



Mathematical modeling of water flow in porous medium with phase changes due freezing and evaporation.

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Porous medium hydrodynamics - standard Richards equation

continuity equation

$$\frac{\partial V}{\partial t} = -\nabla \cdot \vec{q}_l - S$$

- fluxes: diffusion type flow Darcy-Buckingham equation Buckingham(1907)

$$\vec{q} = -K(\theta)(\nabla h + \nabla z),$$

where

- $\nabla z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$
- $\theta(h)$ - water retention curve, and so $K(h)$
- volume: volumetric water content $V = \theta$
- sink term S : root water uptake, typically $S(h)$ Feddes et al.(1978)

Constitutive relations

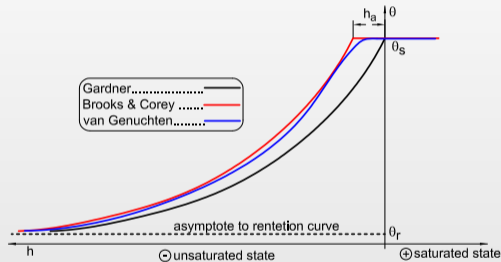


Figure: Retention curve according to Gardner(1958), Brooks and Corey(1964) and van Genuchten(1980).

Mualem(1976) definition for $K(h)$: steep retention curve even steeper $K(h)$

$$K(h) = K_s \begin{cases} \sqrt{\left(\frac{\theta(h)-\theta_r}{\theta_s-\theta_r}\right)} \left(\frac{\int_{\theta_r}^{\theta(h)} \frac{1}{h(\theta)} d\theta}{\int_{\theta_r}^{\theta_s} \frac{1}{h(\theta)} d\theta}\right)^2 & \forall \theta \in (\theta_r, \theta_s) \\ 1, & \theta = \theta_s \end{cases}$$

Richards equation

Richards(1931) equation

$$\frac{d\theta}{dh} \frac{\partial h}{\partial t} = \nabla \cdot K(h) \nabla h + \underbrace{\frac{\partial K(h)}{\partial z}}_{\text{gravity convection}} - S$$

- solution $h(\vec{x}, t)$ [L] - pressure head
- proof existence and uniqueness Alt and Luckhaus(1983)

- term $\frac{\partial K(h)}{\partial z}$ problematic, how to cope if layered environment?
- **solution:** solve it for H - total hydraulic head (at the moment functional)

$$H = h + z \rightarrow \vec{q} = -K(H) \nabla H$$

$$\frac{d\theta}{dh} \frac{\partial H}{\partial t} = \nabla \cdot K(H) \nabla H - S$$

Remark

!It is a macro-scale approach, solution should be understood in terms of probability.!

Water flow coupled with heat flow

$$\vec{q} = -K_{lh}(\theta)\nabla H - K_{lT}\nabla T,$$

- K_{lt} : Hydro/thermal conductivity for liquid (cross term),
- $K_{lt} = K_l \left(hG_w \frac{1}{\gamma_0} \frac{d\gamma}{dT} \right),$

Noborio et al.(1996) model

$$\frac{d\theta}{dh} \frac{\partial h}{\partial t} = \nabla \cdot K(h)\nabla h + \frac{\partial K(h)}{\partial z} + \nabla \cdot K_{lt}\nabla T - S_w$$

$$C_{T_s} \frac{\partial T}{\partial t} = \nabla \cdot \lambda \nabla T - \nabla \cdot C_{T_l} T \vec{q}_l + S_H$$

Remark: Noborio et al.(1996) complete model

$$\vec{q} = -K_{lh}(\theta)\nabla H - K_{lT}\nabla T - K_{lc}\nabla c,$$

- K_{cl} : Hydro/osmotic conductivity for liquid (cross term),
- $K_{cl} = K_l \left(h \frac{1}{\gamma_0} \frac{d\gamma}{dc} + \sigma \frac{d\psi_\pi}{dc} \right)$

