APPENDIX A

A.STATE AUGMENTATION OF PROXSIM1D

State augmentation is a method by which the Kalman-filter may be used to estimate the model parameters (Goodwin and Sin, 1984). Using this approach, the original state vector **X** is augmented by addition of the constant but unknown model parameters, such that the state vector becomes

$$\underline{\mathbf{X}} = \left\{ \begin{array}{c} X_1 \\ \vdots \\ X_N \\ \hdashline \alpha_1 \\ \vdots \\ \alpha_M \end{array} \right\} \qquad \text{(A.1)},$$

where X_j is the model state (ie. matric head or temperature) at node j and α_i is the ith model parameter requiring estimation by the filter. To take account of the augmentation of the state vector, the **A** matrix and **U** vector of the original Kalman-filter propagation equations given by (3.1) and (3.2) are replaced by $\underline{\mathbf{A}}$ and $\underline{\mathbf{U}}$ respectively, where

$$\underline{\mathbf{A}} = \left[\begin{array}{c:c} \mathbf{A} & \frac{\partial}{\partial \alpha}\left(\mathbf{A} \cdot \hat{\mathbf{X}} + \mathbf{U}\right) \\ \hdashline 0 & \mathbf{I} \end{array} \right] \qquad \text{(A.2)},$$

and

$$\underline{\mathbf{U}} = \left\{ \begin{array}{c} \mathbf{U} \\ \hdashline 0 \end{array} \right\} \qquad \text{(A.3)}.$$

The system noise covariance matrix **Q** in (3.2) is replaced by $\underline{\mathbf{Q}}$, where

$$\underline{\mathbf{Q}} = \left[\begin{array}{c:c} \mathbf{Q}_X & 0 \\ \hdashline 0 & \mathbf{Q}_\alpha \end{array}\right] \qquad \text{(A.4)},$$

with $\mathbf{Q}_X$ being the original system noise covariance matrix of the system states **Q**, and $\mathbf{Q}_\alpha$ being the system noise covariance matrix of the system parameters. Finally, the observation matrix **H** of the observation equation given by (3.3) is replaced by $\underline{\mathbf{H}}$, where

$$\underline{\mathbf{H}} = \left[\begin{array}{c:c} \mathbf{H} & \dfrac{\partial}{\partial \alpha}\left(\mathbf{H} \cdot \hat{\mathbf{X}}\right) \end{array}\right] \qquad \text{(A.5)}.$$

Thus, in order to estimate the model parameters using the state augmented Kalman filter, it is necessary to differentiate the model equations with respect to each of the model parameters. However, with the chosen format of the observation equation, the “observations” are independent of the model parameters and no extra work is required. Therefore the following sections present the necessary differentiations required to estimate the model parameters used in PROXSIM1D (Chapter 5) by the state augmented Kalman-filter.

A.1 DIFFERENTIATION OF MOISTURE EQUATION

The moisture equation used by PROXSIM1D is not a simple function of the model parameters. In fact it is a rather complex system, with many variables in the moisture equation being a complex function of the model parameters. Thus, evaluation of the derivates of the moisture equation can not be done directly, but require evaluation through the chain rule.

As the model has the option to use a combination of the Brooks and Corey (1966), Clapp and Hornberger (1978) and van Genuchten (1980) water retention and unsaturated hydraulic conductivity models, derivates with respect to model parameters had to be available that do not require evaluation unless a model option is chosen that requires that particular model parameter. The chain rules which require evaluation for the derivate of the moisture equation with respect to each of the model parameters are given below. The derivative with respect to porosity ϕ is

$$\frac{\partial \psi_j^{n+1}}{\partial \phi} = \frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n}\frac{\partial S_{w_j}^n}{\partial \phi} + \frac{\partial \psi_j^{n+1}}{\partial S_{0\psi_j}^n}\frac{\partial S_{0\psi_j}^n}{\partial \phi} + \frac{\partial \psi_j^{n+1}}{\partial C_{\psi_j}^n}\frac{\partial C_{\psi_j}^n}{\partial \phi} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial \phi} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \phi} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial \phi} \qquad \text{(A.6);}$$

with respect to saturated hydraulic conductivity K_s is

$$\frac{\partial \psi_j^{n+1}}{\partial K_s} = \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial K_s} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial K_s} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial K_s} \qquad \text{(A.7);}$$

with respect to residual soil moisture content θ_r is

$$\frac{\partial \psi_j^{n+1}}{\partial \theta_r} = \frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n}\frac{\partial S_{w_j}^n}{\partial \theta_r} + \frac{\partial \psi_j^{n+1}}{\partial C_{\psi_j}^n}\frac{\partial C_{\psi_j}^n}{\partial \theta_r} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial \theta_r} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \theta_r} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial \theta_r} \qquad \text{(A.8);}$$

with respect to the bubbling capillary pressure ψ_b is

$$\frac{\partial \psi_j^{n}}{\partial \psi_b} = \frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n}\frac{\partial S_{w_j}^n}{\partial \psi_b} + \frac{\partial \psi_j^{n}}{\partial C_{\psi_j}^n}\frac{\partial C_{\psi_j}^n}{\partial \psi_b} \qquad \text{(A.9);}$$

with respect to the saturated soil matric potential ψ_s is

$$\frac{\partial \psi_j^{n}}{\partial \psi_s} = \frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n}\frac{\partial S_{w_j}^n}{\partial \psi_s} + \frac{\partial \psi_j^{n}}{\partial C_{\psi_j}^n}\frac{\partial C_{\psi_j}^n}{\partial \psi_s} \qquad \text{(A.10);}$$

with respect to the van Genuchten soil texture parameter η is

$$\frac{\partial \psi_j^{n+1}}{\partial \eta} = \frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n}\frac{\partial S_{w_j}^n}{\partial \eta} + \frac{\partial \psi_j^{n+1}}{\partial C_{\psi_j}^n}\frac{\partial C_{\psi_j}^n}{\partial \eta} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial \eta} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \eta} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial \eta} \qquad \text{(A.11);}$$

with respect to the van Genuchten soil texture parameter *n* is

$$\frac{\partial \psi_j^{n+1}}{\partial n} = \frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n}\frac{\partial S_{w_j}^n}{\partial n} + \frac{\partial \psi_j^{n+1}}{\partial C_{\psi_j}^n}\frac{\partial C_{\psi_j}^n}{\partial n} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial n} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial n} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial n} \qquad \text{(A.12);}$$

with respect to the Clapp and Hornberger soil texture parameter *b* is

$$\frac{\partial \psi_j^{n+1}}{\partial b} = \frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n}\frac{\partial S_{w_j}^n}{\partial b} + \frac{\partial \psi_j^{n+1}}{\partial C_{\psi_j}^n}\frac{\partial C_{\psi_j}^n}{\partial b} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial b} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial b} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial b} \qquad \text{(A.13);}$$

with respect to the Brooks and Corey pore size distribution index φ is

$$\frac{\partial \psi_j^{n+1}}{\partial \varphi} = \frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n}\frac{\partial S_{w_j}^n}{\partial \varphi} + \frac{\partial \psi_j^{n+1}}{\partial C_{\psi_j}^n}\frac{\partial C_{\psi_j}^n}{\partial \varphi} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial \varphi} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \varphi} + \frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial \varphi} \qquad \text{(A.14);}$$

with respect to the volumetric proportion of quartz θ_3 is

$$\frac{\partial \psi_j^{n+1}}{\partial \theta_3} = 0 \qquad \text{(A.15);}$$

with respect to the volumetric proportion of other minerals θ_4 is

$$\frac{\partial \psi_j^{n+1}}{\partial \theta_4} = 0 \qquad \text{(A.16);}$$

and with respect to the volumetric proportion of organic matter θ_5 is

$$\frac{\partial \psi_j^{n+1}}{\partial \theta_5} = 0 \qquad \text{(A.17).}$$

A.1.1 DERIVATIVES OF MOISTURE EQUATION

The derivatives of the moisture equation which are required for evaluation of the chain rules at node j are given below. The derivative with respect to the water saturation ratio S_w at node j is

$$\frac{\partial \psi_j^{n+1}}{\partial S_{w_j}^n} = -\frac{S_{0\psi_j}^n \left(t^{n+1} - t^n\right)}{\left(S_{0\psi_j}^n S_{w_j}^n + C_{\psi_j}^n\right)^2 \left(z_{j-1} - z_{j+1}\right)} \cdot \begin{pmatrix} D_{\psi l_{j-1}}^n + \dfrac{\left(D_{\psi l_{j-1}}^n + D_{\psi l_j}^n\right)\left(\psi_{j-1}^n - \psi_j^n\right)}{\left(z_{j-1} - z_j\right)} \\ - D_{\psi l_{j+1}}^n - \dfrac{\left(D_{\psi l_j}^n + D_{\psi l_{j+1}}^n\right)\left(\psi_j^n - \psi_{j+1}^n\right)}{\left(z_j - z_{j+1}\right)} \end{pmatrix} \qquad \text{(A.18);}$$

