soilice: Governing Equations

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1 State variables

We assume the following soil volume, mass, energy and temperature relations, all of which are extensive variables:

$$
\begin{aligned}
V &= V_I + V_L + V_S + V_A \\
M &= M_I + M_L + M_S + M_A \\
U &= U_I + U_L + U_S + U_A \\
T &= T_I = T_L = T_S = T_A
\end{aligned} \tag{1}
$$

where V (m^3) is volume, M (kg) is mass, U (J) is internal energy and T (°C) is temperature, and subscripts are for the components liquid, L, ice, I, soil solid matter, S, and air, A.

Equivalent intensive variables, expressed per unit volume, and given by dividing the above expressions (excluding T) by V are

$$
\begin{aligned}
V/V &= 1 = \theta_I + \theta_L + \theta_S + \theta_A \\
M/V &= m = m_I + m_L + m_S + m_A \\
U/V &= u = u_I + u_L + u_S + u_A
\end{aligned} \tag{2}
$$

The density of a component, ρ_i (kg m^{-3}), is

$$\rho_i = \frac{M_i}{V_i} \tag{3}$$

while the mass fraction of a component, m_i (kg m^{-3}) is

$$m_i = \frac{M_i}{V} = \rho_i \theta_i \tag{4}$$

2 Internal energy

Consider a control volume of water V (m^3), of mass M (kg) and temperature T (°C). We define internal energy associated with sensible heat, that is the sensible internal energy, U_s (J), as

$$U_s = Mc_pT \tag{5}$$

where c_p (J kg^{-1} K^{-1}) is the specific heat capacity (which is defined by this equation). Likewise

$$u_s = mc_pT \tag{6}$$

The differential equation for the change in sensible internal energy with time is

$$\frac{du_s}{dt} = \frac{d}{dt}(mc_pT) = mc_p\frac{dT}{dt} + c_pT\frac{dm}{dt} \tag{7}$$

Latent heat is a form of internal energy, called latent internal energy, U_l (J), associated with the chemical bonds between molecules in a particular phase (solid, liquid, gas) of a substance. We assume latent heat is negative in the solid phase, zero in the liquid phase and positive in the vapor phase, hence

$$\begin{aligned} U_{li} &= -M_i\lambda_f \\ U_{ll} &= 0 \\ U_{lv} &= M_v\lambda_v \end{aligned} \tag{8}$$

where λ_f, the amount of heat needed to convert 1 kg of ice to 1 kg of liquid water, is a constant $\approx 3.34 \times 10^5$ J kg^{-1} and $\lambda_v = 2.50 \times 10^6$ J kg^{-1} at $T = 0°$C). Likewise, we can define the intensive variables:

$$\begin{aligned} u_{li} &= -u_i\lambda_f \\ u_{ll} &= 0 \\ u_{lv} &= m_v\lambda_v \end{aligned} \tag{9}$$

Using this convention, the total latent internal energy is

$$u_l = -m_i\lambda_f + m_v\lambda_v \tag{10}$$

and the change in latent internal energy is

$$\frac{du_l}{dt} = -\lambda_f\frac{dm_i}{dt} + \lambda_v\frac{dm_v}{dt} \tag{11}$$

The total internal energy that concerns us in soils is given by the sum of sensible and latent heat, i.e.

$$u = u_s + u_l \tag{12}$$

In a control volume containing ice, liquid water, vapor and soil solids we have

$$u = u_{si} + u_{sl} + u_{sv} + u_{ss} + u_{li} + u_{lv} \tag{13}$$

(Noting that $U_{ll} = 0$).