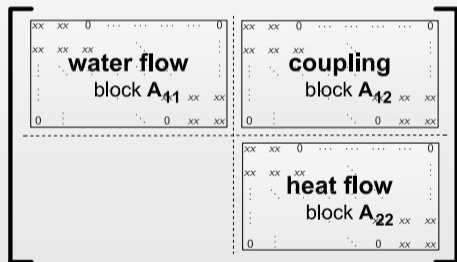
$$\Downarrow$$

$$\frac{d\theta}{dh} \frac{\partial h}{\partial t} = \nabla \cdot K(h)\nabla h + \frac{\partial K(h)}{\partial z} + \nabla \cdot K_{lt}\nabla T + \nabla \cdot K_{lc}\nabla c - S_w,$$

$$C_{T_s} \frac{\partial T}{\partial t} = \nabla \cdot \lambda \nabla T - \nabla \cdot C_{T_l} T \vec{q}_l + S_H,$$

$$R_d(c) \frac{\partial \theta c}{\partial t} = \nabla \cdot \theta \mathbf{D} \nabla c - \nabla \cdot \vec{q} c - r_1 c.$$

Remark: matrix structure for Noborio et al.(1996) wa- ter + heat model



Strategy: single-step block-Jacobi method

$$\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ 0 & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \vec{x}_h \\ \vec{x}_T \end{pmatrix} = \begin{pmatrix} \vec{b}_1 \\ \vec{b}_2 \end{pmatrix}$$

Easy as pie :)

- 1 | solve: $\mathbf{A}_{22}\vec{x}_T = \vec{b}_2$
- 2 | solve: $\mathbf{A}_{11}\vec{x}_h = \vec{b}_1 - \mathbf{A}_{12}\vec{x}_T$

Richards equation with phase changes

Freezing $V = \theta_l + \theta_i$ – given by Dall' Amico et al.(2011)

$$\frac{\partial \theta_l}{\partial t} + \frac{\rho_i}{\rho_l} \frac{\partial \theta_i}{\partial t} = \nabla \cdot K_{lh} \nabla h_l + \nabla \cdot K_{lT} \nabla T + \frac{\partial K_{lh}}{\partial z},$$

$$C_p \frac{\partial T}{\partial t} - \underbrace{L_f \rho_i \frac{\partial \theta_i}{\partial t}}_{\text{latent heat}} = \nabla \cdot \lambda \nabla T - \nabla \cdot C_l \vec{q}_l T.$$

Evaporation $V = \theta_l + \theta_v$ – given by Sakai et al.(2011)

$$\frac{\partial \theta_l}{\partial t} + \frac{\partial \theta_v}{\partial t} = \nabla \cdot (K_{lh} + K_{vh}) \nabla h + \frac{\partial K_{lh}}{\partial z} + \nabla \cdot (K_{lt} + K_{vt}) \nabla T - S$$

$$\bar{c} \frac{\partial T}{\partial t} + \underbrace{L_0 \frac{\partial \theta_v}{\partial t}}_{\text{latent heat}} = \nabla \cdot \lambda(\theta_l) \nabla T - \nabla \cdot (\vec{q}_l C_l + \vec{q}_v C_v) T - \nabla \cdot L_0 \vec{q}_v - C_l S T + S_{heat},$$

Overall strategy freezing + evaporation

- 1 | define relations for θ_i , θ_v , choose approach equilibrium \times non-equilibrium
- 2 | constitutive relations: $K_{lh}(\theta_i)$, $K_{vh}(T, h)$, K_{vT} , $\lambda(\theta)$, ...
- 3 | define problem specific boundary conditions (eg. energy balance for evaporation)

Freezing

Define θ_i

- in porous medium unfrozen water can exist below sub-zero temperatures \rightsquigarrow *cryosuction*
- soil freezing reduces the liquid pressure head \rightsquigarrow water flux towards the freezing front
- soil freezing \equiv soil drying
- approaches (similar to equilibrium \times kinetic sorption)
 - equilibrium (Clausius-Clapeyron theory)
 - non-equilibrium (freezing rate)

Equilibrium approach

Clausius-Clapeyron equation – see Kurylyk and Watanabe(2013)

$$\frac{dp}{dT} = \frac{L_f \rho_l}{T}, \rightsquigarrow \int_{p_l}^{p_w} \frac{dp}{dT} d = \int_{T_f}^T \frac{L_f \rho_l}{T} d,$$

$$h_l = \begin{cases} h_w + \underbrace{\frac{L_f}{g} \ln \frac{T}{T_f}}_{\text{cryosuction}}, & \text{for } T < T_f, \\ h_w, & \text{for } T \geq T_f, \end{cases}$$