with respect to the specific storativity $S_{0\psi}$ at node j is

$$\frac{\partial \psi_j^{n+1}}{\partial S_{0\psi_j}^n} = -\frac{S_{w_j}^n \left(t^{n+1} - t^n\right)}{\left(S_{0\psi_j}^n S_{w_j}^n + C_{\psi_j}^n\right)^2 \left(z_{j-1} - z_{j+1}\right)} \cdot \begin{pmatrix} D_{\psi l_{j-1}}^n + \dfrac{\left(D_{\psi l_{j-1}}^n + D_{\psi l_j}^n\right)\left(\psi_{j-1}^n - \psi_j^n\right)}{\left(z_{j-1} - z_j\right)} \\ - D_{\psi l_{j+1}}^n - \dfrac{\left(D_{\psi l_j}^n + D_{\psi l_{j+1}}^n\right)\left(\psi_j^n - \psi_{j+1}^n\right)}{\left(z_j - z_{j+1}\right)} \end{pmatrix} \qquad \text{(A.19);}$$

with respect to the capillary capacity factor C_ψ at node j is

$$\frac{\partial \psi_j^{n+1}}{\partial C_{\psi_j}^n} = -\frac{\left(t^{n+1} - t^n\right)}{\left(S_{0\psi_j}^n S_{w_j}^n + C_{\psi_j}^n\right)^2 \left(z_{j-1} - z_{j+1}\right)} \cdot \left(\begin{array}{l} D_{\psi l_{j-1}}^n + \dfrac{\left(D_{\psi l_{j-1}}^n + D_{\psi l_j}^n\right)\left(\psi_{j-1}^n - \psi_j^n\right)}{\left(z_{j-1} - z_j\right)} \\ - D_{\psi l_{j+1}}^n - \dfrac{\left(D_{\psi l_j}^n + D_{\psi l_V}^n\right)\left(\psi_j^n - \psi_{j+1}^n\right)}{\left(z_j - z_{j+1}\right)} \end{array} \right) \qquad \text{(A.20);}$$

with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node j–1 is

$$\frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j-1}}^n} = \frac{\left(t^{n+1} - t^n\right)\left(z_{j-1} - z_j + \psi_{j-1}^n - \psi_j^n\right)}{\left(S_{0\psi_j}^n S_{w_j}^n + C_{\psi_j}^n\right)\left(z_{j-1} - z_{j+1}\right)\left(z_{j-1} - z_j\right)} \qquad \text{(A.21);}$$

with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node j is

$$\frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_j}^n} = \frac{\left(t^{n+1} - t^n\right)}{\left(S_{0\psi_j}^n S_{w_j}^n + C_{\psi_j}^n\right)\left(z_{j-1} - z_{j+1}\right)} \cdot \left(\left(\frac{\psi_{j-1}^n - \psi_j^n}{z_{j-1} - z_j} \right) - \left(\frac{\psi_j^n - \psi_{j+1}^n}{z_j - z_{j+1}} \right) \right) \qquad \text{(A.22);}$$

and with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node j+1 is

$$\frac{\partial \psi_j^{n+1}}{\partial D_{\psi l_{j+1}}^n} = -\frac{\left(t^{n+1} - t^n\right)\left(z_j - z_{j+1} + \psi_j^n - \psi_{j+1}^n\right)}{\left(S_{0\psi_j}^n S_{w_j}^n + C_{\psi_j}^n\right)\left(z_{j-1} - z_{j+1}\right)\left(z_j - z_{j+1}\right)} \qquad \text{(A.23).}$$

In order to solve the partial differential equations which model the soil moisture transfer in the soil column, various boundary conditions can be applied, as outlined in section 5.1.1. Therefore, the derivatives of the moisture equation at the surface and bottom nodes depend on the boundary condition applied. If a Dirichlet boundary condition is applied, then the derivatives are zero, but if a Neumann boundary condition is applied, then the derivatives are as given below for the boundary nodes. The derivative with respect to the water saturation ratio S_w at node 2 is

$$\frac{\partial \psi_1^{n+1}}{\partial S_{w_2}^n} = \frac{\partial \psi_2^{n+1}}{\partial S_{w_2}^n} \tag{A.24a}$$,

and at node N–1 is

$$\frac{\partial \psi_N^{n+1}}{\partial S_{w_{N-1}}^n} = \frac{\partial \psi_{N-1}^{n+1}}{\partial S_{w_{N-1}}^n} \tag{A.24b}$$;

with respect to the specific storativity $S_{0\psi}$ at node 2 is

$$\frac{\partial \psi_1^{n+1}}{\partial S_{0\psi_2}^n} = \frac{\partial \psi_2^{n+1}}{\partial S_{0\psi_2}^n} \tag{A.25a}$$,

and at node N–1 is

$$\frac{\partial \psi_N^{n+1}}{\partial S_{0\psi_{N-1}}^n} = \frac{\partial \psi_{N-1}^{n+1}}{\partial S_{0\psi_{N-1}}^n} \tag{A.25b}$$;

with respect to the capillary capacity factor C_ψ at node 2 is

$$\frac{\partial \psi_1^{n+1}}{\partial C_{\psi_2}^n} = \frac{\partial \psi_2^{n+1}}{\partial C_{\psi_2}^n} \tag{A.26a}$$,

and at node N–1 is

$$\frac{\partial \psi_N^{n+1}}{\partial C_{\psi_{N-1}}^n} = \frac{\partial \psi_{N-1}^{n+1}}{\partial C_{\psi_{N-1}}^n} \tag{A.26b}$$;

with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node 1 is

$$\frac{\partial \psi_1^{n+1}}{\partial D_{\psi l_1}^n} = \frac{\partial \psi_2^{n+1}}{\partial D_{\psi l_1}^n} + \frac{2Q_{top}^{\psi}(z_1 - z_2)}{\left(D_{\psi l_1}^n + D_{\psi l_2}^n\right)^2} \tag{A.27a}$$,

and at node N–2 is

$$\frac{\partial \psi_N^{n+1}}{\partial D_{\psi l_{N-2}}^n} = \frac{\partial \psi_{N-1}^{n+1}}{\partial D_{\psi l_{N-2}}^n} \qquad \text{(A.27b);}$$

with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node 2 is

$$\frac{\partial \psi_1^{n+1}}{\partial D_{\psi l_2}^n} = \frac{\partial \psi_2^{n+1}}{\partial D_{\psi l_2}^n} + \frac{2Q_{top}^{\psi}(z_1 - z_2)}{\left(D_{\psi l_1}^n + D_{\psi l_2}^n\right)^2} \qquad \text{(A.28a),}$$

and at node N–1 is

$$\frac{\partial \psi_N^{n+1}}{\partial D_{\psi l_{N-1}}^n} = \frac{\partial \psi_{N-1}^{n+1}}{\partial D_{\psi l_{N-1}}^n} - \frac{2Q_{bot}^{\psi}(z_{N-1} - z_N)}{\left(D_{\psi l_{N-1}}^n + D_{\psi l_N}^n\right)^2} \qquad \text{(A.28b);}$$

and with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node 3 is

$$\frac{\partial \psi_1^{n+1}}{\partial D_{\psi l_3}^n} = \frac{\partial \psi_2^{n+1}}{\partial D_{\psi l_3}^n} \qquad \text{(A.29a),}$$

and at node N is

$$\frac{\partial \psi_N^{n+1}}{\partial D_{\psi l_N}^n} = \frac{\partial \psi_{N-1}^{n+1}}{\partial D_{\psi l_N}^n} - \frac{2Q_{bot}^{\psi}(z_{N-1} - z_N)}{\left(D_{\psi l_{N-1}}^n + D_{\psi l_N}^n\right)^2} \qquad \text{(A.29b).}$$

A.1.2 DERIVATIVES OF CONSTITUTIVE RELATIONS

In this section, the derivatives of the constitutive relations that are required for evaluation of the chain rules at node j are given. The derivative of the water saturation ratio S_w at node j with respect the porosity ϕ is

$$\frac{\partial S_w}{\partial \phi} = -\frac{\theta_l}{\phi^2} + \frac{1}{\phi}\frac{\partial \theta_l}{\partial \phi} \qquad \text{(A.30);}$$

with respect to the residual soil moisture θ_r is

$$\frac{\partial S_w}{\partial \theta_r} = \frac{1}{\phi}\frac{\partial \theta_l}{\partial \theta_r} \qquad \text{(A.31);}$$

with respect to the saturated soil matric potential ψ_s is

$$\frac{\partial S_w}{\partial \psi_s} = \frac{1}{\phi}\frac{\partial \theta_l}{\partial \psi_s} \qquad \text{(A.32);}$$

with respect to the bubbling capillary pressure ψ_b is

$$\frac{\partial S_w}{\partial \psi_b} = \frac{1}{\phi}\frac{\partial \theta_l}{\partial \psi_b} \qquad \text{(A.33);}$$

with respect to the van Genuchten soil texture parameter η is

$$\frac{\partial S_w}{\partial \eta} = \frac{1}{\phi}\frac{\partial \theta_l}{\partial \eta} \qquad \text{(A.34);}$$

with respect to the van Genuchten soil texture parameter n is

$$\frac{\partial S_w}{\partial n} = \frac{1}{\phi}\frac{\partial \theta_l}{\partial n} \qquad \text{(A.35);}$$

with respect to the Clapp and Hornberger soil texture parameter b is

$$\frac{\partial S_w}{\partial b} = \frac{1}{\phi}\frac{\partial \theta_l}{\partial b} \qquad \text{(A.36);}$$

and with respect to the Brooks and Corey pore size distribution index φ is

$$\frac{\partial S_w}{\partial \varphi} = \frac{1}{\phi}\frac{\partial \theta_l}{\partial \varphi} \qquad \text{(A.37).}$$

The derivative of the specific storativity $S_{0\psi}$ with respect to its only dependent parameter ϕ is

$$\frac{\partial S_{0\psi}}{\partial \phi} = -\alpha + \beta \qquad \text{(A.38).}$$

A.1.2.1 Volumetric Liquid Water Content

In this section, the derivatives of the volumetric liquid water content θ_l with respect to each of the dependent soil parameters are given for the three models described in section 5.2.1, being the Brooks and Corey (1966), Clapp and Hornberger (1978) and van Genuchten (1980).

