\psi}{D_{\psi_{N-1}}^n + D_{\psi_N}^n} + 1 \right] \end{array} \right\} \quad (5.22).$$

Another boundary condition that is commonly applied to the base of the soil column is gravity drainage. Under a gravity drainage boundary condition, it is assumed that there is a zero matric potential gradient at the base of the soil column (Braud, 1996). Thus, the soil moisture flux at the base of the column can be estimated from the Buckingham-Darcy equation as

$$Q_{bot}^\psi = -D_{\psi_N} \quad (5.23),$$

and applied to (5.22).

5.2.2 HEAT EQUATION

The conservation of heat content in a porous medium can be expressed by the continuity equation for one-dimensional heat transfer as

$$\frac{\partial S_h}{\partial t} = -\nabla q_h \quad (5.24),$$

where q_h is the heat flux density. S_h is the total heat content per unit bulk volume and has been expressed by de Vries (1958) as

$$S_h = (C_d + c_l \rho_l \theta_l + c_p \rho_l \theta_v)(T - T_{ref}) + L_{ref} \rho_l \theta_v - \rho_l \int_0^{\theta_l} W d\theta_l \quad (5.25),$$

where C_d is the volumetric heat capacity of the dry soil, c_l is the specific heat capacity of liquid water, c_p is the specific heat capacity of water vapour at constant pressure, T_{ref} is an arbitrary reference temperature, L_{ref} is the latent heat of vaporisation at temperature T_{ref} , and W is the differential heat of wetting.

Volumetric heat capacity is the quantity of heat required to raise or lower the temperature of a given volume of material by a given amount. If the quantity of heat refers to a given mass, then it is called the specific heat capacity (Williams, 1982). The latent heat of vaporisation refers to the quantity of heat associated with the phase change from liquid to vapour (Williams, 1982). The differential heat of wetting is the amount of heat released per unit mass of added water when an infinitesimal quantity of free liquid water is added to the soil medium (Milly, 1982).

Ignoring the contribution to heat storage from the differential heat of wetting, the rate of change of heat storage with time can be written as

$$\begin{aligned} \frac{\partial S_h}{\partial t} = & (C_d + c_l \rho_l \theta_l + c_p \rho_l \theta_v) \frac{\partial T}{\partial t} \\ & + \left(c_l \rho_l \frac{\partial \theta_l}{\partial t} + c_p \rho_l \frac{\partial \theta_v}{\partial t} \right) (T - T_{ref}) + L_{ref} \rho_l \frac{\partial \theta_v}{\partial t} \end{aligned} \quad (5.26).$$

Following de Vries (1958), the total heat flux density for both sensible and latent heat in a porous medium is given by

$$q_h = -(\lambda - L\rho_l D_{Tv}) \nabla T + Lq_v + c_l (T - T_{ref}) q_m \quad (5.27),$$

where L is the latent heat of vaporisation of water at temperature T given by (Milly, 1982)

$$L = L_{ref} - (c_l - c_p)(T - T_{ref}) \quad (5.28),$$

and λ is the apparent thermal conductivity, which accounts for the combined effects of simple Fourier heat diffusion and latent heat transport by temperature induced vapour diffusion (Milly, 1982). Thermal conductivity is the rate at which heat transfer can occur within a substance (Williams, 1982).

Substitution of (5.26) and (5.27) into the continuity equation given by (5.24) yields the following governing equation for heat transfer in a one-dimensional soil column

$$C_T \frac{\partial T}{\partial t} = \nabla [(\lambda - \rho_l D_{Tv} L) \nabla T - L q_v - c_l (T - T_{ref}) q_m] - \left(c_l \rho_l \frac{\partial \theta_l}{\partial t} + c_p \rho_l \frac{\partial \theta_v}{\partial t} \right) (T - T_{ref}) - L_{ref} \rho_l \frac{\partial \theta_v}{\partial t} \quad (5.29),$$

where $C_T = C_d + c_l \rho_l \theta_l + c_p \rho_l \theta_v$ is the volumetric heat capacity of the bulk soil medium.

Again, by neglecting the vapour flux, the governing equation for heat transport in a porous medium may be reduced to

$$C_T \frac{\partial T}{\partial t} = \nabla [\lambda \nabla T - c_l (T - T_{ref}) q_l] - c_l \rho_l (T - T_{ref}) \frac{\partial \theta_l}{\partial t} \quad (5.30).$$

Writing (5.3) in explicit finite difference form for node j and time step $n+1$ using the soil discretisation given in Figure 5.1, we obtain

$$T_j^{n+1} = T_j^n + \left(\frac{t^{n+1} - t^n}{C_{T_j}^n} \right) \left\{ \begin{array}{l} \frac{1}{z_{j-1/2} - z_{j+1/2}} \left[\lambda_{j-1/2} \left(\frac{T_{j-1} - T_j}{z_{j-1} - z_j} \right) \right. \\ \left. - \lambda_{j+1/2} \left(\frac{T_j - T_{j+1}}{z_j - z_{j+1}} \right) \right] \\ - \frac{c_l}{z_{j-1} - z_{j+1}} \left[(T_{j-1} - T_{ref}) \mathbf{q}_{l_{j-1}} \right. \\ \left. - (T_{j+1} - T_{ref}) \mathbf{q}_{l_{j+1}} \right] \\ - c_l \rho_l (T_j^n - T_{ref}) \left[\frac{\theta_{l_j}^n - \theta_{l_j}^{n-1}}{t^n - t^{n-1}} \right] \end{array} \right\}^n \quad (5.31),$$