3 Mass and energy balance equations

We will assume that the mass and internal energy in the vapor phase is negligible, hence

$$\begin{aligned} m_v &= 0 \\ u_{sv} &= 0 \\ u_{lv} &= 0 \end{aligned} \tag{14}$$

The mass and energy balance equations are

$$\frac{\partial m}{\partial t} = \frac{\partial m_l}{\partial t} + \frac{\partial m_i}{\partial t} = -\rho_l \nabla \cdot \mathbf{q}_l \tag{15}$$

and

$$\frac{\partial u}{\partial t} = \frac{\partial u_{si}}{\partial t} + \frac{\partial u_{sl}}{\partial t} + \frac{\partial u_{ss}}{\partial t} + \frac{\partial u_{li}}{\partial t} = -\nabla \cdot (\mathbf{j}_a + \mathbf{j}_c + \mathbf{j}_o) \tag{16}$$

where $\mathbf{q}_l$ (m s^{-1}) is the flux of liquid water and $\mathbf{j}_a$, $\mathbf{j}_c$ and $\mathbf{j}_o$ (J m^{-2} s^{-1}) are the advective, conductive, and other heat flux components. Expanding the left hand side of the energy balance equation gives

$$\frac{\partial u}{\partial t} = (m_i c_{pi} + m_l c_{pl} + m_s c_{ps}) \frac{\partial T}{\partial t} + c_{pl} T \frac{\partial m_l}{\partial t} + (c_{pi} T - \lambda_f) \frac{\partial m_i}{\partial t} \tag{17}$$

We define the bulk heat capacity, c_{pb} (J kg^{-1} K^{-1}) as

$$c_{pb} = m_i c_{pi} + m_l c_{pl} + m_s c_{ps} \tag{18}$$

so we have

$$\frac{\partial u}{\partial t} = c_{pb} \frac{\partial T}{\partial t} + c_{pl} T \frac{\partial m_l}{\partial t} + (c_{pi} T - \lambda_f) \frac{\partial m_i}{\partial t} \tag{19}$$

Now we want to eliminate the terms dm_l/dt and dm_i/dt. Under equilibrium conditions (which is a big assumption) a soil control volume should reach a unique state on the basis of the temperature and the total water. We ignore any hysteresis effects. We define the total water content, θ_T (-) as being given by

$$\theta_T = \theta_L + \frac{\rho_I}{\rho_L} \theta_I \tag{20}$$

We defined ψ_e (m) as the effective matric potential, which is associated with θ_T by the soil characteristic curve relationship,

$$\theta_T = \theta(\psi_e) \tag{21}$$

ψ_f (m) is the matric potential that corresponds to the freezing threshold, as defined by the GCE, where (Amankwah et al., 2021):

$$\psi_f = \frac{\lambda_f}{g} \ln\left(\frac{T + T_0}{T_0}\right) \tag{22}$$

where T is the soil temperature in °C, and $T_0 = 273.15$. If $\psi_e \leq \psi_f$ there is no ice in the soil pore space. Now we say

$$\begin{aligned}
&\theta_T = \theta(\psi_e); \quad \theta_L = \theta_T; && \theta_I = 0; && \text{if } \ \psi_e \leq \psi_f \\
&\theta_T = \theta(\psi_e); \quad \theta_L = \theta(\psi_f(T)) = F(T); && \theta_I = \tfrac{\rho_L}{\rho_I}(\theta_T - \theta_L); && \text{if } \ \psi_e > \psi_f
\end{aligned} \tag{23}$$

The function $F(T)$ defines the freezing characteristic curve, and is simply the combination of the GCE and the $\theta(\psi)$ relationship. $\theta(\psi)$ and $F(T)$ can be differentiated, giving

$$\frac{d\theta_T}{d\psi_e} = C(\psi_e) \tag{24}$$

and

$$\frac{d\theta_L}{dT} = F'(T) \tag{25}$$

So we can further say

$$\begin{aligned}
&\frac{d\theta_T}{dt} = C(\psi_e)\frac{d\psi_e}{dt}; \quad \frac{d\theta_L}{dt} = \frac{d\theta_T}{dt}; && \frac{d\theta_I}{dt} = 0; && \text{if } \ \psi_e \leq \psi_f \\
&\frac{d\theta_T}{dt} = C(\psi_e)\frac{d\psi_e}{dt}; \quad \frac{d\theta_L}{dt} = F'(T)\frac{dT}{dt}; && \frac{d\theta_I}{dt} = \frac{\rho_L}{\rho_I}\left(\frac{d\theta_T}{dt} - \frac{d\theta_L}{dt}\right); && \text{if } \ \psi_e > \psi_f
\end{aligned} \tag{26}$$