A.1.2.1.1 Brooks and Corey

The derivative of the volumetric liquid water content as given by the Brooks and Corey (1966) model at node j with respect to porosity ϕ is

$$\frac{\partial \theta_l}{\partial \phi} = \left(\frac{\psi_b}{\psi}\right)^{\varphi} \qquad \psi \le \psi_b \qquad \text{(A.39a)}$$

$$\frac{\partial \theta_l}{\partial \phi} = 1 \qquad \psi > \psi_b \qquad \text{(A.39b);}$$

with respect to the residual soil moisture θ_r is

$$\frac{\partial \theta_l}{\partial \theta_r} = 1 - \left(\frac{\psi_b}{\psi}\right)^{\varphi} \qquad \psi \le \psi_b \qquad \text{(A.40a)}$$

$$\frac{\partial \theta_l}{\partial \theta_r} = 0 \qquad \psi > \psi_b \qquad \text{(A.40b);}$$

with respect to the bubbling capillary pressure ψ_b is

$$\frac{\partial \theta_l}{\partial \psi_b} = \frac{\varphi(\phi - \theta_r)}{\psi_b}\left(\frac{\psi_b}{\psi}\right)^{\varphi} \qquad \psi \leq \psi_b \qquad \text{(A.41a)}$$

$$\frac{\partial \theta_l}{\partial \psi_b} = 0 \qquad \psi > \psi_b \qquad \text{(A.41b);}$$

and with respect to the Brooks and Corey pore size distribution index φ is

$$\frac{\partial \theta_l}{\partial \varphi} = (\phi - \theta_r)\left(\frac{\psi_b}{\psi}\right)^{\varphi} \log_e\left(\frac{\psi_b}{\psi}\right) \qquad \psi \leq \psi_b \qquad \text{(A.42a)}$$

$$\frac{\partial \theta_l}{\partial \varphi} = 0 \qquad \psi > \psi_b \qquad \text{(A.42b).}$$

A.1.2.1.2 Clapp and Hornberger

The derivative of the volumetric liquid water content as given by the Clapp and Hornberger (1978) model at node j with respect to the porosity ϕ is

$$\frac{\partial \theta_l}{\partial \phi} = \left(\frac{\psi_s}{\psi}\right)^{\frac{1}{b}} \qquad W \leq W_i \qquad \text{(A.43a)}$$

$$\frac{\partial \theta_l}{\partial \phi} = -\frac{\theta_l}{\phi} \qquad W_i < W < 1 \qquad \text{(A.43b)}$$

$$\frac{\partial \theta_l}{\partial \phi} = 1 \qquad W = 1 \qquad \text{(A.43c);}$$

with respect to the saturated soil matric potential ψ_s is

$$\frac{\partial\theta_l}{\partial\psi_s} = \frac{\phi}{b\psi_s}\left(\frac{\psi_s}{\psi}\right)^{\frac{1}{b}} \qquad W \le W_i \qquad \text{(A.44a)}$$

$$\frac{\partial\theta_l}{\partial\psi_s} = 0 \qquad W_i < W \qquad \text{(A.44b);}$$

and with respect to the Clapp and Hornberger soil texture parameter b is

$$\frac{\partial\theta_l}{\partial b} = -\frac{\phi}{b^2}\left(\frac{\psi_s}{\psi}\right)^{\frac{1}{b}} \log_e\left(\frac{\psi_s}{\psi}\right) \qquad W \le W_i \qquad \text{(A.45a)}$$

$$\frac{\partial\theta_l}{\partial b} = \frac{(W_i - 1)(\theta_l - \phi)(\phi W_i - \theta_l)}{\left(\begin{array}{l} 2W_i(\phi W_i - \theta_l) + \\ b(W_i - 1)(\phi + \phi W_i - 2\theta_l) \end{array}\right)} \qquad W_i < W < 1 \qquad \text{(A.45b)}$$

$$\frac{\partial\theta_l}{\partial b} = 0 \qquad W = 1 \qquad \text{(A.45c).}$$

A.1.2.1.3 Van Genuchten

The derivative of the volumetric liquid water content as given by the van Genuchten (1980) model at node j with respect to the porosity ϕ is

$$\frac{\partial\theta_l}{\partial\phi} = \Theta \qquad \psi < 0 \qquad \text{(A.46a)}$$

$$\frac{\partial\theta_l}{\partial\phi} = 1 \qquad \psi \ge 0 \qquad \text{(A.46b);}$$

with respect to the residual soil moisture θ_r is

$$\frac{\partial\theta_l}{\partial\theta_r} = 1 - \Theta \qquad \psi < 0 \qquad \text{(A.47a)}$$

$$\frac{\partial\theta_l}{\partial\theta_r} = 0 \qquad \psi \ge 0 \qquad \text{(A.47b);}$$

with respect to the van Genuchten soil texture parameter η is

$$\frac{\partial\theta_l}{\partial\eta} = \frac{m\,n(\theta_r - \phi)(-\eta\psi)^n}{\eta} \cdot \left(\frac{1}{1+(-\eta\psi)^n}\right)^{1+m} \qquad \psi < 0 \qquad \text{(A.48a)}$$

$$\frac{\partial\theta_l}{\partial\eta} = 0 \qquad \psi \geq 0 \qquad \text{(A.48b);}$$

and with respect to the van Genuchten soil texture parameter *n* is

$$\frac{\partial\theta_l}{\partial n} = (\phi - \theta_r)\left(\begin{array}{l} \dfrac{\Theta}{n^2}\log_e\left(\dfrac{1}{1+(-\eta\psi)^n}\right) - \\ \dfrac{m(-\eta\psi)^n \log_e(-\eta\psi)}{\left(1+(-\eta\psi)^n\right)^2} \\ \cdot\left(\dfrac{1}{1+(-\eta\psi)^n}\right)^{-\frac{1}{n}} \end{array}\right) \qquad \psi < 0 \qquad \text{(A.49a)}$$

$$\frac{\partial\theta_l}{\partial n} = 0 \qquad \psi \geq 0 \qquad \text{(A.49b).}$$

A.1.2.2 Capillary Capacity Relationship

In this section, the derivatives of the capillary capacity C_ψ with respect to each of the dependent soil parameters are given for the three models described previously.

A.1.2.2.1 Brooks and Corey

The derivative of the unsaturated capillary capacity as given by the Brooks and Corey (1966) model at node *j* with respect to the porosity ϕ is

$$\frac{\partial C_\psi}{\partial\phi} = -\frac{\varphi}{\psi}\left(\frac{\psi_b}{\psi}\right)^{\varphi} \qquad \psi \leq \psi_b \qquad \text{(A.50a)}$$

$$\frac{\partial C_\psi}{\partial\phi} = 0 \qquad \psi > \psi_b \qquad \text{(A.50b);}$$

with respect to the residual soil moisture θ_r is

$$\frac{\partial C_\psi}{\partial \theta_r} = \frac{\varphi}{\psi}\left(\frac{\psi_b}{\psi}\right)^{\varphi} \qquad \psi \le \psi_b \qquad \text{(A.51a)}$$

$$\frac{\partial C_\psi}{\partial \theta_r} = 0 \qquad \psi > \psi_b \qquad \text{(A.51b);}$$

with respect to the bubbling capillary pressure ψ_b is

$$\frac{\partial C_\psi}{\partial \psi_b} = \frac{\varphi^2\left(\theta_r - \phi\right)}{\psi^2}\left(\frac{\psi_b}{\psi}\right)^{(\varphi-1)} \qquad \psi \le \psi_b \qquad \text{(A.52a)}$$

$$\frac{\partial C_\psi}{\partial \psi_b} = 0 \qquad \psi > \psi_b \qquad \text{(A.52b);}$$

and with respect to the Brooks and Corey pore size distribution index φ is

$$\frac{\partial C_\psi}{\partial \varphi} = \frac{\left(\theta_r - \phi\right)}{\psi}\left(\frac{\psi_b}{\psi}\right)^{\varphi}\left(1 + \varphi \log_e\left(\frac{\psi_b}{\psi}\right)\right) \qquad \psi \le \psi_b \qquad \text{(A.53a)}$$

$$\frac{\partial C_\psi}{\partial \varphi} = 0 \qquad \psi > \psi_b \qquad \text{(A.53b).}$$