where

$$\lambda_{j-1/2} = \frac{\lambda_{j-1} + \lambda_j}{2} \quad (5.32a)$$

$$\lambda_{j+1/2} = \frac{\lambda_j + \lambda_{j+1}}{2} \quad (5.32b)$$

and can be easily vectorised as

$$\{T_j\}^{n+1} = \left\{ \begin{array}{l} \frac{(t^{n+1} - t^n)(\lambda_{j-1}^n + \lambda_j^n)}{C_{T_j}^n(z_{j-1} - z_{j+1})(z_{j-1} - z_j)} - \frac{(t^{n+1} - t^n)c_l \mathbf{q}_{l_{j-1}}^n}{C_{T_j}^n(z_{j-1} - z_{j+1})} \\ 1 - \left(\frac{(t^{n+1} - t^n)}{C_{T_j}^n(z_{j-1} - z_{j+1})} \left[\frac{\lambda_{j-1}^n + \lambda_j^n}{z_{j-1} - z_j} + \frac{\lambda_j^n + \lambda_{j+1}^n}{z_j - z_{j+1}} \right] \right) \\ - \frac{(t^{n+1} - t^n)c_l \rho_l}{C_{T_j}^n} \left[\frac{\theta_{l_j}^n - \theta_{l_j}^{n-1}}{t^n - t^{n-1}} \right] \\ \frac{(t^{n+1} - t^n)(\lambda_j^n + \lambda_{j+1}^n)}{C_{T_j}^n(z_{j-1} - z_{j+1})(z_j - z_{j+1})} + \frac{(t^{n+1} - t^n)c_l \mathbf{q}_{l_{j+1}}^n}{C_{T_j}^n(z_{j-1} - z_{j+1})} \end{array} \right\}^T \left\{ \begin{array}{l} T_{j-1} \\ T_j \\ T_{j+1} \end{array} \right\}^n \\ + \left\{ \begin{array}{l} \frac{(t^{n+1} - t^n)c_l T_{ref}}{C_{T_j}^n} \left[\frac{\mathbf{q}_{l_{j-1}}^n - \mathbf{q}_{l_{j+1}}^n}{z_{j-1} - z_{j+1}} \right] \\ + \frac{(t^{n+1} - t^n)c_l \rho_l T_{ref}}{C_{T_j}^n} \left[\frac{\theta_{l_j}^n - \theta_{l_j}^{n-1}}{t^n - t^{n-1}} \right] \end{array} \right\} \quad (5.33).$$

Equation (5.33) requires knowledge of the soil temperature and apparent thermal conductivity both above and below the node of interest. Hence, this equation cannot be used to solve for the soil temperature at the top and bottom boundary of the one-dimensional soil column. In order to solve for the transfer of heat storage in the soil column, boundary conditions must be applied. The simplest boundary conditions to apply are a fixed soil temperature at both the top and bottom of the soil column. However, a more realistic boundary condition, especially at the soil surface, is a heat flux boundary condition.

If there is a heat flux boundary condition at the soil surface of Q_{top}^T (positive upward), then the heat flux density equation for one-dimensional heat transfer, neglecting the vapour component, can be written as

$$Q_{top}^T = -\lambda \nabla T + c_l (T - T_{ref}) \mathbf{q}_l \quad (5.34).$$

Writing (5.34) in explicit finite difference form for the surface node (node 1) at time step $n+1$ and rearranging, we obtain

$$T_1^{n+1} = T_2^{n+1} + \frac{(z_1 - z_2)}{\lambda_{1/2}^n} [c_l (T_1^n - T_{ref}) \mathbf{q}_{l_1}^n - Q_{top}^T] \quad (5.35).$$

Substitution of (5.31) for T_2^{n+1} and vectorising yields

$$\begin{aligned}
\{T_1\}^{n+1} = & \left\{ \begin{aligned} & \left(\frac{(t^{n+1} - t^n)(\lambda_1^n + \lambda_2^n)}{C_{T_2}^n(z_1 - z_3)(z_1 - z_2)} - \frac{(t^{n+1} - t^n)c_l q_{l_1}^n}{C_{T_2}^n(z_1 - z_3)} \right) \\ & + \frac{2(z_1 - z_2)c_l q_{l_1}^n}{\lambda_1^n + \lambda_2^n} \end{aligned} \right\}^T \\
& 1 - \left\{ \begin{aligned} & \left(\frac{(t^{n+1} - t^n)}{C_{T_2}^n(z_1 - z_3)} \left[\frac{\lambda_1^n + \lambda_2^n}{z_1 - z_2} + \frac{\lambda_2^n + \lambda_3^n}{z_2 - z_3} \right] \right) \\ & - \frac{(t^{n+1} - t^n)c_l \rho_l}{C_{T_2}^n} \left[\frac{\theta_{l_2}^n - \theta_{l_2}^{n-1}}{t^n - t^{n-1}} \right] \end{aligned} \right\} \begin{Bmatrix} T_1 \\ T_2 \\ T_3 \end{Bmatrix}^n \\
& \left(\frac{(t^{n+1} - t^n)(\lambda_2^n + \lambda_3^n)}{C_{T_2}^n(z_1 - z_3)(z_2 - z_3)} + \frac{(t^{n+1} - t^n)c_l q_{l_3}^n}{C_{T_2}^n(z_1 - z_3)} \right) \\
& + \left\{ \begin{aligned} & \left(\frac{(t^{n+1} - t^n)c_l T_{ref}}{C_{T_2}^n} \left[\frac{q_{l_1}^n - q_{l_3}^n}{z_1 - z_3} \right] \right) \\ & + \frac{(t^{n+1} - t^n)c_l \rho_l T_{ref}}{C_{T_2}^n} \left[\frac{\theta_{l_2}^n - \theta_{l_2}^{n-1}}{t^n - t^{n-1}} \right] \end{aligned} \right\} \\
& - \frac{2(z_1 - z_2)}{\lambda_1^n + \lambda_2^n} [c_l T_{ref} q_{l_1}^n + Q_{top}^T] \end{aligned} \quad (5.36).
\end{aligned}$$