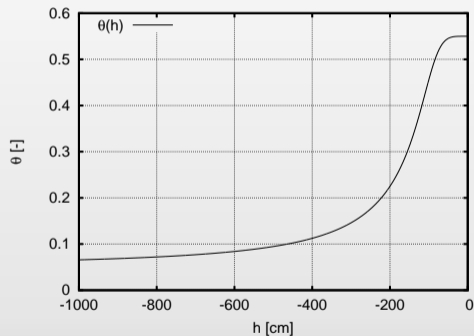
Why $h_I \times h_W$

Use of standard retention curve for θ_i !!

$$\theta_w = \theta(h_w),$$

$$\theta_I = \theta(h_I),$$

$$\theta_i = \theta_w - \theta_I.$$



volume term (time derivative term)

- due to the density differences of ice and water $\theta_{w_eq} = \theta_w + \left(\frac{\rho_i}{\rho_l} - 1 \right) \theta_i$,

- time derivative term becomes $\frac{\partial \theta_{w_eq}}{\partial t} = C(h_w) \frac{\partial h_w}{\partial t} + \left(\frac{\rho_i}{\rho_l} - 1 \right) \frac{\partial \theta_i}{\partial t}$,

- The term $\frac{\partial \theta_i}{\partial t}$ can then be expressed as follows (since $\theta_i = \theta_w - \theta_l$):

$$\frac{\partial \theta_i}{\partial t} = \frac{\partial \theta_w}{\partial t} - \frac{\partial \theta_l}{\partial t} = C(h_w) \frac{\partial h_w}{\partial t} - C(h_l) \frac{\partial h_l}{\partial t}$$

- to avoid two unknowns h_w and h_l use Clapeyron $\rightsquigarrow h_l(h_w, T)$ and so

$$C(h_l) \frac{\partial h_l}{\partial t} = C(h_l) \left(\frac{dh_l}{dh_w} \frac{\partial h_w}{\partial t} + \frac{dh_l}{dT} \frac{\partial T}{\partial t} \right)$$

Term $\frac{dh_l}{dT}$

Term $\frac{dh_l}{dT}$ is discontinuous

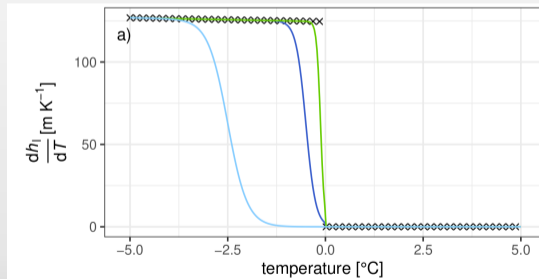
$$\frac{dh_l}{dT} = \begin{cases} \frac{L_f}{T_g} & \text{for } T < T_f, \\ 0 & \text{for } T \geq T_f, \end{cases},$$

$$\frac{\partial \theta_i}{\partial t} = \frac{\partial \theta_w - \theta_l}{\partial t} = C(h_w) \frac{\partial h_w}{\partial t} - C(h_l) \frac{dh_l}{dh_w} \frac{\partial h_w}{\partial t} -$$

$$- C(h_l) \frac{dh_l}{dT} \frac{\partial T}{\partial t} =$$

$$= \left(C(h_w) - C(h_l) \frac{dh_l}{dh_w} \right) \frac{\partial h_w}{\partial t} - C(h_l) \frac{dh_l}{dT} \frac{\partial T}{\partial t}$$

Discontinuous term $\frac{dh_l}{dT}$, regularization with sin function



Heat transport equation

$$C_p \frac{\partial T}{\partial t} - L_f \rho_i \frac{\partial \theta_i}{\partial t} = \nabla \cdot \lambda \nabla T - \nabla \cdot C_l \vec{q}_l T,$$

- Identical approach for θ_i

$$\frac{\partial \theta_i}{\partial t} = \left(C(h_w) - C(h_l) \frac{dh_l}{dh_w} \right) \frac{\partial h_w}{\partial t} - C(h_l) \frac{dh_l}{dT} \frac{\partial T}{\partial t}$$

$$C_p \frac{\partial T}{\partial t} - L_f \rho_i \frac{\partial \theta_i}{\partial t} = \left(C_p - L_f \rho_i C(h_l) \frac{dh_l}{dT} \right) \frac{\partial T}{\partial t} - L_f \rho_i \left(C(h_w) - C(h_l) \frac{dh_l}{dh_w} \right) \frac{\partial h_w}{\partial t}$$