A.1.2.2.2 Clapp and Hornberger

The derivative of the unsaturated capillary capacity as given by the Clapp and Hornberger (1978) model at node j with respect to the porosity ϕ is

$$\frac{\partial C_\psi}{\partial \phi} = -\frac{1}{b\psi}\left(\frac{\psi}{\psi_s}\right)^{-\frac{1}{b}} \qquad W \le W_i \qquad \text{(A.54a)}$$

$$\frac{\partial C_\psi}{\partial \phi} = \frac{\phi(\phi - 6\theta + n_w \phi)}{m_w(\phi - 2\theta + n_w \phi)^2} \qquad W_i < W < 1 \qquad \text{(A.54b)}$$

$$\frac{\partial C_\psi}{\partial \phi} = 0 \qquad W = 1 \qquad \text{(A.54c);}$$

with respect to the saturated soil matric potential ψ_s is

$$\frac{\partial C_\psi}{\partial \psi_s} = -\frac{\phi}{b^2 \psi_s^2}\left(\frac{\psi}{\psi_s}\right)^{\left(-\frac{1+b}{b}\right)} \qquad W \le W_i \qquad \text{(A.55a)}$$

$$\frac{\partial C_\psi}{\partial \psi_s} = 0 \qquad W_i < W \qquad \text{(A.55b);}$$

and with respect to the Clapp and Hornberger soil texture parameter b is

$$\frac{\partial C_\psi}{\partial b} = \frac{\phi}{b^3 \psi}\left(\frac{\psi}{\psi_s}\right)^{-\frac{1}{b}}\left(b - \log_e\left(\frac{\psi}{\psi_s}\right)\right) \qquad W \le W_i \qquad \text{(A.56a)}$$

$$\begin{aligned}\frac{\partial C_\psi}{\partial b} = & \frac{2\phi^2 (W_i - 1)(\theta_l - \phi)(W_i \phi - \theta_l)}{\left[\begin{array}{l} m_w(\phi - 2\theta_l + n_w \phi)^2 \\ \left(\begin{array}{l} 2W_i(W_i\phi - \theta_l) + \\ b(W_i - 1)(\phi - 2\theta_l + W_i\phi) \end{array}\right) \end{array}\right]} \\ & - \frac{W_i \phi^2 (W_i - 1)^3 (\phi - 2\theta_l + W_i \phi)}{\psi_i \left(\begin{array}{l} 2W_i(W_i\phi - \theta_l) + \\ b(W_i - 1)(\phi - 2\theta_l + W_i\phi) \end{array}\right)^2}\end{aligned} \qquad W_i < W < 1 \qquad \text{(A.56b)}$$

$$\frac{\partial C_\psi}{\partial b} = 0 \qquad W = 1 \qquad \text{(A.56c).}$$

A.1.2.2.3 Van Genuchten

The derivative of the unsaturated capillary capacity as given by the van Genuchten (1980) model at node *j* with respect to the porosity ϕ is

$$\frac{\partial C_\psi}{\partial \phi} = \frac{\eta}{m-1}\Theta^{\frac{1}{m}}\left(1-\Theta^{\frac{1}{m}}\right)^m \cdot \left(\frac{m-1+\Theta^{\frac{1}{m}}}{\Theta^{\frac{1}{m}}-1} - \frac{\Theta\left(1+\frac{m\Theta^{\frac{1}{m}}}{\Theta^{\frac{1}{m}}-1}\right)(\phi-\theta_r)}{\theta_l-\theta_r} \right) \qquad \psi < 0 \qquad \text{(A.57a)}$$

$$\frac{\partial C_\psi}{\partial \phi} = 0 \qquad \psi \geq 0 \qquad \text{(A.57b);}$$

with respect to the residual soil moisture θ_r is

$$\frac{\partial C_\psi}{\partial \theta_r} = \frac{1}{(m-1)(\theta-\theta_r)} \cdot \left(\eta\Theta^{\frac{1}{m}}\left(1-\Theta^{\frac{1}{m}}\right)^{m-1} \cdot \left(\theta_l\left(m-1+\Theta^{\frac{1}{m}}\right) + \theta_r\left(m-1-\Theta+\Theta^{1+\frac{1}{m}} + m\Theta^{1+\frac{1}{m}} - \Theta^{\frac{1}{m}}\right) - \phi\Theta\left(\Theta^{\frac{1}{m}}-1+m\Theta^{\frac{1}{m}}\right) \right) \right) \qquad \psi < 0 \qquad \text{(A.58a)}$$

$$\frac{\partial C_\psi}{\partial \theta_r} = 0 \qquad \psi \geq 0 \qquad \text{(A.58b);}$$

with respect to the van Genuchten soil texture parameter η is

$$\frac{\partial C_\psi}{\partial \eta} = \frac{m}{m-1}\Theta^{\frac{1}{m}}\left(1-\Theta^{\frac{1}{m}}\right)^{m}\left(\theta_r - \phi\right)\cdot \left(\begin{array}{l} 1-\left(\dfrac{n\left(\phi-\theta_r\right)\left(-\eta\psi\right)^n}{\theta_l-\theta_r}\right)\cdot \\ \left(\left(1+\dfrac{m\Theta^{\frac{1}{m}}}{\Theta^{\frac{1}{m}}-1}\right)\left(\dfrac{1}{1+\left(-\eta\psi\right)^n}\right)^{1+m}\right)\end{array}\right) \qquad \psi < 0 \qquad \text{(A.59a)}$$

$$\frac{\partial C_\psi}{\partial \eta} = 0 \qquad \psi \geq 0 \qquad \text{(A.59b);}$$

and with respect to the van Genuchten soil texture parameter n is

$$\frac{\partial C_\psi}{\partial n} = \eta\Theta^{\frac{1}{m}}\left(\begin{array}{l} \dfrac{1}{n^2(n-1)}\left(\begin{array}{l}\left(1-\Theta^{\frac{1}{m}}\right)^{-\frac{1}{n}}\left(\theta_r-\phi\right)\cdot \\ \left(\begin{array}{l}(n-1)^2\left(\Theta^{\frac{1}{m}}-1\right)\log_e\left(1-\Theta^{\frac{1}{m}}\right)+ \\ n\left(\begin{array}{l} n(n-1)\left(\Theta^{\frac{1}{m}}-1\right)+ \\ \left(n+\Theta^{\frac{1}{m}}-2n\Theta^{\frac{1}{m}}\right)\log_e\Theta\end{array}\right)\end{array}\right)\end{array}\right) \\ -\dfrac{1}{(m-1)(\theta_l-\theta_r)}\cdot \\ \left(\begin{array}{l}(\theta_r-\phi)^2\left(1-\Theta^{\frac{1}{m}}\right)^m\left(1+\dfrac{m\Theta^{\frac{1}{m}}}{\Theta^{\frac{1}{m}}-1}\right)\cdot \\ \left(\begin{array}{l}\dfrac{\Theta\log_e}{n^2}\left(\dfrac{1}{1+(-\eta\psi)^n}\right)- \\ \dfrac{m(-\eta\psi)^n\log_e(-\eta\psi)}{\left(1+(-\eta\psi)^n\right)^2}\left(\dfrac{1}{1+(-\eta\psi)^n}\right)^{-\frac{1}{n}}\end{array}\right)\end{array}\right)\end{array}\right) \qquad \psi < 0 \qquad \text{(A.60a)}$$

$$\frac{\partial C_\psi}{\partial n} = 0 \qquad \psi \geq 0 \qquad \text{(A.60b).}$$

A.1.2.3 Isothermal Liquid Hydraulic Conductivity

In this section, the derivatives of the isothermal liquid hydraulic conductivity with respect to each of the dependent soil parameters are given for the three models described previously.