Likewise, if there is a specified heat flux of Q_{bot}^T (positive upward) at the base of the soil column, then the heat flux density equation for one-dimensional heat transfer can be written as

$$Q_{bot}^T = -\lambda \nabla T + c_l (T - T_{ref}) \mathfrak{q}_l \quad (5.37).$$

Writing in explicit finite difference form for the bottom node (node N) at time step $n+1$ and rearranging, we obtain

$$T_N^{n+1} = T_{N-1}^{n+1} - \frac{(z_{N-1} - z_N)}{\lambda_{N-1/2}^n} [c_l (T_N^n - T_{ref}) \mathfrak{q}_{l_N}^n - Q_{bot}^T] \quad (5.38).$$

Substitution of (5.31) for T_{N-1}^{n+1} and vectorising yields

$$\begin{aligned}
\{T_N\}^{n+1} = & \left\{ 1 - \left[\frac{(t^{n+1} - t^n)(\lambda_{N-2}^n + \lambda_{N-1}^n)}{C_{T_{N-1}}^n (z_{N-2} - z_N)(z_{N-2} - z_{N-1})} - \frac{(t^{n+1} - t^n)c_l q_{I_{N-2}}^n}{C_{T_{N-1}}^n (z_{N-2} - z_N)} \right] \right. \\
& \left. - \left[\frac{(t^{n+1} - t^n)}{C_{T_{N-1}}^n (z_{N-2} - z_N)} \left[\frac{\lambda_{N-2}^n + \lambda_{N-1}^n}{z_{N-2} - z_{N-1}} + \frac{\lambda_{N-1}^n + \lambda_N^n}{z_{N-1} - z_N} \right] \right] \right. \\
& \left. - \left[\frac{(t^{n+1} - t^n)c_l \rho_l \left[\frac{\theta_{I_{N-1}}^n - \theta_{I_{N-1}}^{n-1}}{t^n - t^{n-1}} \right]}{C_{T_{N-1}}^n} \right] \right\} \left\{ \begin{matrix} T_{N-2} \\ T_{N-1} \\ T_N \end{matrix} \right\}^n \\
& \left(\frac{(t^{n+1} - t^n)(\lambda_{N-1}^n + \lambda_N^n)}{C_{T_{N-1}}^n (z_{N-2} - z_N)(z_{N-1} - z_N)} + \frac{(t^{n+1} - t^n)c_l q_{I_N}^n}{C_{T_{N-1}}^n (z_{N-2} - z_N)} \right) \\
& - \frac{2(z_{N-1} - z_N)c_l q_{I_N}^n}{\lambda_{N-1}^n + \lambda_N^n} \\
& + \left\{ \frac{(t^{n+1} - t^n)c_l T_{ref} \left[\frac{q_{I_{N-2}}^n - q_{I_N}^n}{z_{N-2} - z_N} \right]}{C_{T_{N-1}}^n} \right. \\
& + \left. \frac{(t^{n+1} - t^n)c_l \rho_l T_{ref} \left[\frac{\theta_{I_{N-1}}^n - \theta_{I_{N-1}}^{n-1}}{t^n - t^{n-1}} \right]}{C_{T_{N-1}}^n} \right\} \\
& + \frac{2(z_{N-1} - z_N)}{\lambda_{N-1}^n + \lambda_N^n} [c_l T_{ref} q_{I_N}^n + Q_{bot}^T]
\end{aligned} \tag{5.39}$$

Another boundary condition that is commonly applied to the base of the soil column is advection. Under the advection boundary condition, it is assumed that there is a zero temperature gradient at the base of the soil column and that heat transfer is just the heat content of the water flowing through the bottom of the soil column. Thus, neglecting the vapour terms, the heat flux at the base of the column can be estimated from the heat flux density equation in (5.27) as

$$Q_{bot}^T = c_l (T_N^n - T_{ref}^n) q_{I_N}^n \tag{5.40},$$

and applied to (5.39).

The liquid component of the mass flux rate q_l , which is required for evaluation of the heat transfer equations, can be estimated from the Buckingham-Darcy equation. At the surface node, this may be expressed as

$$q_{I_1}^n = \rho_l \left[-D_{\psi_{1/2}}^n \left(\frac{\psi_1 - \psi_2}{z_1 - z_2} \right)^n - D_{\psi_{1/2}}^n \right] \tag{5.41}.$$

However, if there is a specified evaporation rate or a specified precipitation rate, which is not in excess of the infiltration rate, the flux at the surface node need not be estimated from (5.41).

