APPARENT HEAT CAPACITY APPROACH BASED ON QIN ET AL.

VOLUMETRIC HEAT CAPACITY $C = \rho c$

SPECIFIC HEAT CAPACITY

(A) $$H(x,T) = \int_0^T C(x,s)\,ds + \rho_\ell L\,\theta_\ell(x,T)$$

VOLUMETRIC ENTHALPY $[J/m^3]$

(B) $$\theta_\ell(x,T) = \eta(x)\cdot\begin{cases} 1 & t>t^* \\ a|T|^{-b} & t<t^* \end{cases} \quad ; \quad t^* = \left(\frac{1}{a}\right)^b$$

$$H(x,T) = \underbrace{\int_0^T \sum_i \frac{V_i\,C_i(x,s)}{V_T}\,ds}\; + \rho_\ell L\,\theta_\ell(x,T)$$

$$= \theta_\ell(x,T)\,C_\ell T + \theta_i(x,T)\,C_i T + \theta_a(x,T)\,C_a T + (1-\varphi)\,C_R T + L\theta_\ell(x,T)$$

$$= \theta_\ell(x,T)\left[C_\ell T + L\right] + (\theta_w - \theta_\ell)\,C_i T + (\varphi - \theta_w)\,C_a T + (1-\varphi)\,C_R T$$

TOTAL WATER CONTENT

IS THIS THE SAME $\eta(x)$ FROM (B)?

WHAT IS $\eta(x)$ IN (B)? IF $t>t^*$ THEN ALL WATER IS UNFROZEN, MEANING $\theta_\ell(x) = \eta(x)$, SO $\eta(x)$ IS LIKE THE TOTAL WATER CONTENT.

(C) $$H(x,T) = \theta_\ell(x,T)\left[C_\ell T + L\right] + \left(\eta(x) - \theta_\ell(x,T)\right)C_i T + \left(\varphi(x) - \eta(x)\right)C_a T + \left(1 - \varphi(x)\right)C_R T$$

WHERE:

- $\theta_\ell(x,T)$ IS GIVEN IN (B)
- $\eta(x)$ IS DEFINED BY W.T. DEPTH + VAN GENUCHTEN
- $\varphi(x)$ IS A STIPULATED MODEL PARAMETER THAT MAY VARY WITH DEPTH.

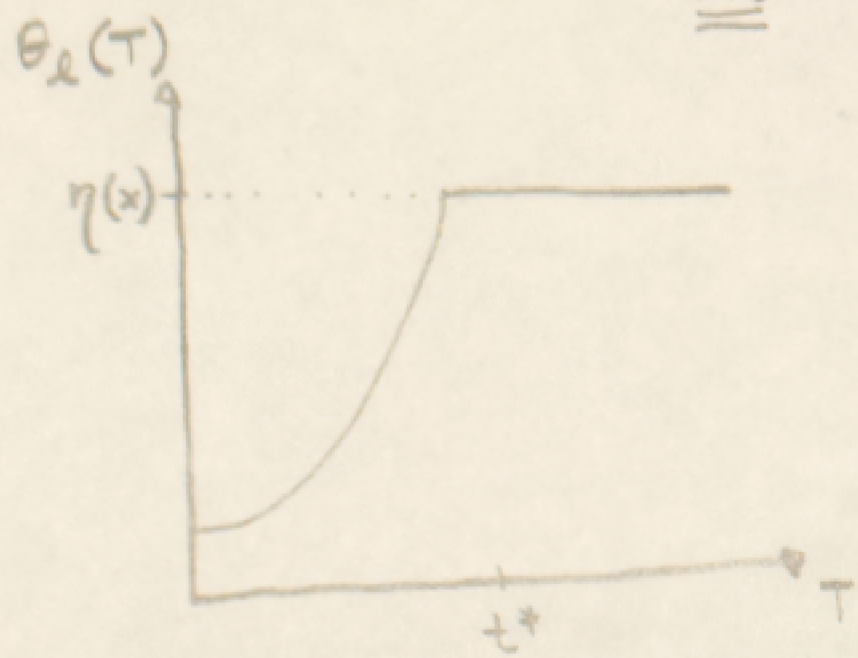
SPECIFIC HEAT CAPACITY

$$(1) \quad \overline{\rho H} = \rho_\ell \, \theta_\ell(x,T)\left[c_\ell T + L\right] + \left(\eta(x) - \theta_\ell(x,T)\right)\rho_i c_i T + \left(\varphi(x) - \eta(x)\right)\rho_a c_a T$$