Now, consider first the case where $\psi_e \leq \psi_f$ (i.e. the soil is unfrozen). We have

$$\frac{\partial m_l}{\partial t} = \frac{\partial m}{\partial t}; \quad \frac{\partial m_i}{\partial t} = 0 \tag{27}$$

Substituting this into Equation 19 we have

$$\frac{\partial T}{\partial t} = \frac{\dfrac{\partial u}{\partial t} - c_{pl}T\dfrac{\partial m}{\partial t}}{c_{pb}} \tag{28}$$

Next consider the case where $\psi_e > \psi_f$ (i.e. the soil is frozen). This time we have

$$\frac{\partial m_l}{\partial t} = \rho_l F'(T)\frac{\partial T}{\partial t} \tag{29}$$

and

$$\frac{\partial m_i}{\partial t} = \frac{\partial m}{\partial t} - \frac{\partial m_l}{\partial t} = \frac{\partial m}{\partial t} - \rho_l F'(m,T)\frac{\partial T}{\partial t} \tag{30}$$

Substituting these expressions into the Equation 19 we get

$$\frac{\partial T}{\partial t} = \frac{\dfrac{\partial u}{\partial t} - (c_{pi}T - \lambda_f)\dfrac{\partial m}{\partial t}}{c_{pb} + \rho_l F'(T)((c_{pl} - c_{pi})T + \lambda_f)} \tag{31}$$

which may then be solved by replacing the derivative terms on the right hand side with the net fluxes. Note, in Ireson et al. (2026 in prep) these derivative terms are expanded, and the equations are further simplified. Here, we do not take this extra step, since the soilice model calculates $\partial u/\partial t$ and $\partial m/\partial t$ directly, and those values are substituted directly into Equations 28 and 31. Hence our governing equations are consistent with those presented in Ireson et al. (2026 in prep).

4 Finite difference formulation

For a one-dimensional vertical model, with z (m) representing the depth below the ground surface, it is good practice to use a block-centred grid, where z_n denotes the midpoint of a cell, and $z_{n-1/2}$ and $z_{n+1/2}$ are the depths of the top and bottom faces of the cell, respectively. Consider that the profile is discretized into N cells, with $N+1$ faces. Using the method of lines we reduce our system of two PDEs to a system of $2N$ ODEs, as follows. Considering a single control volume at depth index n, we can write

$$\begin{aligned} \left.\frac{dm_l}{dt}\right|_n + \left.\frac{dm_i}{dt}\right|_n &= -\rho_l \nabla \cdot \mathbf{q}_n \\ \left.\frac{du}{dt}\right|_n &= -\nabla \cdot \mathbf{j}_n \end{aligned} \tag{32}$$

where $\nabla \cdot \mathbf{q}_n$ and $\nabla \cdot \mathbf{j}_n$ are the net fluxes of mass and energy into the control volume. Expressing these equations with total mass, m and temperature T as the dependent variables we have

$$\left.\frac{dm}{dt}\right|_n = -\rho_l \nabla \cdot \mathbf{q}_n \tag{33}$$

$$\left.\frac{du}{dt}\right|_n = -\nabla \cdot \mathbf{j}_n \tag{34}$$

$$\left.\frac{dT}{dt}\right|_n = \begin{cases} \dfrac{\left.\frac{du}{dt}\right|_n - c_{pl} T_n \left.\frac{dm}{dt}\right|_n}{c_{pb}}, & \psi_{e,n} \leq \psi_{f,n} \\ \dfrac{\left.\frac{du}{dt}\right|_n - (c_{pi} T_n - \lambda_f) \left.\frac{dm}{dt}\right|_n}{c_{pb} + \rho_l f'(m_n, T_n)((c_{pl} - c_{pi}) T_n + \lambda_f)}, & \psi_{e,n} > \psi_{f,n} \end{cases} \tag{35}$$