Constitutive relations

water flow equation

- hydraulic conductivity: K_{lh_u} – unfrozen, standard Mualem(1976), according to Lundin(1990)

$$K_{lh} = 10^{-\Omega\alpha_{th}} K_{lh,u},$$

according to Hansson et al.(2004): Ω – empirical impedance factor [-],

$$\alpha_{th} = \frac{\theta_i}{\theta_i + \theta_l - \theta_r}.$$

heat transport equation

- thermal conductivity for freezing soil

$$\lambda = C_1 + C_2(\theta + F\theta_i) - (C_1 - C_4) \exp(-[C_3(\theta + F\theta_i)]^{C_5}),$$

coefficients C_1, \dots, C_5 some estimates can be found in literature, eg. Campbell(1985),

F – difference in thermal conductivities ice and water

as expected a lot of parameters :), but all well documented in literature

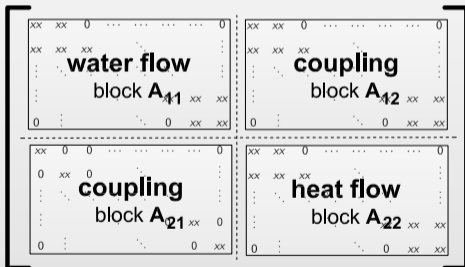
Boundary and initial conditions

- **initial conditions:** no special comment needed :)
- **boundary conditions:** use of Dirichlet/Neumann, semi-permeable boundary, etc., no special comment needed :)

Entire model review

$$\begin{aligned}
 & \left(C(h_w) \frac{\rho_i}{\rho_l} - \left(\frac{\rho_i}{\rho_l} - 1 \right) \frac{dh_l}{dh_w} C(h_l) \right) \frac{\partial H_w}{\partial t} + \overbrace{C(h_l) \bar{\Phi}_r \frac{dh_l}{dT} \left(\frac{\rho_i}{\rho_l} - 1 \right) \frac{\partial T}{\partial t}}^{\text{coupling term}} = \\
 & = \nabla \cdot K_{lh} \nabla H_w + \underbrace{\nabla \cdot \left(K_{lh} \bar{\Phi}_r \frac{L_f}{gT} + K_{IT} \right) \nabla T}_{\text{coupling term}}, \\
 & \overbrace{\left(C(h_l) \frac{dh_l}{dh_w} - C(h_w) \right) L_f \rho_i \frac{\partial H_w}{\partial t}}^{\text{coupling term}} + \left(C_p + C(h_l) L_f \rho_i \bar{\Phi}_r \frac{dh_l}{dT} \right) \frac{\partial T}{\partial t} = \\
 & = \nabla \cdot \lambda \nabla T - C_l \bar{q}_l \nabla T.
 \end{aligned}$$

Matrix structure and linear algebra strategy



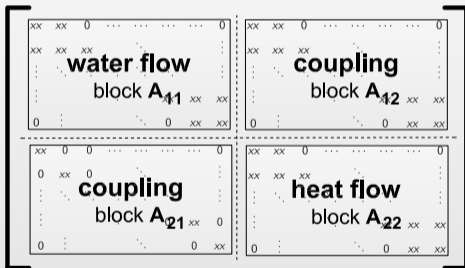
Recommendations

- block-Jacobi doesn't really work here, despite some popular implementations (Hydrus, etc.)
- coupling blocks

$$\begin{aligned}
 & \left(C(h_w) \frac{\rho_l}{\rho_i} - \left(\frac{\rho_l}{\rho_i} - 1 \right) \frac{dh_l}{dh_w} C(h_l) \right) \frac{\partial H_w}{\partial t} + \overbrace{C(h_l) \bar{\Phi}_r \frac{dh_l}{dT} \left(\frac{\rho_l}{\rho_i} - 1 \right) \frac{\partial T}{\partial t}}^{\text{coupling term}} = \\
 & = \nabla \cdot K_{ib} \nabla H_w + \underbrace{\nabla \cdot \left(K_{ib} \bar{\Phi}_r \frac{L_f}{gT} + K_{JT} \right) \nabla T}_{\text{coupling term}}, \\
 & \underbrace{\left(C(h_l) \frac{dh_l}{dh_w} - C(h_w) \right) L_f \rho_l \frac{\partial H_w}{\partial t}}_{\text{coupling term}} + \left(C_p + C(h_l) L_f \rho_l \bar{\Phi}_r \frac{dh_l}{dT} \right) \frac{\partial T}{\partial t} = \\
 & = \nabla \cdot \lambda \nabla T - C_i \bar{q}_i \nabla T.
 \end{aligned}$$

contains time derivatives !

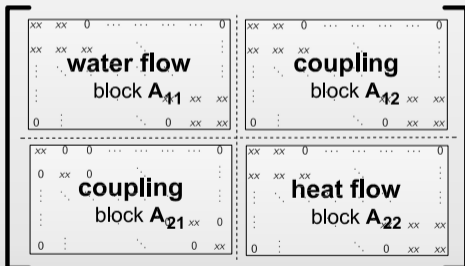
Matrix structure and linear algebra strategy



Why block-Jacobi doesn't work?

- solution requires short time steps
- short time steps – increases dominances of both the **main** and **outer** diagonal
- well-known fact for non-diagonally dominant system Jacobi and Gauss-Seidel doesn't work
- compared to eg. dual permeability model, decreasing time step doesn't increase dominance of the main diagonal

Matrix structure and linear algebra strategy



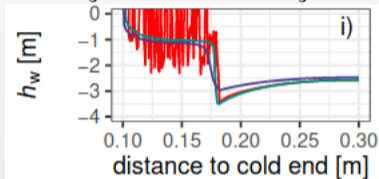
Solution

- use sparse matrix structure and sparse matrix solvers
- for 1D problems LU decomposition still ok, we successfully applied Cuthill and McKee(1969) reordering
 - system is non-symmetric
 - reordering algorithm developed for SPD systems
 - **consequence:** optimal pivot selection is not guaranteed, however, throughout all of our simulations all fine :)
- for 2D problems we use CG for normal equations, however still incomplete, major coefficients jumps, etc.

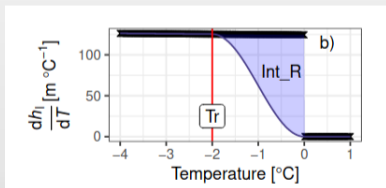
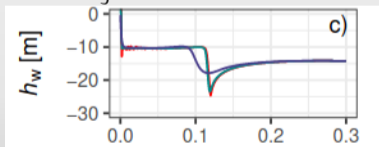
Discontinuity in time derivative term

$$\frac{dh_l}{dT} = \begin{cases} \frac{L_f}{T_g} & \text{for } T < T_f, \\ 0 & \text{for } T \geq T_f, \end{cases}$$

- if not regularized – solution goes oscillating

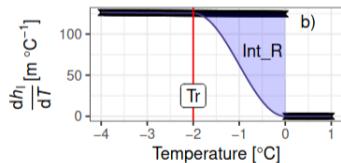


- if over-regularized – solution oversmoothed



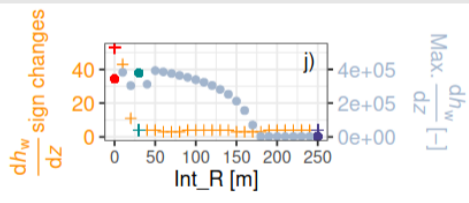
Discontinuity in time derivative term

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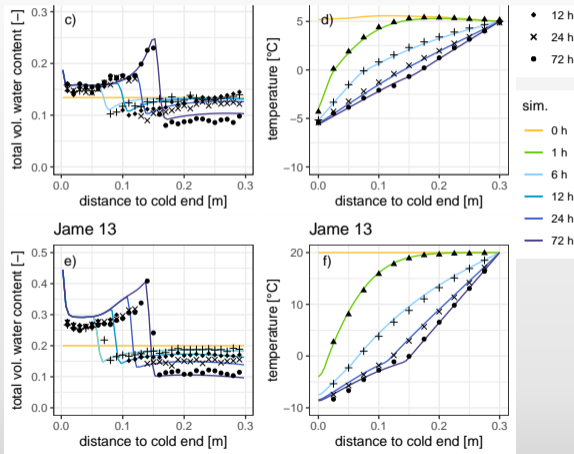
The right amount of regularization

- maintain minimal amount of solution h_w sign changes with maximal solution gradients



Model testing

- Numerical model was tested on laboratory data from Jame(1977) experiment
- model parameters were measured, only Ω impedance factor optimized



Short comment on nonequilibrium approach

Given by Peng(2016) and extended by Blöcher(2022)

$$\frac{\partial \theta_i}{\partial t} = v_f,$$

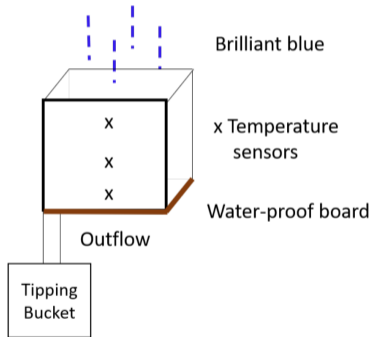
$$v_f = \begin{cases} \beta(\theta_l - \theta_{l,cl})(T_f - T)^{1/3} & \text{for } T < T_f, \\ 0 & \text{for } T \geq T_f, \end{cases}$$

where equilibrium water content $\theta_{l,cl}$ is computed from Clausius-Clapeyron

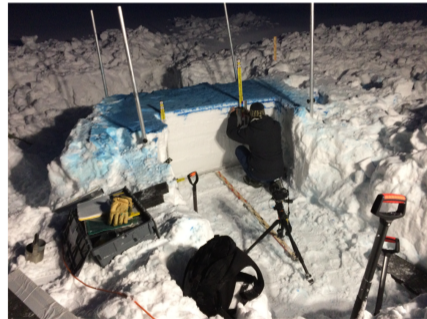
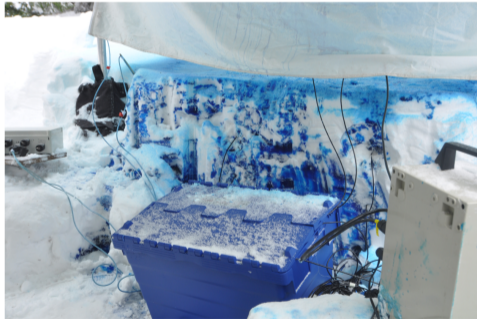
- for melting the model is not completely accurate, if $T = T_f \rightsquigarrow v_f = 0$, if some ice still present it can't melt any further
- fixed by Blöcher(2022)

$$v_f = \frac{\theta_{i,eq} - \theta_i}{\beta}$$

Application – rain on snow



Application – rain on snow



Application – rain on snow -> goals

- to mimic the rain water penetration into a snowpack
- to describe the changing liquid water content in snow
- to create a prediction system for avalanche warning = still future :)

Evaporation + evapotranspiration modeling

Governing equation

Following Saito et al.(2006) + Sakai et al.(2011)

$$\frac{\partial \theta_l}{\partial t} + \frac{\partial \theta_v}{\partial t} = \nabla \cdot (K_{lh} + K_{vh}) \nabla h + \frac{\partial K_{lh}}{\partial z} + \nabla \cdot (K_{lt} + K_{vt}) \nabla T - S$$

$$\bar{c} \frac{\partial T}{\partial t} + L_0 \frac{\partial \theta_v}{\partial t} = \nabla \cdot \lambda(\theta_l) \nabla T - \nabla \cdot (\bar{q}_l C_l + \bar{q}_v C_v) T - \nabla \cdot L_0 \bar{q}_v - C_l S T + S_{heat},$$

$$\bar{c} = C_s(1 - \theta_s) + C_l \theta_l + C_v \theta_v$$

Model structure

- definition for θ_v
- constitutive functions
- boundary and initial conditions

vapour content

Defined by Philip and De Vries(1957)

$$\theta_v = (\theta_s - \theta_v) H_r \frac{\rho_{sv}}{\rho_l}$$

Relative humidity:

$$H_r = \begin{cases} \exp\left(\frac{hMg}{RT}\right), & \text{if } h < 0 \\ 1, & \text{if } h \geq 0 \end{cases}$$

saturated vapour density

$$\rho_{sv} = 10^{-3} \frac{\exp\left(31.3716 - \frac{6014.79}{T} - 7.925 \times 10^{-3} T\right)}{T}$$

liquid water density

$$\rho_l = 1000 - 7.370 \times 10^{-3} (T - 3.98)^2 + 3.790 \times 10^{-5} (T - 3.98)^3$$

and so

$$\theta_v(h, T) \rightsquigarrow \frac{\partial \theta_v}{\partial t} = \frac{d\theta_v}{dh} \frac{\partial h}{\partial t} + \frac{d\theta_v}{dT} \frac{\partial T}{\partial t}$$

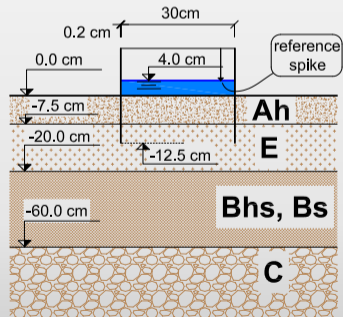
Fluxes

$$\vec{q}_l = -K_{lh} (\nabla h + \nabla z) - K_{vh} \nabla h - K_{lT} \nabla T - K_{vT} \nabla T,$$

$$\vec{q}_T = -\lambda(\theta) \nabla T + C_l \vec{q}_l T.$$

We have a problem

We can't avoid gravity convection term $\frac{\partial K_{lh}}{\partial z}$, how to cope with layered medium? Probably some *transition layer*



Constitutive relations

- hydraulic conductivity for liquid K_{lh} , K_{lT} already defined
- hydraulic conductivity for vapour K_{vh} , K_{vT} (see Nassar and Horton(1989); Nassar and Horton(1997))

$$K_{vh} = \frac{D}{\rho_w} \rho_{sv} \frac{Mg}{RT} H_r$$

$$K_{vt} = \frac{D}{\rho_l} \eta H_r \frac{d\rho_{sv}}{dT}$$

- thermal conductivity Chung and Horton(1987)

$$\lambda(\theta) = \lambda(\theta) = \lambda_0(\theta) + \beta \|\vec{q}_l\|_2,$$

$$\lambda_0(\theta) = b_1 + b_2\theta_l + b_3\sqrt{\theta_l}$$

where b_1 , b_2 , b_3 defined for sand, loam and clay. Empirical relation, overdried clay can reach negative conductivity!

Boundary conditions

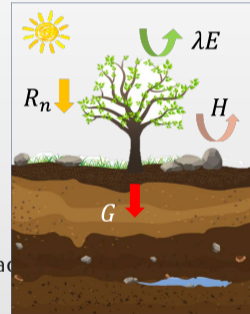
For bottom profile standard, for top – energy balance equation basically Neumann type boundary for both water flow and heat flow model

$$R_n - H - L_0 E - G = 0,$$

- R_n – net radiation [$\text{W}\cdot\text{m}^{-2}$]
- H – sensible heat flux density [$\text{W}\cdot\text{m}^{-2}$]
- E – evaporation rate flux [$\text{m}\cdot\text{s}^{-1}$]
- G – surface heat flux density [$\text{W}\cdot\text{m}^{-2}$]

$$E = \frac{\rho_{vs} - \rho_{va}}{r_h + r_s},$$

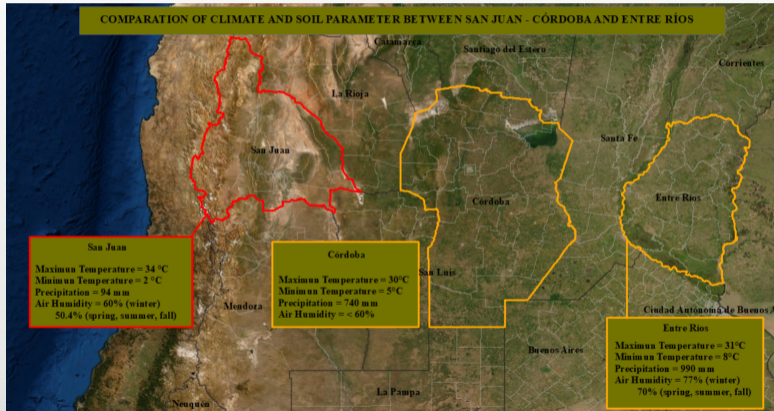
- $r_h + r_s$ – resistance factor
- ρ_{vs} – water vapor density at the soil surface
- ρ_{va} – atmospheric vapor density



meteo data included

T_{air} , wind speed, solar radiation, cloudiness, air humidity

Application: Finca ECOHUMUS, provincia San Juan, Argentina



Vineyard modeling

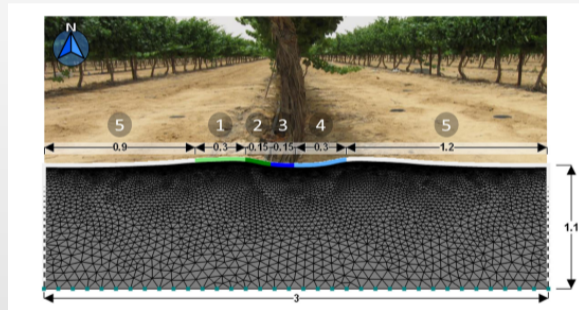
Calicatas observadas y descripción

Calicata 1

Este suelo está compuesto por una capa superior de suelo franco arcilloso a franco arcillo limoso (50 cm) (figura 2), lo que se considera muy bueno para el desarrollo de las raíces por su capacidad de contener e intercambiar nutrientes. A los 10 cm de profundidad se observan raíces y el 80% se desarrolla entre los 30 y 40 cm (figura 3) por lo que existe un impedimento para el desarrollo de la raíz en profundidad.

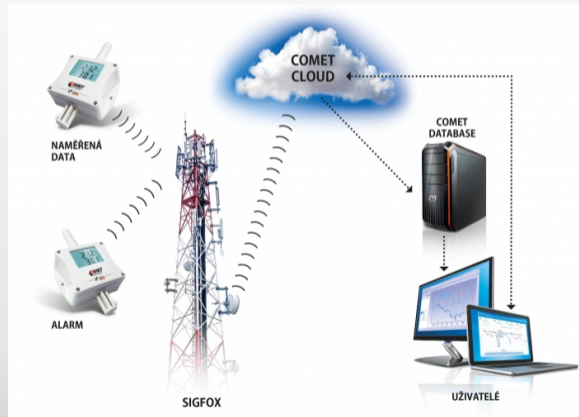


Figura 1. Perfil de suelo tipo serio Belgrano.



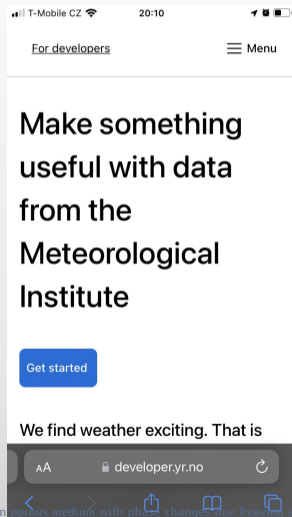
Data observations - initial conditions

- system of dielectric tensionmeters at different soil depths (Decagon Devices, Inc.)
- data time step 1 hrs



Boundary conditions value

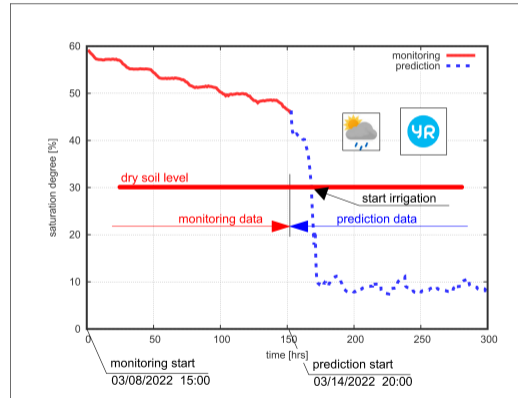
- meteorological data for **energy balance equation** obtained from `http://yr.no`
- they provide for free API interface
- \$ `"curl -s 'https://api.met.no/weathe..."`
- for defined longitude + latitude we obtain JSON data file with 10 days weather forecast, hourly time step! FOR FREE!!
- they provide exactly everything what we need for evaporation modeling



System PRAGASY

PRedicting soil moisture dynamics for efficient irriGAtion management (smart farming SYStems)

- system of sensors for measuring soil water content + temperature
- predicting the future development of soil water dynamics using yr.no (weather forecast) + drutes.org (soil moisture dynamics model)
- forecasting for up to 7 days
- providing the exact amount of irrigation water demand – to avoid over/under saturation states – optimal conditions for defined crop type
- predicting risks of water shortage for upcoming days – warning system providing alerts and exact timeline for optimal irrigation based on weather forecast and crop water consumption.



Gracias por su atención...

¿Preguntas?



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