A.1.2.3.1 Brooks and Corey

The derivative of the isothermal liquid hydraulic conductivity as given by the Brooks and Corey (1966) model at node j with respect to the porosity ϕ is

$$\frac{\partial D_{\psi l}}{\partial \phi} = -\frac{cK_s}{(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^c + \frac{K_s(2+3\varphi)}{\varphi(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{c-1}\frac{\partial \theta_l}{\partial \phi} \qquad \text{(A.61);}$$

with respect to the saturated hydraulic conductivity K_s is

$$\frac{\partial D_{\psi l}}{\partial K_s} = \left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^c \qquad \text{(A.62);}$$

with respect to the residual soil moisture θ_r is

$$\frac{\partial D_{\psi l}}{\partial \theta_r} = \frac{cK_s(\theta_l-\phi)}{(\phi-\theta_r)(\theta_l-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^c + \frac{K_s(2+3\varphi)}{\varphi(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{c-1}\frac{\partial \theta_l}{\partial \theta_r} \qquad \text{(A.63);}$$

with respect to the bubbling capillary pressure ψ_b is

$$\frac{\partial D_{\psi l}}{\partial \psi_b} = \frac{K_s(2+3\varphi)}{\varphi(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{c-1}\frac{\partial \theta_l}{\partial \psi_b} \qquad \text{(A.64);}$$

with respect to the saturated soil matric potential ψ_s is

$$\frac{\partial D_{\psi l}}{\partial \psi_s} = \frac{K_s(2+3\varphi)}{\varphi(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{c-1}\frac{\partial \theta_l}{\partial \psi_s} \qquad \text{(A.65);}$$

with respect to the van Genuchten soil texture parameter η is

$$\frac{\partial D_{\psi l}}{\partial \eta} = \frac{K_s(2+3\varphi)}{\varphi(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{c-1}\frac{\partial \theta_l}{\partial \eta} \qquad \text{(A.66);}$$

with respect to the van Genuchten soil texture parameter n is

$$\frac{\partial D_{\psi l}}{\partial n} = \frac{K_s(2+3\varphi)}{\varphi(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{c-1}\frac{\partial \theta_l}{\partial n} \qquad \text{(A.67);}$$

with respect to the Clapp and Hornberger soil texture parameter b is

$$\frac{\partial D_{\psi l}}{\partial b} = \frac{K_s(2+3\varphi)}{\varphi(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{c-1}\frac{\partial \theta_l}{\partial b} \qquad \text{(A.68);}$$

and with respect to the Brooks and Corey pore size distribution index φ is

$$\begin{aligned}\frac{\partial D_{\psi l}}{\partial \varphi} = &-\frac{2K_s(\theta_l-\theta_r)^3}{\varphi^2(\phi-\theta_r)^3}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{\frac{2}{\varphi}}\log_e\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right) \\ &+\frac{K_s(2+3\varphi)}{\varphi(\phi-\theta_r)}\left(\frac{\theta_l-\theta_r}{\phi-\theta_r}\right)^{c-1}\frac{\partial \theta_l}{\partial \varphi}\end{aligned} \qquad \text{(A.69).}$$

A.1.2.3.2 Clapp and Hornberger

The derivative of the isothermal liquid hydraulic conductivity as given by the Clapp and Hornberger (1978) model at node j with respect to the porosity ϕ is

$$\frac{\partial D_{\psi l}}{\partial \phi} = -\frac{K_s\theta_l^3(3+2b)}{\phi^4}\left(\frac{\theta_l}{\phi}\right)^{2b} + \frac{K_s(3+2b)}{\phi}\left(\frac{\theta_l}{\phi}\right)^{2+2b}\frac{\partial \theta_l}{\partial \phi} \qquad \text{(A.70);}$$

with respect to the saturated hydraulic conductivity K_s is

$$\frac{\partial D_{\psi l}}{\partial K_s} = \left(\frac{\theta_l}{\phi}\right)^{3+2b} \quad \text{(A.71);}$$

with respect to the residual soil moisture θ_r is

$$\frac{\partial D_{\psi l}}{\partial \theta_r} = \frac{K_s(3+2b)}{\phi}\left(\frac{\theta_l}{\phi}\right)^{2+2b} \frac{\partial \theta_l}{\partial \theta_r} \quad \text{(A.72);}$$

with respect to the bubbling capillary pressure ψ_b is

$$\frac{\partial D_{\psi l}}{\partial \psi_b} = \frac{K_s(3+2b)}{\phi}\left(\frac{\theta_l}{\phi}\right)^{2+2b} \frac{\partial \theta_l}{\partial \psi_b} \quad \text{(A.73);}$$

with respect to the saturated soil matric potential ψ_s is

$$\frac{\partial D_{\psi l}}{\partial \psi_s} = \frac{K_s(3+2b)}{\phi}\left(\frac{\theta_l}{\phi}\right)^{2+2b} \frac{\partial \theta_l}{\partial \psi_s} \quad \text{(A.74);}$$

with respect to the van Genuchten soil texture parameter η is

$$\frac{\partial D_{\psi l}}{\partial \eta} = \frac{K_s(3+2b)}{\phi}\left(\frac{\theta_l}{\phi}\right)^{2+2b} \frac{\partial \theta_l}{\partial \eta} \quad \text{(A.75);}$$

with respect to the van Genuchten soil texture parameter n is

$$\frac{\partial D_{\psi l}}{\partial n} = \frac{K_s(3+2b)}{\phi}\left(\frac{\theta_l}{\phi}\right)^{2+2b} \frac{\partial \theta_l}{\partial n} \quad \text{(A.76);}$$

with respect to the Clapp and Hornberger soil texture parameter b is

$$\frac{\partial D_{\psi l}}{\partial b} = 2K_s \left(\frac{\theta_l}{\phi}\right)^{3+2b} \log_e \left(\frac{\theta_l}{\phi}\right) + \frac{K_s(3+2b)}{\phi}\left(\frac{\theta_l}{\phi}\right)^{2+2b} \frac{\partial \theta_l}{\partial b} \quad \text{(A.77);}$$

and with respect to the Brooks and Corey pore size distribution index φ is

$$\frac{\partial D_{\psi l}}{\partial \varphi} = \frac{K_s(3+2b)}{\phi}\left(\frac{\theta_l}{\phi}\right)^{2+2b} \frac{\partial \theta_l}{\partial \varphi} \qquad \text{(A.78).}$$

A.1.2.3.3 Van Genuchten

The derivative of the isothermal liquid hydraulic conductivity as given by the van Genuchten (1980) model at node j with respect to the saturated hydraulic conductivity K_s is

$$\frac{\partial D_{\psi l}}{\partial K_s} = \frac{\left(1 - (-\eta\psi)^{n-1}\left(1 + (-\eta\psi)^n\right)^{-m}\right)^2}{\left(1 + (-\eta\psi)^n\right)^{\frac{m}{2}}} \qquad \psi < 0 \qquad \text{(A.79a)}$$

$$\frac{\partial D_{\psi l}}{\partial K_s} = 1 \qquad \psi \geq 0 \qquad \text{(A.79b);}$$

with respect to the van Genuchten soil texture parameter η is

$$\frac{\partial D_{\psi l}}{\partial \eta} = -\frac{1}{2\eta^3\psi^2}\left(\begin{array}{l} \dfrac{K_s(-\eta\psi)^n}{\left(1+(-\eta\psi)^n\right)^{1+\frac{5m}{2}}} \cdot \\ \left((-\eta\psi)^n + \eta\psi\left(1+(-\eta\psi)^n\right)^m\right) \cdot \\ \left(\begin{array}{l} 4\left(1+(-\eta\psi)^n\right) + \\ n\left(\begin{array}{l} 5m(-\eta\psi)^n - 4(-\eta\psi)^n \\ + m\eta\psi\left(1+(-\eta\psi)^n\right)^m - 4 \end{array}\right) \end{array}\right) \end{array}\right) \qquad \psi < 0 \qquad \text{(A.80a)}$$

$$\frac{\partial D_{\psi l}}{\partial \eta} = 0 \qquad \psi \geq 0 \qquad \text{(A.80b);}$$

and with respect to the van Genuchten soil texture parameter n is

$$\frac{\partial D_{\psi l}}{\partial n} = -\frac{1}{2n^2\eta^2\psi^2}\left(\begin{array}{l} K_s\left(1+(-\eta\psi)^n\right)^{\frac{1}{2}\left(\frac{1}{n}-7\right)}\left(\begin{array}{l} \eta\psi\left(1+(-\eta\psi)^n\right)+ \\ (-\eta\psi)^n\left(1+(-\eta\psi)^n\right)^{\frac{1}{n}} \end{array} \right) \\ \cdot\left(\begin{array}{l} n(-\eta\psi)^n\left(\begin{array}{l} \eta\psi(n-1)\left(1+(-\eta\psi)^n\right) \\ +\left(1+(-\eta\psi)^n\right)^{\frac{1}{n}}\cdot \\ \left(n(-\eta\psi)^n-5(-\eta\psi)^n-4n\right) \end{array} \right) \\ \cdot\log_e(-\eta\psi)+ \\ \left(1+(-\eta\psi)^n\right)\left(\begin{array}{l} \eta\psi\left(1+(-\eta\psi)^n\right)+ \\ 5(-\eta\psi)^n\left(1+(-\eta\psi)^n\right)^{\frac{1}{n}} \end{array} \right) \\ \cdot\log_e\left(1+(-\eta\psi)^n\right) \end{array} \right) \end{array} \right) \qquad \psi < 0 \qquad \text{(A.81a)}$$

$$\frac{\partial D_{\psi l}}{\partial n} = 0 \qquad \psi \geq 0 \qquad \text{(A.81b).}$$

A.2 DIFFERENTIATION OF TEMPERATURE EQUATION

As with the moisture equation, the temperature equation used by PROXSIM1D is a rather complex system with many variables in the temperature equation being a complex function of the model parameters. Thus, evaluation of the derivates of the temperature equation can not be done directly, but require evaluation through the chain rule. The chain rules which require evaluation for the derivate of the temperature equation with respect to each of the model parameters are given below. The derivative with respect to porosity ϕ is

$$
\begin{aligned}
\frac{\partial T_j^{n+1}}{\partial \phi} = {} & \frac{\partial T_j^{n+1}}{\partial C_{T_j}^n}\frac{\partial C_{T_j}^n}{\partial \phi} + \frac{\partial T_j^{n+1}}{\partial \lambda_{j-1}^n}\frac{\partial \lambda_{j-1}^n}{\partial \phi} + \frac{\partial T_j^{n+1}}{\partial \lambda_j^n}\frac{\partial \lambda_j^n}{\partial \phi} + \frac{\partial T_j^{n+1}}{\partial \lambda_{j+1}^n}\frac{\partial \lambda_{j+1}^n}{\partial \phi} \\
& + \frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j-1}}^n}\left(\frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_{j-2}}^n}\frac{\partial D_{\psi l_{j-2}}^n}{\partial \phi} + \frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial \phi} + \frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \phi}\right) \\
& + \frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j+1}}^n}\left(\frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \phi} + \frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial \phi} + \frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_{j+2}}^n}\frac{\partial D_{\psi l_{j+2}}^n}{\partial \phi}\right) \\
& + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n}\frac{\partial \theta_{l_j}^n}{\partial \phi} + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}}\frac{\partial \theta_{l_j}^{n-1}}{\partial \phi}
\end{aligned}
\quad \text{(A.82);}
$$

with respect to saturated hydraulic conductivity K_s is

$$
\begin{aligned}
\frac{\partial T_j^{n+1}}{\partial K_s} = {} & \frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j-1}}^n}\left(\frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_{j-2}}^n}\frac{\partial D_{\psi l_{j-2}}^n}{\partial K_s} + \frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial K_s} + \frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial K_s}\right) \\
& + \frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j+1}}^n}\left(\frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial K_s} + \frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial K_s} + \frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_{j+2}}^n}\frac{\partial D_{\psi l_{j+2}}^n}{\partial K_s}\right)
\end{aligned}
\quad \text{(A.83);}
$$

with respect to residual soil moisture content θ_r is

$$
\begin{aligned}
\frac{\partial T_j^{n+1}}{\partial \theta_r} = {} & \frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j-1}}^n}\left(\frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_{j-2}}^n}\frac{\partial D_{\psi l_{j-2}}^n}{\partial \theta_r} + \frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial \theta_r} + \frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \theta_r}\right) \\
& + \frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j+1}}^n}\left(\frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \theta_r} + \frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial \theta_r} + \frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_{j+2}}^n}\frac{\partial D_{\psi l_{j+2}}^n}{\partial \theta_r}\right) \\
& + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n}\frac{\partial \theta_{l_j}^n}{\partial \theta_r} + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}}\frac{\partial \theta_{l_j}^{n-1}}{\partial \theta_r}
\end{aligned}
\quad \text{(A.84);}
$$

with respect to the bubbling capillary pressure ψ_b is

$$
\frac{\partial T_j^{n+1}}{\partial \psi_b} = \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n}\frac{\partial \theta_{l_j}^n}{\partial \psi_b} + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}}\frac{\partial \theta_{l_j}^{n-1}}{\partial \psi_b} \quad \text{(A.85);}
$$

with respect to the saturated soil matric potential ψ_s is

$$\frac{\partial T_j^{n+1}}{\partial \psi_s} = \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n} \frac{\partial \theta_{l_j}^n}{\partial \psi_s} + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}} \frac{\partial \theta_{l_j}^{n-1}}{\partial \psi_s} \tag{A.86}$$

with respect to the van Genuchten soil texture parameter η is

$$\begin{aligned}\frac{\partial T_j^{n+1}}{\partial \eta} = {} & \frac{\partial T_j^{n+1}}{\partial q_{l_{j-1}}^n} \left(\frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_{j-2}}^n} \frac{\partial D_{\psi l_{j-2}}^n}{\partial \eta} + \frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_{j-1}}^n} \frac{\partial D_{\psi l_{j-1}}^n}{\partial \eta} + \frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_j}^n} \frac{\partial D_{\psi l_j}^n}{\partial \eta} \right) \\ & + \frac{\partial T_j^{n+1}}{\partial q_{l_{j+1}}^n} \left(\frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_j}^n} \frac{\partial D_{\psi l_j}^n}{\partial \eta} + \frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_{j+1}}^n} \frac{\partial D_{\psi l_{j+1}}^n}{\partial \eta} + \frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_{j+2}}^n} \frac{\partial D_{\psi l_{j+2}}^n}{\partial \eta} \right) \\ & + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n} \frac{\partial \theta_{l_j}^n}{\partial \eta} + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}} \frac{\partial \theta_{l_j}^{n-1}}{\partial \eta}\end{aligned} \tag{A.87}$$

with respect to the van Genuchten soil texture parameter n is

$$\begin{aligned}\frac{\partial T_j^{n+1}}{\partial n} = {} & \frac{\partial T_j^{n+1}}{\partial q_{l_{j-1}}^n} \left(\frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_{j-2}}^n} \frac{\partial D_{\psi l_{j-2}}^n}{\partial n} + \frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_{j-1}}^n} \frac{\partial D_{\psi l_{j-1}}^n}{\partial n} + \frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_j}^n} \frac{\partial D_{\psi l_j}^n}{\partial n} \right) \\ & + \frac{\partial T_j^{n+1}}{\partial q_{l_{j+1}}^n} \left(\frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_j}^n} \frac{\partial D_{\psi l_j}^n}{\partial n} + \frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_{j+1}}^n} \frac{\partial D_{\psi l_{j+1}}^n}{\partial n} + \frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_{j+2}}^n} \frac{\partial D_{\psi l_{j+2}}^n}{\partial n} \right) \\ & + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n} \frac{\partial \theta_{l_j}^n}{\partial n} + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}} \frac{\partial \theta_{l_j}^{n-1}}{\partial n}\end{aligned} \tag{A.88}$$

with respect to the Clapp and Hornberger soil texture parameter b is

$$\begin{aligned}\frac{\partial T_j^{n+1}}{\partial b} = {} & \frac{\partial T_j^{n+1}}{\partial q_{l_{j-1}}^n} \left(\frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_{j-2}}^n} \frac{\partial D_{\psi l_{j-2}}^n}{\partial b} + \frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_{j-1}}^n} \frac{\partial D_{\psi l_{j-1}}^n}{\partial b} + \frac{\partial q_{l_{j-1}}^n}{\partial D_{\psi l_j}^n} \frac{\partial D_{\psi l_j}^n}{\partial b} \right) \\ & + \frac{\partial T_j^{n+1}}{\partial q_{l_{j+1}}^n} \left(\frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_j}^n} \frac{\partial D_{\psi l_j}^n}{\partial b} + \frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_{j+1}}^n} \frac{\partial D_{\psi l_{j+1}}^n}{\partial b} + \frac{\partial q_{l_{j+1}}^n}{\partial D_{\psi l_{j+2}}^n} \frac{\partial D_{\psi l_{j+2}}^n}{\partial b} \right) \\ & + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n} \frac{\partial \theta_{l_j}^n}{\partial b} + \frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}} \frac{\partial \theta_{l_j}^{n-1}}{\partial b}\end{aligned} \tag{A.89}$$

with respect to the Brooks and Corey pore size distribution index φ is

$$\begin{aligned}\frac{\partial T_j^{n+1}}{\partial \varphi} = &\frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j-1}}^n}\left(\frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_{j-2}}^n}\frac{\partial D_{\psi l_{j-2}}^n}{\partial \varphi}+\frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_{j-1}}^n}\frac{\partial D_{\psi l_{j-1}}^n}{\partial \varphi}+\frac{\partial \mathrm{q}_{l_{j-1}}^n}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \varphi}\right)\\ &+\frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j+1}}^n}\left(\frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_j}^n}\frac{\partial D_{\psi l_j}^n}{\partial \varphi}+\frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_{j+1}}^n}\frac{\partial D_{\psi l_{j+1}}^n}{\partial \varphi}+\frac{\partial \mathrm{q}_{l_{j+1}}^n}{\partial D_{\psi l_{j+2}}^n}\frac{\partial D_{\psi l_{j+2}}^n}{\partial \varphi}\right)\\ &+\frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n}\frac{\partial \theta_{l_j}^n}{\partial \varphi}+\frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}}\frac{\partial \theta_{l_j}^{n-1}}{\partial \varphi}\end{aligned} \quad \text{(A.90);}$$

with respect to the volumetric proportion of quartz θ_3 is

$$\frac{\partial T_j^{n+1}}{\partial \theta_3} = \frac{\partial T_j^{n+1}}{\partial C_{T_j}^n}\frac{\partial C_{T_j}^n}{\partial \theta_3}+\frac{\partial T_j^{n+1}}{\partial \lambda_{j-1}^n}\frac{\partial \lambda_{j-1}^n}{\partial \theta_3}+\frac{\partial T_j^{n+1}}{\partial \lambda_j^n}\frac{\partial \lambda_j^n}{\partial \theta_3}+\frac{\partial T_j^{n+1}}{\partial \lambda_{j+1}^n}\frac{\partial \lambda_{j+1}^n}{\partial \theta_3} \quad \text{(A.91);}$$