Expanding the flux terms we have

$$\begin{aligned} -\rho_l \nabla \cdot \mathbf{q}_n &= \frac{(q_{l,n-1/2} - q_{l,n+1/2})\rho_l}{z_{n+1/2} - z_{n-1/2}} \\ -\nabla \cdot \mathbf{j}_n &= \frac{(j_{a,n-1/2} - j_{a,n+1/2}) + (j_{c,n-1/2} - j_{c,n+1/2}) + (j_{o,n-1/2} - j_{o,n+1/2})}{z_{n+1/2} - z_{n-1/2}} \end{aligned} \tag{36}$$

Here the individual flux terms are given by

$$\begin{aligned} q_{l,n-1/2} &= -K_{n-1/2} \left(\frac{\psi_n - \psi_{n-1}}{z_i - z_{n-1}} - 1 \right) \\ q_{l,n+1/2} &= -K_{n+1/2} \left(\frac{\psi_{n+1} - \psi_n}{z_{n+1} - z_n} - 1 \right) \\ j_{a,n-1/2} &= q_{l,n-1/2} \rho_l c_{pl} T_{n-1} \\ j_{a,n+1/2} &= q_{l,n+1/2} \rho_l c_{pl} T_n \\ j_{c,n-1/2} &= -\kappa_{n-1/2} \left(\frac{T_n - T_{n-1}}{z_n - z_{n-1}} \right) \\ j_{c,n+1/2} &= -\kappa_{n+1/2} \left(\frac{T_{n+1} - T_n}{z_{n+1} - z_n} \right) \end{aligned} \tag{37}$$

For the advected heat fluxes here we assume the water flux is positive in the z direction, such that T_{n-1} is the downstream temperature at point $n - 1/2$, and T_n is the upstream temperature at point $n + 1/2$. Alternative formulations for advection may be considered, but we will not expand on this here. The term j_o will be zero for all n

except $n = 1$ or $n = N$, that is the upper and lower boundary condition, where a specified direct heat flux (e.g. from net radiation or the geothermal heat flux) may be applied.

Consider a soil profile subject to a vertical infiltration flux q_a (m s^{-1}), a drainage flux, q_d (m s^{-1}) and an evaporative loss term q_e (m s^{-1}). The following boundary conditions can be used, where index $n = 1$ represents the ground surface and $n = N$ is the lower boundary:

$$\begin{aligned}
q_{l,1/2} &= q_a - q_e \\
q_{l,N+1/2} &= q_d \\
j_{a,1/2} &= j_{a,T} \\
j_{c,1/2} &= j_{g,T} \\
j_{a,N+1/2} &= j_{a,B} \\
j_{c,N+1/2} &= j_{g,B} \\
j_{o,1/2} &= j_r - j_h - j_e \\
j_{o,N+1/2} &= 0
\end{aligned} \tag{38}$$

where all j terms have units (J m^{-2} s^{-1}), and $j_{a,T}$ is advection with net infiltrating water, $j_{g,T}$ is the ground heat flux, driven by conduction across the soil surface (important when there is snow on the ground), j_r is net radiation, j_h is the sensible heat lost (advection with the movement of air), j_e is the latent heat lost to evaporation (advection of water vapor), $j_{a,B}$ is advection with water draining out the base of the soil and $j_{g,B}$ is the conductive heat flux across the lower boundary. The different flux terms in Eq 38 may be zero under different scenarios (e.g. snow cover, bare soil, etc) or assumptions.

We have here a system of ordinary differential equations which we solve using an ODE solver using the method described in Ireson et al (2023).