If the boundary condition applied to the base of the soil column for solving the one-dimensional unsaturated flow equation is a specified matric potential rather than a moisture flux, the liquid mass flux at the base of the soil column may be estimated from the Buckingham-Darcy equation as

$$q_{l_N}^n = \rho_l \left[-D_{\psi_{N-1/2}}^n \left(\frac{\psi_{N-1} - \psi_N}{z_{N-1} - z_N} \right)^n - D_{\psi_{N-1/2}}^n \right] \quad (5.42).$$

For the intermediate nodes in the soil discretisation, the liquid mass flux can be estimated from the following finite element representation of the Buckingham-Darcy equation as

$$q_{l_j}^n = \rho_l \left\{ -\frac{1}{2} \left[\begin{array}{l} D_{\psi_{j-1/2}}^n \left(\frac{\psi_{j-1} - \psi_j}{z_{j-1} - z_j} \right)^n \\ + D_{\psi_{j+1/2}}^n \left(\frac{\psi_j - \psi_{j+1}}{z_j - z_{j+1}} \right)^n \end{array} \right] - D_{\psi_j}^n \right\} \quad (5.43).$$

5.3 CONSTITUTIVE RELATIONS

In order to evaluate the soil moisture and heat transfer equations presented, it is necessary to evaluate the constitutive relations. This section presents the most commonly used equations for evaluating the constitutive relations.

5.3.1 WATER RETENTION RELATIONSHIP

Numerous water retention relationships have been presented in literature. The three most commonly used models are presented below, being those of Brooks and Corey (1966), Clapp and Hornberger (1978) and van Genuchten (1980).

5.3.1.1 Brooks and Corey

$$\theta_l = (\phi - \theta_r) \left(\frac{\psi_b}{\psi} \right)^\phi + \theta_r \quad \psi \leq \psi_b \quad (5.44a)$$

$$\theta_l = \phi \quad \psi > \psi_b \quad (5.44b),$$

where ϕ is the soil porosity, θ_r is the residual soil water content, ψ_b is the bubbling capillary pressure, and ϕ is a pore size distribution index.

5.3.1.2 Clapp and Hornberger

$$\psi = \psi_s \left(\frac{\theta_l}{\phi} \right)^{-b} \quad W \leq W_i \quad (5.45a)$$

$$\psi = -m_w \left(\frac{\theta_l}{\phi} - n_w \right) \left(\frac{\theta_l}{\phi} - 1 \right) \quad W_i < W < 1 \quad (5.45b)$$

$$\psi = 0, \theta_l = \phi \quad W = 1 \quad (5.45c),$$

where

$$W = \frac{\theta_l}{\phi} \quad (5.45d)$$

$$m_w = \frac{\psi_i}{(1 - W_i)^2} - \frac{\psi_i b}{W_i (1 - W_i)} \quad (5.45e)$$

$$n_w = 2W_i - \left(\frac{\psi_i b}{m_w W_i} \right) - 1 \quad (5.45f),$$

and ψ_s is the saturated soil matric potential, ϕ is the soil porosity and b is a soil texture parameter. W_i is considered for operational purposes as the air entry point, occurring between $0.8 < W_i < 1$. Clapp and Hornberger (1978) have suggested that $W_i = 0.92$ is a useful estimate, limited by $W_i > b/(b+1)$. ψ_i is the matric potential that corresponds with θ_i from (5.45d).

5.3.1.3 Van Genuchten

$$\theta_i = (\phi - \theta_r) \left[\frac{1}{1 + (-\eta\psi)^n} \right]^m + \theta_r \quad \psi < 0 \quad (5.46a)$$

$$\theta_i = \phi \quad \psi \geq 0 \quad (5.46b)$$

where η , n and m are soil texture parameters. The parameters n and m are related to each other by

$$m = 1 - \frac{1}{n} \quad 0 < m < 1 \quad (5.46c),$$

and are related to the Brooks and Corey (1966) parameters by (van Genuchten, 1980)

$$\eta = -\frac{1}{\psi_b} \quad (5.46d)$$

$$n = \phi + 1 \quad (5.46e).$$

5.3.2 CAPILLARY CAPACITY RELATIONSHIP

The capillary capacity $C_\psi = \partial\theta/\partial\psi$ may be estimated by differentiating the water retention relationships given above. Therefore, the capillary capacity for the three water retention relationships described above are as follows.

5.3.2.1 Brooks and Corey

$$\frac{\partial \theta_l}{\partial \psi} = -\frac{\phi(\phi - \theta_r)}{\psi} \left(\frac{\psi_b}{\psi} \right)^\phi \quad \psi \leq \psi_b \quad (5.47a)$$

$$\frac{\partial \theta_l}{\partial \psi} = 0 \quad \psi > \psi_b \quad (5.47b)$$

5.3.2.2 Clapp and Hornberger

$$\frac{\partial \theta_l}{\partial \psi} = -\frac{\phi}{b\psi} \left(\frac{\psi}{\psi_s} \right)^{-\frac{1}{b}} \quad W \leq W_i \quad (5.48a)$$

$$\frac{\partial \theta_l}{\partial \psi} = \frac{\phi^2}{m_w(\phi - 2\theta + n_w\phi)} \quad W_i < W < 1 \quad (5.48b)$$

$$\frac{\partial \theta_l}{\partial \psi} = 0 \quad W = 1 \quad (5.48c)$$

5.3.2.3 Van Genuchten

$$\frac{\partial \theta_l}{\partial \psi} = \frac{\eta m(\phi - \theta_r)}{1 - m} \Theta^{\frac{1}{m}} \left(1 - \Theta^{\frac{1}{m}} \right)^m \quad \psi < 0 \quad (5.49a)$$

$$\frac{\partial \theta_l}{\partial \psi} = 0 \quad \psi \geq 0 \quad (5.49b),$$

where

$$\Theta = \left[\frac{1}{1 + (-\eta\psi)^n} \right]^m = \frac{\theta_l - \theta_r}{\phi - \theta_r} \quad (5.49c).$$

5.3.3 ISOTHERMAL LIQUID HYDRAULIC CONDUCTIVITY

The isothermal liquid hydraulic conductivity D_{ψ_l} is simply the unsaturated hydraulic conductivity K . The three models described here for the liquid hydraulic conductivity are those of Brooks and Corey (1966), Clapp and Hornberger (1978) and van Genuchten (1980).

5.3.3.1 Brooks and Corey

$$K = K_s \left(\frac{\theta_l - \theta_r}{\phi - \theta_r} \right)^c \quad (5.50a),$$

where K_s is the saturated hydraulic conductivity and c is a soil texture parameter given by

$$c = \frac{2 + 3\phi}{\phi} \quad (5.50b).$$

5.3.3.2 Clapp and Hornberger

$$K = K_s \left(\frac{\theta}{\phi} \right)^{2b+3} \quad (5.51)$$

5.3.3.3 Van Genuchten

$$K = K_s \Theta^{\frac{1}{2}} \left[1 - \left(1 - \Theta^{\frac{1}{m}} \right)^m \right]^2 \quad \psi \leq 0 \quad (5.52a)$$

or

$$K = K_s \frac{\left\{ 1 - (-\eta\psi)^{n-1} \left[1 + (-\eta\psi)^n \right]^{-m} \right\}^2}{\left[1 + (-\eta\psi)^n \right]^{\frac{m}{2}}} \quad \psi \leq 0 \quad (5.52b)$$

and

$$K = K_s \quad \psi > 0, \theta = \phi \quad (5.52c)$$

5.3.4 THERMAL LIQUID DIFFUSIVITY

The thermal liquid diffusivity D_{Tl} has been defined by Philip and de Vries (1957) as

$$D_{Tl} = K\gamma\psi \quad (5.53),$$

where γ is the temperature coefficient of water surface tension. γ is temperature dependent, but Philip and de Vries (1957) suggest that the constant value $-2.09 \times 10^{-3} \text{ }^\circ\text{C}^{-1}$ may reasonably be adopted as representative for the temperature range 10°C to 30°C .

5.3.5 ISOTHERMAL VAPOUR CONDUCTIVITY

The isothermal vapour conductivity D_{ψ_l} has been defined by Philip and de Vries (1957) as

$$D_{\psi_v} = \frac{\xi D_{atm} (\phi - \theta) g}{\rho_l} \frac{P_{atm}}{P_{atm} - e} \frac{\rho_v}{R_v (T + 273)} \quad (5.54),$$

where ξ is the tortuosity factor for diffusion of gases in soils allowing for the extra path length, and is approximately 0.67 (de Vries, 1958); g is the acceleration due to gravity (981 cm s^{-2}); R_v is the gas constant of water vapour ($4.615 \times 10^6 \text{ erg g}^{-1}$); ϕ is the soil porosity; T is the soil temperature ($^\circ\text{C}$); P_{atm} is the atmospheric pressure, which for practical purposes may be taken as 101 kPa; e is partial pressure of water vapour (kPa) given by

$$e = 0.611 \exp\left(\frac{17.27T}{T + 237.3}\right) RH_{soil} \quad (5.55).$$

RH_{soil} is the relative humidity of the soil, which is a measure of the affinity of water and soil particles, reflecting the forces by which water is retained through depression of its vapour pressure below that of free water (Sasamori, 1970), given by the Kelvin law as

$$RH_{soil} = \exp\left(\frac{\psi g}{R_v (T + 273)}\right) \quad (5.56),$$

and D_{atm} is the molecular diffusion coefficient of water vapour in air given by

$$D_{atm} = 4.42 \times 10^{-4} \frac{(T + 273)^{2.3}}{P_{atm}} \quad (5.57).$$

5.3.6 THERMAL VAPOUR DIFFUSIVITY

The thermal vapour diffusivity has been defined by Philip and de Vries (1957) as

$$D_{Tv} = \frac{\xi D_{atm} (\phi - \theta) \beta RH_{soil}}{\rho_l} \frac{P_{atm}}{P_{atm} - e} \quad (5.58),$$

where $\beta = d\rho_v/dT = 1.05 \times 10^{-6} \text{ g cm}^{-3} \text{ }^\circ\text{C}^{-1}$ at 20°C, and is representative for 10°C to 30°C (Philip and de Vries, 1957), and ρ_o is the density of saturated water vapour.

5.3.7 HEAT CAPACITY

The volumetric heat capacity of a soil is a weighted average of the heat capacities of its components (de Vries, 1963),

$$C_T = \sum_{i=1}^5 C_i \theta_i \quad (5.59)$$

where θ_i and C_i are the volumetric fraction and the volumetric heat capacity of the i th soil constituent. The five components are: (i) water; (ii) air, given by $\theta_2 = \phi - \theta_1$;

Table 5.1: Properties of soil constituents (Milly, 1984).

Constituent	<i>i</i>	C_i $\text{cal cm}^{-3} \text{ }^\circ\text{C}^{-1}$	λ_i $\text{cal cm}^{-1} \text{ s}^{-1} \text{ }^\circ\text{C}^{-1}$	g_i
Liquid Water	1	1.0	1.37×10^3	...
Air	2	3×10^4	$6 \times 10^5 + \lambda_{vap}$	see (5.61)
Quartz	3	0.46	2.1×10^2	0.125
Other Minerals	4	0.46	7×10^3	0.125
Organic Matter	5	0.6	6×10^4	0.5

(iii) quartz particles; (iv) other minerals; and (v) organic matter. The heat capacities suggested for these constituents are listed in Table 5.1.

5.3.8 THERMAL CONDUCTIVITY

The effective thermal conductivity of a moist soil is given by de Vries (1963) as

$$\lambda = \frac{\sum_{i=1}^5 k_i \theta_i \lambda_i}{\sum_{i=1}^5 k_i \theta_i} \quad (5.60a),$$

where λ_i is the thermal conductivity of the i th constituent as given in Table 5.1 and k_i is the ratio of the average temperature gradient in the i th constituent to the average temperature gradient of the bulk medium. A conceptual model is (Kimball *et al.*, 1976)

$$k_i = \frac{2}{3} \left[1 + \left(\frac{\lambda_i}{\lambda_1} - 1 \right) g_i \right]^{-1} + \frac{1}{3} \left[1 + \left(\frac{\lambda_i}{\lambda_1} - 1 \right) (1 - 2g_i) \right]^{-1} \quad (5.60b),$$

where the liquid phase is considered continuous and g_i is the “shape factor” of the i th constituent. For the solid particles, constant values as given in Table 5.1 are assumed. No value is needed for g_1 since its coefficient is zero. The value of g_2 is

considered as a function of soil moisture content as follows (Kimball *et al.*, 1976; Milly, 1984).

$$g_2 = 0.013 + \left(\frac{0.022}{\theta_{4.2}} + \frac{0.298}{\phi} \right) \theta_l \quad \theta_l < \theta_{4.2} \quad (5.61a)$$

$$g_2 = 0.035 + \frac{0.298}{\phi} \theta_l \quad \theta_{4.2} < \theta_l \quad (5.61b),$$

where $\theta_{4.2}$ is the volumetric soil moisture content corresponding to ψ from $4.2 = \log(-\psi)$.

The effective thermal conductivity of the air-filled pores, enhanced by vapour distillation (Philip and de Vries, 1957), is given by

$$\lambda_2 = \lambda_a + \lambda_{vap} \quad (5.62a),$$

where λ_a is the thermal conductivity of the dry air alone and λ_{vap} is the increase in the thermal conductivity of the pores due to vapour distillation, given by Philip and de Vries (1957) as

$$\lambda_{vap} = LD_{atm} RH_{soil} \beta \frac{P_{atm}}{P_{atm} - e} \quad (5.62b),$$

where $\beta = d\rho_v/dT$.

In estimating L from (5.28), L_{ref} may be taken as 591.6 cal g^{-1} at 10°C , c_p as $0.449 \text{ cal g}^{-1} \text{ }^\circ\text{C}^{-1}$ and c_l as $1.0 \text{ cal g}^{-1} \text{ }^\circ\text{C}^{-1}$ (Monteith and Unsworth, 1990).

5.3.9 COMPRESSIBILITY COEFFICIENTS

The typical ranges of compressibility coefficients for various types of geologic materials is given in Table 5.2, along with the well known value for compressibility of water. The value selected for soil compressibility was $\alpha = 10^{-5} \text{ cm}^{-1} \text{ H}_2\text{O}$.

Table 5.2: Range of values of compressibility (Freeze and Cherry, 1979).

	Compressibility, α	
	Pa^{-1}	$\text{cm}^{-1} \text{H}_2\text{O}$
Clay	$10^{-6} - 10^{-8}$	$10^{-4} - 10^{-6}$
Sand	$10^{-7} - 10^{-9}$	$10^{-5} - 10^{-7}$
Gravel	$10^{-8} - 10^{-10}$	$10^{-6} - 10^{-8}$
Water (β)	4.4×10^{-10}	4.3×10^{-8}

5.4 TIME STEPPING PROCEDURE

The size of the computational time step can be determined automatically by a procedure that limits the magnitude of changes in the state variable to some specified values, subject to the modulus of the eigenvalues being less than or equal to 1 (Gerald and Wheatley, 1989) and the current time step size being not greater than 1.2 times the previous time step size (Celia and Gray, 1992). The procedure presented here is that suggested by Milly (1982) for a fully implicit backward difference scheme. For matric potential, we define

$$\varepsilon_{\psi}^n = \max_j \left| \frac{\psi_j^n - \psi_j^{n-1}}{\psi_j^n} \right| \quad (5.63a),$$

and for temperature,

$$\varepsilon_T^n = \max_j |T_j^n - T_j^{n-1}| \quad (5.63b).$$

Given specified targets for maximum change in matric potential and soil temperature at any node in the soil column of $\hat{\varepsilon}_{\psi}$ and $\hat{\varepsilon}_T$ respectively, the new time step size (generally the order of seconds) can be forecast according to the rule

$$(\Delta t)^{n+1} = (\Delta t)^n \left[\max \left(\frac{\varepsilon_{\psi}^n}{\hat{\varepsilon}_{\psi}}, \frac{\varepsilon_T^n}{\hat{\varepsilon}_T} \right) \right]^{-1} \quad (5.64).$$

5.5 MODEL EVALUATION

The one-dimensional soil moisture and heat transfer model PROXSIM1D has been compared with the Galerkin finite element model of Milly (1982) SPLaSHWaTr (Simulation Program for Land-Surface Heat and Water Transport). In the simulations, the initial conditions were -50 cm matric head and 20°C temperature uniform throughout a 100 cm deep soil profile. The water retention and unsaturated hydraulic conductivity relationships used were those of van Genuchten (1980) and the soil parameters were as given in Table 5.3.

In the comparison, six different boundary conditions were applied: (i) evaporation of 0.5 cm day^{-1} ($5.8\text{e}-6$ cm s^{-1}) and soil heat flux of 400 langley day^{-1} ($4.62\text{e}-3$ cal s^{-1} cm^{-2}) at the soil surface, zero moisture and heat flux at 100 cm depth; (ii) evaporation of 0.5 cm day^{-1} and soil heat flux of 400 langley day^{-1} at the soil surface, matric head of -50 cm and soil temperature of 20°C at 100 cm depth; (iii) matric head of -100 cm and soil temperature of 10°C at soil surface, zero moisture and heat flux at 100 cm depth; (iv) matric head of -100 cm and soil temperature of 10°C at soil surface, matric head of -50 cm and soil temperature of 20°C at 100 cm depth; (v) evaporation of 0.5 cm day^{-1} and soil heat flux of 400 langley day^{-1} at the soil surface, gravity drainage and advection at 100 cm depth; and (vi) precipitation of 30 mm hour^{-1} ($-8.33\text{e}-4$ cm s^{-1}) and soil heat

Table 5.3: Soil parameters used in evaluation of PROXSIM1D.

Total Soil Depth	100 cm
Number of Nodes	31
Soil Thermal and Hydraulic Parameters	Clay Loam
	$K_s = 25$ cm day^{-1}
	$\phi = 0.54$
	$\theta_r = 0.2$
	$\eta = 0.008$
	$n = 1.8$
	Proportion of Quartz = 0.03
	Proportion of Other Minerals = 0.41
	Proportion of Organic Matter = 0.02
Initial Conditions	20°C , -50 cm Matric Head

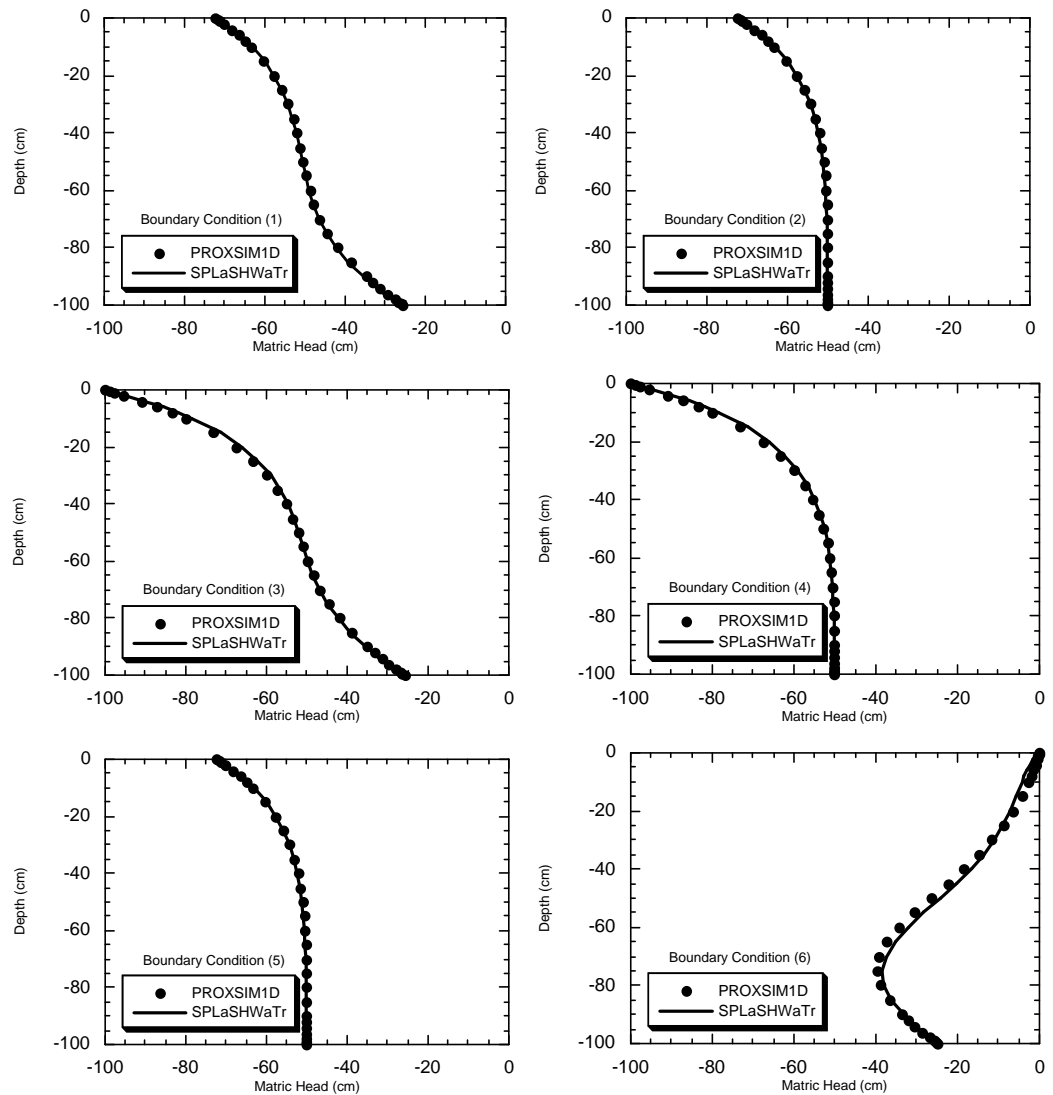


Figure 5.2: Comparison of soil moisture profile simulation results from PROXSIM1D and SPLaSHWaTr under six different boundary conditions.

flux of $400 \text{ langley day}^{-1}$ at the soil surface, zero moisture and heat flux at 100 cm depth.