with respect to the volumetric proportion of other minerals θ_4 is

$$\frac{\partial T_j^{n+1}}{\partial \theta_4} = \frac{\partial T_j^{n+1}}{\partial C_{T_j}^n}\frac{\partial C_{T_j}^n}{\partial \theta_4}+\frac{\partial T_j^{n+1}}{\partial \lambda_{j-1}^n}\frac{\partial \lambda_{j-1}^n}{\partial \theta_4}+\frac{\partial T_j^{n+1}}{\partial \lambda_j^n}\frac{\partial \lambda_j^n}{\partial \theta_4}+\frac{\partial T_j^{n+1}}{\partial \lambda_{j+1}^n}\frac{\partial \lambda_{j+1}^n}{\partial \theta_4} \quad \text{(A.92);}$$

and with respect to the volumetric proportion of organic matter θ_5 is

$$\frac{\partial T_j^{n+1}}{\partial \theta_5} = \frac{\partial T_j^{n+1}}{\partial C_{T_j}^n}\frac{\partial C_{T_j}^n}{\partial \theta_5}+\frac{\partial T_j^{n+1}}{\partial \lambda_{j-1}^n}\frac{\partial \lambda_{j-1}^n}{\partial \theta_5}+\frac{\partial T_j^{n+1}}{\partial \lambda_j^n}\frac{\partial \lambda_j^n}{\partial \theta_5}+\frac{\partial T_j^{n+1}}{\partial \lambda_{j+1}^n}\frac{\partial \lambda_{j+1}^n}{\partial \theta_5} \quad \text{(A.93)}$$

A.2.1 DERIVATIVES OF TEMPERATURE EQUATION

The derivatives of the temperature equation which require evaluation for evaluation of the chain rules at node *j* are given below. The derivative with respect to the volumetric heat capacity C_T at node *j* is

$$\frac{\partial T_j^{n+1}}{\partial C_{T_j}^n} = -\frac{\left(t^{n+1}-t^n\right)}{\left(C_{T_j}^n\right)^2\left(z_{j-1}-z_{j+1}\right)}\left(\begin{array}{l}\left(\begin{array}{l}\dfrac{\left(\lambda_{j-1}^n+\lambda_j^n\right)\left(T_{j-1}^n-T_j^n\right)}{z_{j-1}-z_j} \\ -\dfrac{\left(\lambda_j^n+\lambda_{j+1}^n\right)\left(T_j^n-T_{j+1}^n\right)}{z_j-z_{j+1}}\end{array}\right) \\ -c_l\left(\begin{array}{l}\left(T_{j-1}^n-T_{ref}\right)q_{l_{j-1}}^n \\ -\left(T_{j+1}^n-T_{ref}\right)q_{l_{j+1}}^n\end{array}\right)\end{array}\right) + \left(\frac{t^{n+1}-t^n}{\left(C_{T_j}^n\right)^2}\right)c_l\rho_l\left(T_j^n-T_{ref}\right)\left(\frac{\theta_{l_j}^n-\theta_{l_j}^{n-1}}{t^n-t^{n-1}}\right) \quad \text{(A.94);}$$

with respect to the thermal conductivity λ at node j–1 is

$$\frac{\partial T_j^{n+1}}{\partial \lambda_{j-1}^n} = \frac{\left(t^{n+1}-t^n\right)\left(T_{j-1}^n-T_j^n\right)}{C_{T_j}^n\left(z_{j-1}-z_{j+1}\right)\left(z_{j-1}-z_j\right)} \quad \text{(A.95);}$$

with respect to the thermal conductivity λ at node j is

$$\frac{\partial T_j^{n+1}}{\partial \lambda_j^n} = \frac{\left(t^{n+1}-t^n\right)}{C_{T_j}^n\left(z_{j-1}-z_{j+1}\right)}\left(\left(\frac{T_{j-1}^n-T_j^n}{z_{j-1}-z_j}\right)-\left(\frac{T_j^n-T_{j+1}^n}{z_j-z_{j+1}}\right)\right) \quad \text{(A.96);}$$

with respect to the thermal conductivity λ at node j+1 is

$$\frac{\partial T_j^{n+1}}{\partial \lambda_{j-1}^n} = -\frac{\left(t^{n+1}-t^n\right)\left(T_j^n-T_{j+1}^n\right)}{C_{T_j}^n\left(z_{j-1}-z_{j+1}\right)\left(z_j-z_{j+1}\right)} \quad \text{(A.97);}$$

with respect to the liquid mass flux q_l at node j–1 is

$$\frac{\partial T_j^{n+1}}{\partial q_{l_{j-1}}^n} = -\frac{c_l\left(t^{n+1}-t^n\right)\left(T_{j-1}^n-T_{ref}\right)}{C_{T_j}^n\left(z_{j-1}-z_{j+1}\right)} \quad \text{(A.98);}$$

with respect to the liquid mass flux q_l at node j+1 is

$$\frac{\partial T_j^{n+1}}{\partial \mathrm{q}_{l_{j+1}}^n} = \frac{c_l\left(t^{n+1} - t^n\right)\left(T_{j+1}^n - T_{ref}\right)}{C_{T_j}^n\left(z_{j-1} - z_{j+1}\right)} \quad \text{(A.99);}$$

with respect to volumetric liquid water content θ_l at node j time step n is

$$\frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^n} = -\frac{c_l \rho_l\left(t^{n+1} - t^n\right)\left(T_j^n - T_{ref}\right)}{C_{T_j}^n\left(t^n - t^{n-1}\right)} \quad \text{(A.100);}$$

and with respect to volumetric liquid water content θ_l at node j time step n–1 is

$$\frac{\partial T_j^{n+1}}{\partial \theta_{l_j}^{n-1}} = \frac{c_l \rho_l\left(t^{n+1} - t^n\right)\left(T_j^n - T_{ref}\right)}{C_{T_j}^n\left(t^n - t^{n-1}\right)} \quad \text{(A.101).}$$

In order to solve the partial differential equations which model the soil temperature transfer in the soil column, various boundary conditions can be applied, as outlined in section 5.1.2. Therefore, the derivatives of the temperature equation at the surface and bottom nodes depend on the boundary condition applied. If a Dirichlet boundary condition is applied, then the derivatives are zero, but if a Neumann boundary condition is applied, the derivatives are as given below for the boundary nodes. The derivative with respect to the volumetric heat capacity C_T at node 2 is

$$\frac{\partial T_1^{n+1}}{\partial C_{T_2}^n} = \frac{\partial T_2^{n+1}}{\partial C_{T_2}^n} \quad \text{(A.102a),}$$

and at node N–1 is

$$\frac{\partial T_N^{n+1}}{\partial C_{T_{N-1}}^n} = \frac{\partial T_{N-1}^{n+1}}{\partial C_{T_{N-1}}^n} \quad \text{(A.102b);}$$

with respect to the thermal conductivity λ at node 1 is

$$\frac{\partial T_1^{n+1}}{\partial \lambda_1^n} = \frac{\partial T_2^{n+1}}{\partial \lambda_1^n} + \frac{2\left(Q_{top}^T - c_l \mathrm{q}_{l_1}^n \left(T_1^n - T_{ref}\right)\right)(z_1 - z_2)}{\left(\lambda_1^n + \lambda_2^n\right)^2} \qquad \text{(A.103a),}$$

and at node N–2 is

$$\frac{\partial T_N^{n+1}}{\partial \lambda_{N-2}^n} = \frac{\partial \psi_{N-1}^{n+1}}{\partial \lambda_{N-2}^n} \qquad \text{(A.103b);}$$

with respect to the thermal conductivity λ at node 2 is

$$\frac{\partial T_1^{n+1}}{\partial \lambda_2^n} = \frac{\partial T_2^{n+1}}{\partial \lambda_2^n} + \frac{2\left(Q_{top}^T - c_l \mathrm{q}_{l_1}^n \left(T_1^n - T_{ref}\right)\right)(z_1 - z_2)}{\left(\lambda_1^n + \lambda_2^n\right)^2} \qquad \text{(A.104a),}$$

and at node N–1 is

$$\frac{\partial T_N^{n+1}}{\partial \lambda_{N-1}^n} = \frac{\partial T_{N-1}^{n+1}}{\partial \lambda_{N-1}^n} - \frac{2\left(Q_{bot}^T - c_l \mathrm{q}_{l_N}^n \left(T_N^n - T_{ref}\right)\right)(z_{N-1} - z_N)}{\left(\lambda_{N-1}^n + \lambda_N^n\right)^2} \qquad \text{(A.104b);}$$

with respect to the thermal conductivity λ at node 3 is

$$\frac{\partial T_1^{n+1}}{\partial \lambda_3^n} = \frac{\partial T_2^{n+1}}{\partial \lambda_3^n} \qquad \text{(A.105a),}$$