5 Hydraulic and thermal properties

Now, we need expressions for M, M', F and F', all of which we can get from the van Genuchten equations combined with the GCE equation.

$$S_e = (1 + (\alpha\psi)^n)^{-m} \tag{39}$$

$$\theta = M(\psi) = \theta_r + (\theta_{sat} - \theta_r)S_e \tag{40}$$

$$\frac{d\theta}{d\psi} = M'(\psi) = \frac{-\alpha m(\theta_{sat} - \theta_r)}{1 - m} S_e^{1/m} \left(1 - S_e^{1/m}\right)^m \tag{41}$$

The GCE:

$$\psi_f(T) = \frac{\lambda_f}{g} \ln\left(\frac{T + T_0}{T_0}\right) \approx \frac{L_f}{g}\left(\frac{T}{T_0}\right) \tag{42}$$

and

$$\begin{aligned}
F(T) &= M\left(\psi_f(T)\right) \\
&= \theta_r + (\theta_{sat} - \theta_r)\left(1 + \left(\tfrac{\alpha L_f T}{g T_0}\right)^n\right)^{-m}
\end{aligned} \tag{43}$$

For the derivative of the SFC let us define

$$S_f = \left(1 + \left(\frac{\alpha L_f T}{g T_0}\right)^n\right)^{-m} \tag{44}$$

Then

$$F'(T) = \frac{-\alpha L_f m(\theta_s - \theta_r)}{g T_0 (1-m)} S_f^{1/m}\left(1 - S_f^{1/m}\right)^m \tag{45}$$

Finally we need to define the hydraulic conductivity. In unfrozen conditions this is

$$K(\psi) = K_s S_e^{1/2}\left(1 - \left(1 - S_e^{1/m}\right)^m\right) \tag{46}$$

In unfrozen conditions, we are still seeking an ideal relationship for $K_f(\psi_e, T)$. For now we use impedence relationship

$$K_f(\psi_e, T) = K(\psi_e)^{-10\theta_I} \tag{47}$$

The bulk thermal conductivity can estimated as the volume weighted geometric mean of each component, with the equation

$$\kappa = \kappa_I^{\theta_L} \kappa_L^{\theta_L} \kappa_S^{\theta_S} \kappa_A^{\theta_A} \tag{48}$$

The soil dependent parameters and soil independent constants used in the above equations are summarized below in Table 1 and 2, respectively.

Symbol	Description	Values for loam	Units
θ_r	Residual water content	0.218	-
θ_{sat}	Saturated water content	0.520	-
α	van Genuchten parameter	1.15	m^{-1}
n	van Genuchten parameter	2.03	-
m	van Genuchten parameter	$1-(1/n)$	-
η	van Genuchten parameter	0.5	-
K_s	Saturated hydraulic conductivity	3.76×10^{-6}	m s^{-1}
c_{ps}	Soil solids specific heat capacity	850	J kg^{-1} K^{-1}
κ_S	Soil solids thermal conductivity	2.9	J s^{-1} m^{-1} K^{-1}
ρ_S	Soil solids density	2600	kg m^{-3}
q	Applied uniform flux for transport only	0	m s $^{-1}$
impedence	Impedence parameter for frozen K	0	(-)

Table 1: Model parameters are specific to the soil properties

Symbol	Description	Values for loam	Units
ρ_l	Density of liquid water	1000	kg m^{-3}
ρ_i	Density of ice	918	kg m^{-3}
ρ_a	Default air density	1.293	kg m^{-3}
c_{pl}	Specific heat capacity of liquid water	4180	J kg^{-1} K^{-1}
c_{pi}	Specific heat capacity of ice	2100	J kg^{-1} K^{-1}
κ_l	Thermal conductivity of liquid water	0.56	J s^{-1} m^{-1} K^{-1}
κ_i	Thermal conductivity of ice	2.2	J s^{-1} m^{-1} K^{-1}
κ_i	Thermal conductivity of air	0.025	J s^{-1} m^{-1} K^{-1}
λ_f	Latent heat of fusion	0.334×10^{6}	J kg^{-1}

Table 2: Model constants that should not change for different soil properties

6 References

Ireson, A. M., Spiteri, R. J., Clark, M. P., & Mathias, S. A. (2023). A simple, efficient, mass-conservative approach to solving Richards' equation (openRE, v1.0). Geoscientific Model Development, 16(2), 659–677. https://doi.org/10.5194/gmd-16-659-2023