SPECIFIC ENTHALPY [J/kg]

$$+ \left(1 - \varphi(x)\right)\rho_R c_R T$$

DISCONTINUITY IN $\theta_\ell(x,T)$? <u>NO</u>




$$\theta_\ell(T) = \eta(x) \begin{cases} 1 & t > t^* \\ a(-T)^{-b} & t < t^* \end{cases}$$

$$\underbrace{t^* = -\left(\frac{1}{a}\right)^{-\frac{1}{b}}}$$

THIS IS DIFFERENT THAN QIN ET AL. REPORTS, BUT MATCHES THE THEORY OF LEVELL (1956) CORRECTLY.

HOW DO WE HANDLE $K(x,T)$?

→ QIN ET AL. USES AN EMPIRICAL RELATIONSHIP:

$$K(x,T) = 0.798 + 1.3904 \cdot \eta(x)$$

BUT THIS WOULDN'T CHANGE WITH FREEZE AND THAW SINCE $\eta(x)$ IS LIKE THE TOTAL WATER CONTENT, WHICH IS UNCHANGING IN OUR SIMULATIONS.

→ COMMON TO USE THE GEOMETRIC MEAN:

$$K(x,T) = \prod_i^N K_i^{\theta_i}$$

*MANY OTHER, MORE COMPLEX $K(x,T)$ MODELS EXIST. HE ET AL. GIVES A THOROUGH REVIEW.

→ GEOTOP USES MIXING MODEL:

$$(2) \quad K(x,T) = \left[\sum_i^N \theta_i \sqrt{K_i}\right]^2 \quad \text{COSENZA ET AL. (2003)}$$

*SHOULD WE CONSIDER ORGANIC CONTENT?*

(3) $$\frac{\partial(\overline{\rho H})}{\partial t} - \frac{\partial}{\partial z}\left(\kappa \frac{\partial T}{\partial z}\right) = 0$$

SEMI-IMPLICIT FORMULATION:

$$\frac{d(\overline{\rho H})}{dT}\frac{\partial T}{\partial t} - \frac{\partial}{\partial z}\left(\kappa \frac{\partial T}{\partial z}\right) = 0$$

$$\overline{\rho H}' = \frac{d}{dT}\begin{cases} \rho_\ell \eta (c_\ell T + L) + (\varphi - \eta)\rho_a c_a T + (1-\varphi)\rho_R c_R T & t > t^* \\ \rho_\ell \eta (a(-T)^{-b})(c_\ell T + L) + (\eta - \eta(a(-T)^{-b}))\rho_i c_i T + \ldots \\ \quad (\varphi - \eta)\rho_a c_a T + (1-\varphi)\rho_R c_R T & t \leq t^* \end{cases}$$

$$= \begin{cases} \eta \rho_\ell c_\ell + (\varphi - \eta)\rho_a c_a + (1-\varphi)\rho_R c_R & t > t^* \\ ab\eta\rho_\ell (c_\ell T + L)(-T)^{(-1-b)} + a\eta\rho_\ell c_\ell (-T)^{-b} + \ldots \\ \left[-ab\eta\rho_i c_i T (-T)^{(-1-b)}\right] + \eta\rho_i c_i (1 - a(-T)^{-b}) + \ldots \\ (\varphi - \eta)\rho_a c_a + (1-\varphi)\rho_R c_R & t < t^* \end{cases}$$

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$$(\overline{\rho H}')_j^n \frac{T_j^{n+1} - T_j^n}{\Delta t} - \frac{1}{\Delta z}\left[\kappa_{j+1/2}^n \frac{T_{j+1}^{n+1} - T_j^{n+1}}{\Delta z} - \kappa_{j-1/2}^n \frac{T_j^{n+1} - T_{j-1}^{n+1}}{\Delta z}\right] = 0$$

$$-\left[\frac{\kappa_{j-1/2}^n}{\Delta z^2}\right] T_{j-1}^{n+1} + \left[\frac{(\overline{\rho H}')_j^n}{\Delta t} + \frac{(\kappa_{j+1/2}^n + \kappa_{j-1/2}^n)}{\Delta z^2}\right] T_j^{n+1} - \left[\frac{\kappa_{j+1/2}^n}{\Delta z^2}\right] T_{j+1}^{n+1} = \ldots$$

$$\frac{(\overline{\rho H}')_j^n}{\Delta t} T_j^n \quad \text{FOR } j = 2:J-1$$

BC:

- TRANSIENT $T(t)$ AT $j = 1$
- GRADIENT $\frac{dT}{dx}$ AT $j = J$

Equations from Qin et al. (2017):

$$H(x,T) = \int_0^T C(x,s)ds + \rho_l L\theta_l(x,T)$$

$$\theta_l(x,T) = \eta(x)\begin{cases} 1 & t > t^* \\ a|T|^{-b} & t < t^* \end{cases}$$

$$t^* = \left(\frac{1}{a}\right)^b$$

Here, $H$ is like a volumetric enthalpy, $C$ is the volumetric heat capacity, and $\eta(x)$ is like a maximum water content at position $x$ in the soil column. This value can therefore range between $\theta_r$ and $\theta_s$ and will be controlled by the soil parameters and the water table depth.

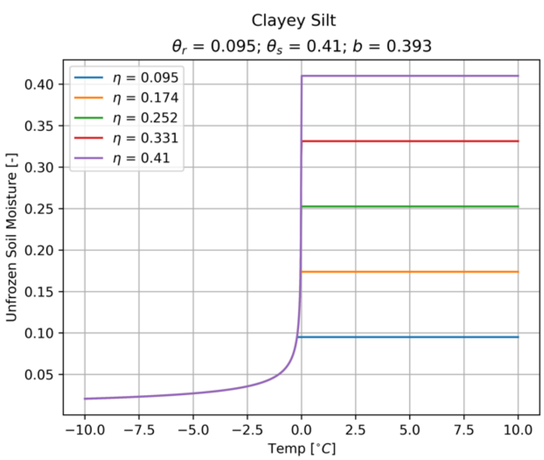
Unfrozen Soil Moisture Curves ($\theta_l \sim T$):

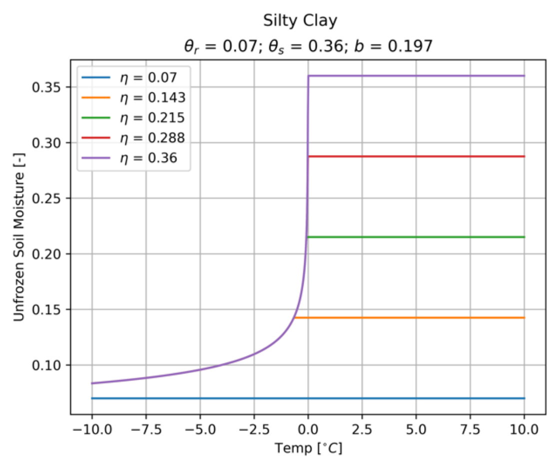
Looking at Levell (1956) which Qin et al. (2017) uses for the soil moisture expression, I believe it should be written as:

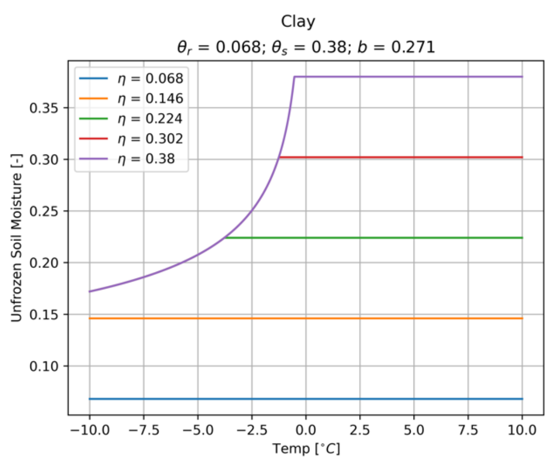
$$\theta_l(x,T) = \eta(x)\begin{cases} 1 & t > t^* \\ a(-T)^{-b} & t < t^* \end{cases}$$

$$t^* = -\left(\frac{1}{a}\right)^{-\left(\frac{1}{b}\right)}$$

This produces plots for soil moisture curves that look like the following:




The reason for a freezing point depression for clay with $\eta = \theta_s$ is that $t^* \to 0$ as $a \to 0$, but $a$ is always non-zero in the Levell (1956) model. It can grow small as $\eta$ grows, but it never reaches zero.