The results of this evaluation are given in Figure 5.2 for soil moisture and Figure 5.3 for soil temperature, after a simulation time of 1 hour. These results show that despite the explicit linearisation, PROXSIM1D does an excellent job of modelling the non-linear solution to the soil moisture and heat transfer of SPLaSHWaTr.

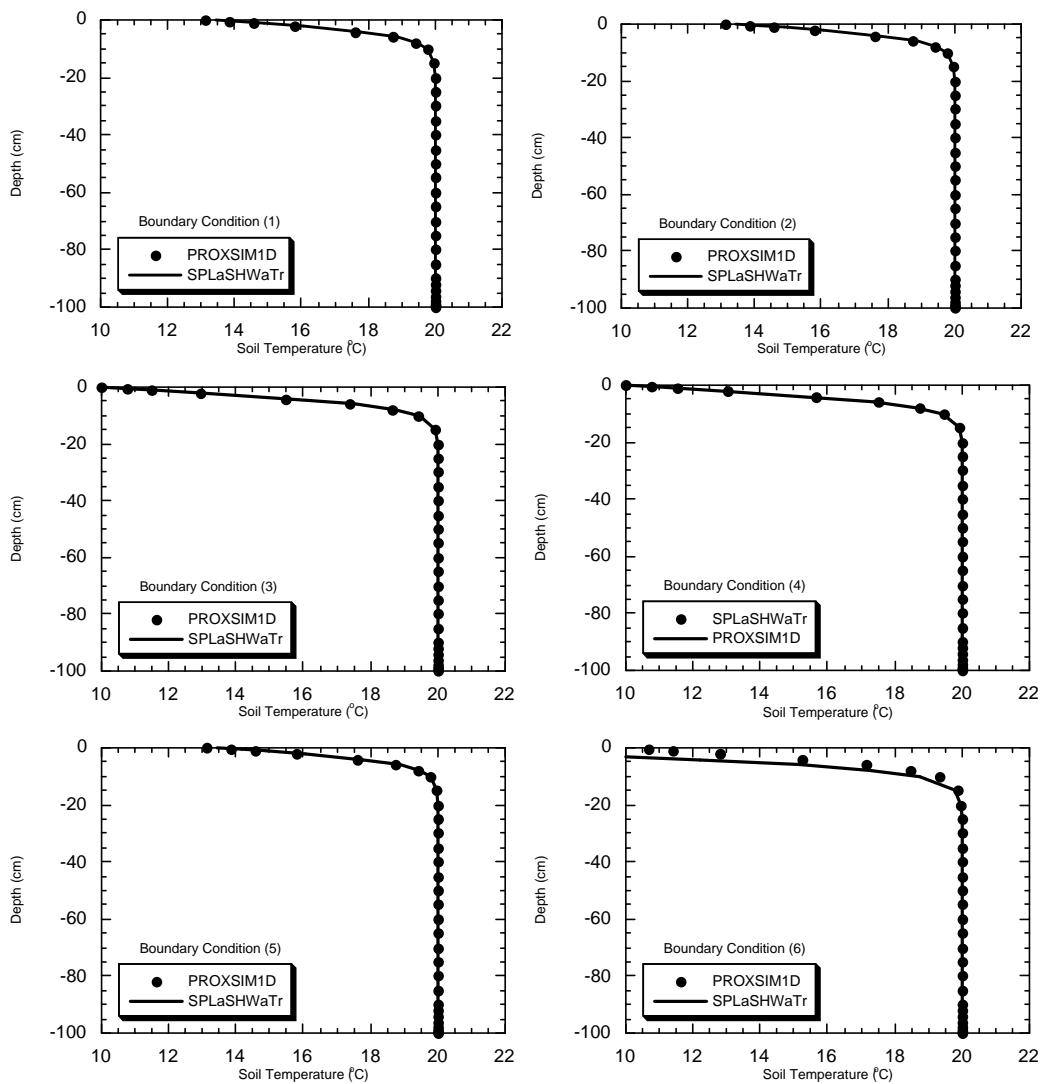


Figure 5.3: Comparison of soil temperature profile simulation results from PROXSIM1D and SPLaSHWaTr under six different boundary conditions.

5.6 CHAPTER SUMMARY

In order to infer near-surface soil moisture content from microwave remote sensing observations, an estimate of the near-surface soil temperature is required. Hence, in order to update a hydrologic model with near-surface soil moisture measurements from remote sensing observations, the soil temperature profile must be forecast, in addition to the soil moisture profile.

This chapter has developed the model equations for forecasting of the soil moisture and temperature profiles by the explicit model PROXSIM1D, which is used in the synthetic study of Chapter 6. This model has been shown to have an excellent agreement with the SPLaSHWaTr implicit model.