and at node N is

$$\frac{\partial T_N^{n+1}}{\partial \lambda_N^n} = \frac{\partial T_{N-1}^{n+1}}{\partial \lambda_N^n} - \frac{2\left(Q_{bot}^T - c_l \mathrm{q}_{l_N}^n \left(T_N^n - T_{ref}\right)\right)(z_{N-1} - z_N)}{\left(\lambda_{N-1}^n + \lambda_N^n\right)^2} \qquad \text{(A.105b);}$$

with respect to the liquid mass flux q_l at node 1 is

$$\frac{\partial T_1^{n+1}}{\partial \mathrm{q}_{l_1}^n} = \frac{\partial T_2^{n+1}}{\partial \mathrm{q}_{l_1}^n} + \frac{2c_l\left(T_1^n - T_{ref}\right)(z_1 - z_2)}{\left(\lambda_1^n + \lambda_2^n\right)} \qquad \text{(A.106a),}$$

and at node N–2 is

$$\frac{\partial T_N^{n+1}}{\partial \mathrm{q}_{l_{N-2}}^n} = \frac{\partial T_{N-1}^{n+1}}{\partial \mathrm{q}_{l_{N-2}}^n} \qquad \text{(A.106b);}$$

with respect to the liquid mass flux q_l at node 3 is

$$\frac{\partial T_1^{n+1}}{\partial \mathrm{q}_{l_3}^n} = \frac{\partial T_2^{n+1}}{\partial \mathrm{q}_{l_3}^n} \qquad \text{(A.107a),}$$

and at node N is

$$\frac{\partial T_N^{n+1}}{\partial \mathrm{q}_{l_N}^n} = \frac{\partial T_{N-1}^{n+1}}{\partial \mathrm{q}_{l_N}^n} - \frac{2c_l\left(T_N^n - T_{ref}\right)\left(z_{N-1} - z_N\right)}{\left(\lambda_{N-1}^n + \lambda_N^n\right)} \qquad \text{(A.107b);}$$

with respect to volumetric liquid water content θ_l at node 2 time step n is

$$\frac{\partial T_1^{n+1}}{\partial \theta_{l_2}^n} = \frac{\partial T_2^{n+1}}{\partial \theta_{l_2}^n} \qquad \text{(A.108a),}$$

and at node N–1 time step n is

$$\frac{\partial T_N^{n+1}}{\partial \theta_{l_{N-1}}^n} = \frac{\partial T_{N-1}^{n+1}}{\partial \theta_{l_{N-1}}^n} \qquad \text{(A.108b);}$$

and with respect to volumetric liquid water content θ_l at node 2 time step n–1 is

$$\frac{\partial T_1^{n+1}}{\partial \theta_{l_2}^{n-1}} = \frac{\partial T_2^{n+1}}{\partial \theta_{l_2}^{n-1}} \qquad \text{(A.109a),}$$

and at node N–1 time step n–1 is

$$\frac{\partial T_N^{n+1}}{\partial \theta_{l_{N-1}}^{n-1}} = \frac{\partial T_{N-1}^{n+1}}{\partial \theta_{l_{N-1}}^{n-1}} \tag{A.109b}$$

The partial differential equations which model the transfer of heat energy within a soil column are a function of the liquid mass flux. The liquid mass flux is not a function of the soil parameters itself, but rather a function of the constitutive relations, which are a function of the soil parameters. Therefore, the derivatives of the liquid mass flux with respect to the constitutive relations are required, and are given below. The derivative with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node j–1 is

$$\frac{\partial \mathrm{q}_{l_j}^n}{\partial D_{\psi l_{j-1}}^n} = -\frac{\rho_l\left(\psi_{j-1}^n - \psi_j^n\right)}{4\left(z_{j-1} - z_j\right)} \tag{A.110}$$

with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node j is

$$\frac{\partial \mathrm{q}_{l_j}^n}{\partial D_{\psi l_j}^n} = -\rho_l\left(1 + \frac{1}{4}\left(\left(\frac{\psi_{j-1}^n - \psi_j^n}{z_{j-1} - z_j}\right) + \left(\frac{\psi_j^n - \psi_{j+1}^n}{z_j - z_{j+1}}\right)\right)\right) \tag{A.111}$$

and with respect to the liquid hydraulic conductivity $D_{\psi l}$ at node j+1 is

$$\frac{\partial \mathrm{q}_{l_j}^n}{\partial D_{\psi l_{j+1}}^n} = -\frac{\rho_l\left(\psi_j^n - \psi_{j+1}^n\right)}{4\left(z_j - z_{j+1}\right)} \tag{A.112}$$

At the boundary nodes, the liquid mass flux is modelled using slightly different relationships. Therefore, different derivates are obtained for the boundary nodes. The derivative with respect to liquid hydraulic conductivity $D_{\psi l}$ at nodes 1 and 2 are

$$\frac{\partial \mathrm{q}_{l_1}^n}{\partial D_{\psi l_1}^n} = \frac{\partial \mathrm{q}_{l_1}^n}{\partial D_{\psi l_2}^n} = -\frac{\rho_l}{2}\left(1 + \frac{\left(\psi_1^n - \psi_2^n\right)}{\left(z_1 - z_2\right)}\right) \tag{A.113a}$$

and at nodes N–1 and N are

$$\frac{\partial \mathrm{q}_{l_N}^{n}}{\partial D_{\psi l_{N-1}}^{n}} = \frac{\partial \mathrm{q}_{l_N}^{n}}{\partial D_{\psi l_N}^{n}} = -\frac{\rho_l}{2}\left(1 + \frac{\left(\psi_{N-1}^{n} - \psi_{N}^{n}\right)}{\left(z_{N-1} - z_{N}\right)}\right) \qquad \text{(A.113b).}$$

A.2.2 DERIVATIVES OF CONSTITUTIVE RELATIONS

In this section, the derivatives of the constitutive relations that require evaluation in order to evaluate the chain rules at node j are given.

A.2.2.1 Volumetric Heat Capacity

In this section, the derivatives of the volumetric heat capacity with respect to each of the dependent soil parameters are given. The derivative of the volumetric heat capacity C_T at node j with respect to porosity ϕ is

$$\frac{\partial C_T}{\partial \phi} = C_2 \qquad \text{(A.114);}$$

with respect to the proportion of quartz θ_3 is

$$\frac{\partial C_T}{\partial \theta_3} = C_3 \qquad \text{(A.115);}$$

with respect to the proportion of other minerals θ_4 is

$$\frac{\partial C_T}{\partial \theta_4} = C_4 \qquad \text{(A.116);}$$

and with respect to the proportion of other minerals θ_5 is

$$\frac{\partial C_T}{\partial \theta_5} = C_5 \qquad \text{(A.117).}$$

A.2.2.2 Thermal Conductivity

In this section, the derivatives of the thermal conductivity with respect to each of the dependent soil parameters are given. The derivative of the thermal conductivity λ at node j with respect to porosity ϕ is

$$\frac{\partial\lambda}{\partial\phi} = \frac{\left(\left(k_2\lambda_2 \sum_{i=1}^{5} k_i\theta_i \right) - \left(k_2 \sum_{i=1}^{5} k_i\theta_i\lambda_i \right) + \frac{\begin{pmatrix} \frac{2}{3}0.298\theta_1(3g_2-1)\theta_2\lambda_1(\lambda_1-\lambda_2)^2 \\ \cdot(\lambda_1(1+g_2)-\lambda_2(g_2-1))\cdot \\ \begin{pmatrix} k_1\theta_1(\lambda_1-\lambda_2)-k_4\theta_4\lambda_2-k_5\theta_5\lambda_2+ \\ k_3\theta_3(\lambda_3-\lambda_2)+k_4\theta_4\lambda_4+k_5\theta_5\lambda_5 \end{pmatrix} \end{pmatrix}}{\phi^2(2g_2(\lambda_1-\lambda_2)+\lambda_2)^2((g_2-1)\lambda_1-g_2\lambda_2)^2} \right)}{\left(\sum_{i=1}^{5} k_i\theta_i \right)^2} \qquad \text{(A.118);}$$

with respect to the proportion of quartz θ_3 is

$$\frac{\partial\lambda}{\partial\theta_3} = \frac{k_3\lambda_3}{\sum_{i=1}^{5} k_i\theta_i} - \frac{k_3\sum_{i=1}^{5} k_i\theta_i\lambda_i}{\left(\sum_{i=1}^{5} k_i\theta_i \right)^2} \qquad \text{(A.119);}$$

with respect to the proportion of other minerals θ_4 is

$$\frac{\partial\lambda}{\partial\theta_4} = \frac{k_4\lambda_4}{\sum_{i=1}^{5} k_i\theta_i} - \frac{k_4\sum_{i=1}^{5} k_i\theta_i\lambda_i}{\left(\sum_{i=1}^{5} k_i\theta_i \right)^2} \qquad \text{(A.120);}$$

and with respect to the proportion of other minerals θ_5 is

$$\frac{\partial \lambda}{\partial \theta_5} = \frac{k_5 \lambda_5}{\sum_{i=1}^{5} k_i \theta_i} - \frac{k_5 \sum_{i=1}^{5} k_i \theta_i \lambda_i}{\left(\sum_{i=1}^{5} k_i \theta_i \right)^2} \qquad \text{(A.121).}$$