Enthalpy ($H$):

Redefining the volumetric enthalpy as:

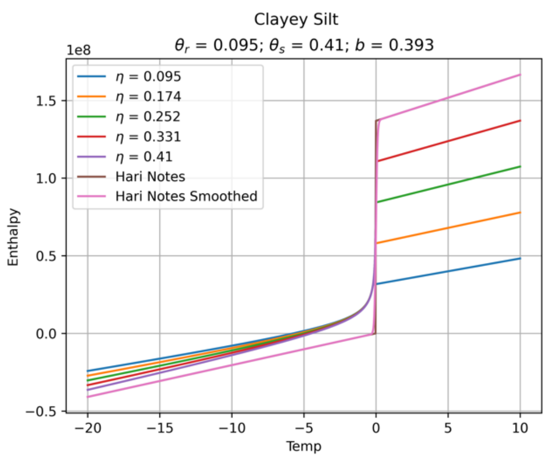
$$\rho H(x,T) = \int_0^T \sum_{i=0}^{n} \frac{V_i}{V_T} \rho_i c_i(x,s) ds \ + \rho_l L \theta_l(x,t)$$

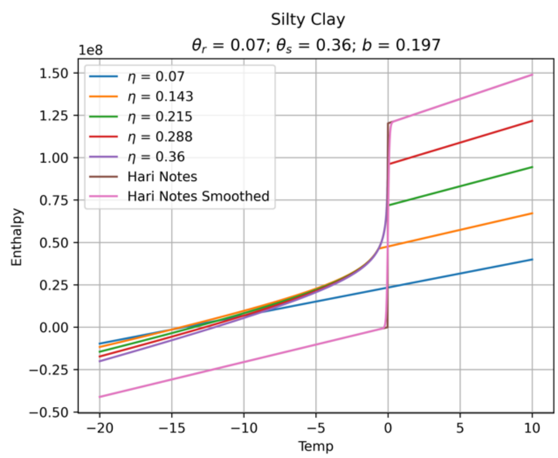
where $H$ is now the specific enthalpy (with units $[J/kg]$) and $c_i$ is the specific heat capacity of the $i^{th}$ component of the soil (i.e. water, ice, air, and soil grains). Now, we can derive:

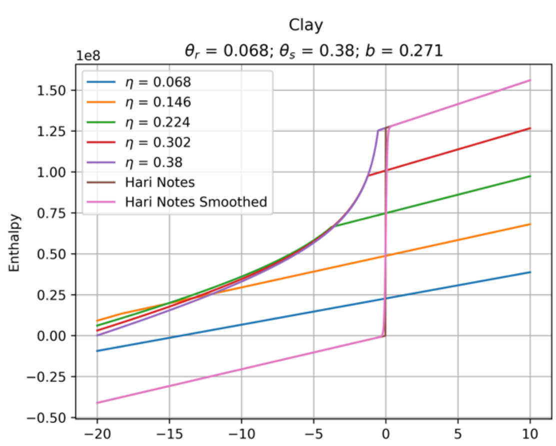
$$\rho H = \rho_l \theta_l(x,T)[c_l T + L] + (\eta(x) - \theta_l(x,T)\rho_i c_i T + \big(\phi(x) - \eta(x)\big)\rho_a c_a T + \big(1 - \phi(x)\big)\rho_r c_r T$$

This is similar to the expression in Hari's notes on the apparent heat capacity approach, but we have generalized it to include the air phase, allow for coexisting water and ice, and allowed the soil to be less than fully saturated.

We can plot this expression for different soil types:



In the finite difference scheme, we need the derivative of the enthalpy expression with respect to temperature, $T$.

$$\frac{d(\rho H)}{dT} = \begin{cases} \eta\rho_l c_l + (\phi - \eta)\rho_a c_a + (1-\phi)\rho_r c_r & t > t^* \\ ab\eta\rho_l(c_l T + L)(-T)^{-1-b} + a\eta\rho_l c_l(-T)^{-b} - ab\eta\rho_i c_i T(-T)^{-1-b} + \cdots \\ \eta\rho_i c_i(1 - a(-T)^{-b}) + (\phi - \eta)\rho_a c_a + (1-\phi)\rho_r c_r & t < t^* \end{cases}$$

There is a discontinuity in this expression at $t^*$.

We can plot this expression for different soil types: