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Modeling Vadose Zone Hydrology: Lecture Notes

Derek M. Heeren
University of Nebraska - Lincoln, derek.heeren@unl.edu

Dean Eisenhauer
University of Nebraska-Lincoln, deisenhauer1@unl.edu

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Derek M. Heeren and Dean E. Eisenhauer
Department of Biological Systems Engineering
University of Nebraska Lincoln
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Abstract
Modeling Vadose Zone Hydrology is a graduate-level course offered biennially in the Department of Biological Systems Engineering. Topics included hydraulic properties of porous media, application of Darcy's Law in variably saturated media, hydrologic and transport processes in the vadose zone, and solution of steady and unsteady flow problems using numerical techniques. A graphical approach for characterizing vertical one-dimensional problems with energy head profiles was emphasized. Common one-dimensional flow and transport problems were solved analytically. The course was taught using a combination of lecture notes and PowerPoint presentations. The lecture notes from 2021, captured using the Microsoft Whiteboard app with a Microsoft Surface, are presented here. The lecture notes are open access (CC BY-NC 4.0) and may be useful to other instructors in vadose zone hydrology or soil physics.

Background
The Modeling Vadose Zone Hydrology course was initially developed by Dean Eisenhauer and Derrel Martin; it was subsequently taught by Dean Eisenhauer for many years. Derek Heeren began teaching the course in 2014 and updated the course materials. The lecture notes presented here represent how the course was taught until 2021. The course is now taught by a different instructor and contains notably different course contents and structure.

Acknowledgements
We recognize that a course reflects a discipline which is shaped by many individuals. We acknowledge the students, guest lecturers, and others who influenced the course. A few of the lecture notes were adapted from courses which Derek Heeren had taken at Oklahoma State University. Tiffany Messer co-taught the class in 2018. Finally, we are thankful to the Department of Biological Systems Engineering and the Institute of Agriculture and Natural Resources at the University of Nebraska-Lincoln for their support of this course.

Citation
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Syllabus and Schedule

Modeling Vadose Zone Hydrology
AGEN/BSEN/CIVE/GEOL 957
Spring 2021

Instructor:

Derek M. Heeren, Ph.D., P.E., Associate Professor
241 L.W. Chase; Office Phone: 472-8577
E-Mail: derek.heeren@unl.edu

Prerequisites:

MATH 221/821 Differential Equations or equivalent
BSEN 350 Soil and Water Resources Engineering, or NRES 453/853 Hydrology, or equivalent

Course Description:

Principles and modeling of fluid flow and solute transport in the vadose zone. Topics include hydraulic properties of variably saturated media, application of Darcy's Law in variably saturated media, hydrologic and transport processes in the vadose zone, and solution of steady and unsteady flow problems using numerical techniques including finite element methods. Contemporary vadose zone models will be applied to engineering flow and transport problems. Review and synthesis of classic and contemporary research literature on vadose zone hydrology will be embedded in the course.

Educational Objectives:

Students who complete this course will be:

- Literate in their understanding of the vadose zone and its importance in hydrologic processes, agriculture, and environmental issues.
- Literate in their understanding of the key properties of fluids, porous media and solutes, and how the properties are estimated and described mathematically, including a graphical approach for characterizing problems with energy head profiles.
- Competent in formulating and analytically solving commonly encountered steady and transient one-dimensional isotropic fluid flow and solute transport problems in the vadose zone.
- Competent in using numerical methods and models (HYDRUS 1D) to model fluid flow and solute transport in the vadose zone.
- Familiar with a base of key classic published research literature, and a selection of current research literature pertaining to vadose zone hydrology.

Text:

Radcliffe, D. E., & Šimůnek, J. 2010. *Soil Physics with HYDRUS*. CRC Press.

Software:

HYDRUS 1D (public domain), https://www.pc-progress.com/

Course Schedule:

Date	Modules (topics)	Readiness Tests	Reading
Jan. 26	Introduction to Vadose Zone Hydrology (vadose zone defined, vadose zone significance)		Ch. 1
Section 1: Fluids in Porous Media			
Jan. 28	Soil and Water Properties (soil solid phase, capillarity, fluid energy states)		Ch. 1, 2.4, 2.7
Feb. 2	Hydrostatic equilibrium (hydrostatic equilibrium, tensiometers, lab tour)	RT 1 (Ch. 1, 2.4, 2.7)	Ch. 2
Feb. 4	Soil Water Retention Curves (retention curve principles, lab tour, retention curve hydrostatics)		Ch. 2.9; van Genuchten (1980)
Feb. 9	Retention Curve Models (equations and parameters, pedotransfer functions)	RT 2 (Ch. 2, except 2.6)	Ch. 2.10; Schaap et al. (2001), Saxton & Rawls (2006)
Section 2: Steady Water Flow			
Feb. 11	Darcy's Law (Henry Darcy and the making of a law, lab tour)		Ch. 3.1, 3.2; Brown (2002)
Feb. 16	Poiseuille Flow & K_s (the Poiseuille equation, application to porous media)	RT 3 (Ch3.1, 3.2; Brown, 2002)	Ch. 3.2, 3.6
Feb. 18	Spatial Variability in K_s (measurements and statistics, flow in layered media)		Ch. 3.2, 3.4, 3.6; Kutilek & Nielsen (1994)
Feb. 23	[no new material]	RT 4 (Ch. 3.2, 3.4, 3.6; Kutilek & Nielsen, 1994)	
Feb. 25	Unsaturated Hydraulic Conductivity [$K(h)$ defined, lab tour, $K(h)$ equations]		Ch. 3.3, 3.4
Mar. 2	Steady Unsaturated Flow (Buckingham-Darcy equation, macroscopic capillary length)		Ch. 3.3
Mar. 4	Numerical Integration for Unsaturated Flow (the integral solution, application to a lagoon)		Ch. 3.3
Mar. 9	Graphical Approach for Steady Flow (vertical flow above a water table, downward unsaturated flow in layered media)	RT 5 (Ch. 3.3)	Ch. 3.3
Section 3: Transient Water Flow			
Mar. 11	Richards Equation (introduction, water content form)		Ch. 5.1, 5.2; Richards (1931)

Mar. 16	*[prep for exam]*		
Mar. 18	*Midterm Exam*		Ch. 1-3; related materials
Mar. 23	Solving RE over a Domain (initial and boundary conditions)		Ch. 5.2
Mar. 25	HYDRUS for Flow (infiltration example, deep percolation demonstration)		Ch. 5.4.1, 5.5; HYDRUS-1D Manual
Mar. 30	Numerical Methods for RE (discretization, practical guidelines, numerical stability, explicit method, implicit method)	RT 6 (Ch. 5.1, 5.2, 5.4.1)	Ch. 5.3; Cella et al. (1990)
Apr. 1	Horizontal Infiltration / Imbibition (Bruce-Klute lab test, sorptivity, water content form ODE, measuring diffusivity)		Klute & Dirksen (1986)
Apr. 6	Infiltration (overview, Green & Ampt, Mein & Larson)	RT 7 (Ch. 5.3, imbibition)	Ch. 5.4
Apr. 8	Preferential Flow (overview, Source-Responsive Model)	RT 8 (Ch. 5.4)	Ch. 5.8
Section 4: Solute Transport			
Apr. 13	Solute Transport Processes (advection and diffusion, thought experiment, hydrodynamic dispersion)		Ch. 6.1, 6.2
Apr. 15	Advection-Dispersion Equation (derivation, analytical solutions, nitrate leaching example, lab tour)		Ch. 6.3.1-6.3.3
Apr. 20	Numerical Methods for Transport (ADE discretization, practical guidelines, HYDRUS demo)	RT 9 (Ch. 6.1 – 6.3.3)	Ch. 6.5-6.7
Apr. 22	Adsorption (isotherms, ADE, HYDRUS demo) *Project Presentations*		Ch. 6.3.4
Apr. 27	Preferential Transport (nonequilibrium, phosphorus leaching example)	RT 10 (Ch. 6.3.4, 6.5)	Ch. 6.3.8; Šimůnek & van Genuchten (2008), Heeren et al. (2017), Freiberger et al. (2018)
Apr. 29	*Project Presentations*		
May 4 (3:30 – 5:30)	*Final Exam*		Ch. 5-6; related materials

Section 1: Fluids in Porous Media

Soil Phases

Volume

$$\left[V = \overbrace{V_g + V_l}^{V_v \to \text{void}} + V_s \right] \Big/ V$$

↳ total

$$1 = a + \theta + \frac{V_s}{V}$$

$$\phi = \text{porosity} = \frac{V_v}{V}$$

Mass

$$m = \cancel{m_g}^{\,0} + m_l + m_s$$

bulk density $= \rho_b = \dfrac{m_s}{V}$

particle density $= \rho_s \approx 2.65\ g/cm^3$ (mineral)

↳ lower if much OM

$$\phi = 1 - \frac{\rho_b}{\rho_s}$$

Water Content

$$\theta = \frac{V_l}{V}$$

$$\theta_g = \frac{m_l}{m_s}$$

↳ gravimetric

$$\theta = \frac{\rho_b}{\rho_w}\,\theta_g$$

Capillarity

Interface between 2 fluids

Contact point between 2 fluids & a solid
- wetting fluid (water climbs tube, adhesion)
- non-wetting fluid

Contact angle = α

$\alpha < 90^\circ \Rightarrow$ wetting fluid

(measure angle through the fluid of interest

Mercury: $\alpha > 90$ (nw)

air $\Rightarrow$ wetting fluid

Water drop on wax paper

Forest fire, Lawn highom } temporarily hydrophobic

$$h_{cr} = \frac{2\sigma \cos(\alpha)}{\rho_w g r}$$

σ : surface tension, water

r = radius capillary tube

"capillary pressure" $= P_c = P_{nw} - P_w$

$$[P_c > 0]$$

- applicable 2 immiscible fluids
- fluid mechanics: curved surface $\Rightarrow$ must be pressure diff

Fluid Energy States

Potential

$\psi \;[=]\; Pa, psi$

$\psi_m = \psi_w - \psi_{nw} = \psi_w - \psi_a$

↳ matric

$\left[\psi_m < 0\right]$

$\psi_m = -P_c$

$\psi_m = \psi_w$ if $\psi_a = 0$ (atmospheric)

"osmotic potential" $= \psi_s$

↳ solute

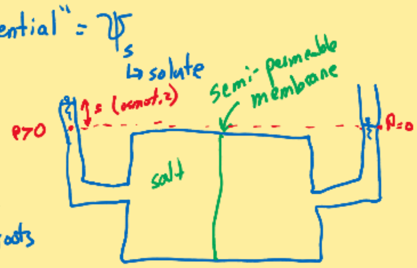
$\psi_s < 0$

add salt → lowers energy

→ flow → higher pressure

plays a role in plant roots

porous media → no effect (no membr.)



Unsaturated Soil:

$\psi_t = \psi_z + \psi_m + \cancel{\psi_s}^{\,0} + \psi_a$

↳ total ↳ gravitation, datum, z positive upwards

$\psi_t = \psi_z + \psi_m + \psi_a$ $\qquad\qquad$ $\psi_m = \psi_w - \psi_a$

$\psi_t = \psi_z + \psi_w$

Head

pressure = $\frac{\text{energy}}{\text{volume}}$

$E = F \cdot L$

$P = \frac{E}{V} = \frac{F \cdot L}{L^3} = \frac{F}{L^2}$

"head" $= \frac{\text{energy}}{\text{unit wt.}} = \frac{E}{F} = \frac{\cancel{F} \cdot L}{\cancel{F}} = L$

- common in VZH
- convenient (elev.)

$\psi = \rho g h$ → head

↳ e.g. water, Hg

$h = \frac{\psi_w}{\rho g}$

↳ pressure head of water

$h_m = h - a$

↳ matric $\qquad$ ↳ air

$H_t = z + h_m + \cancel{s}^{\,0} + a$

↳ total $\quad$ ↳ elev $\quad$ (h_m: → Table) $\quad$ ↳ osmotic head $\quad$ ↳ air

$H_t = z + h_m + a$

$H = z + h$

hydraulic head ↳ water

if $a = 0$, $h = h_m$

Hydrostatic Equilibrium

$H = h + z$

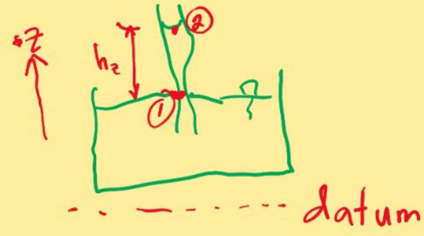
Bernoulli

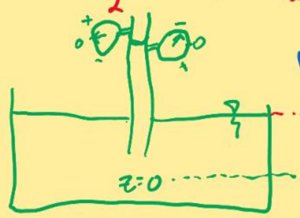
$H_1 = H_2$

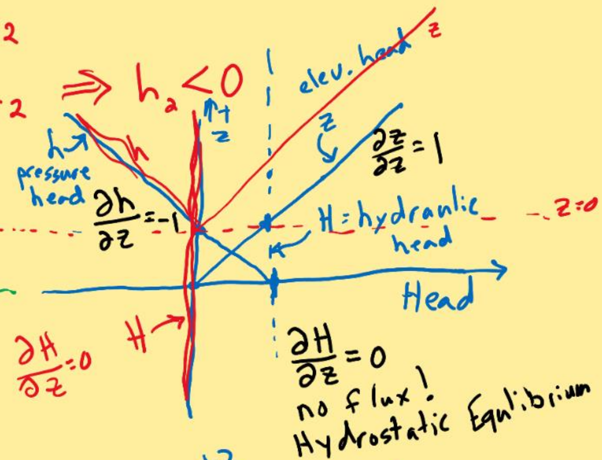
$\cancel{h_1}^{\,0} + z_1 = h_2 + z_2$

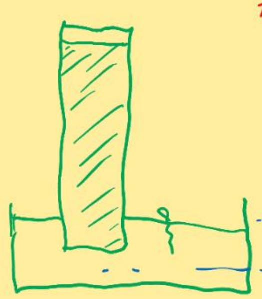
$z_1 = h_2 + z_2$

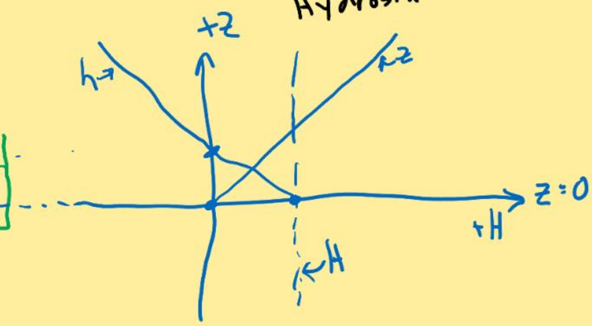
$h_2 = z_1 - z_2 \Rightarrow h_2 < 0$











Tensiometers

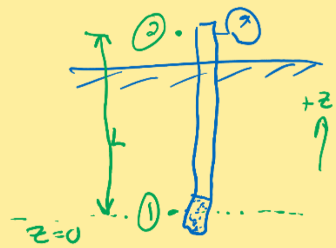
Bernoulli:

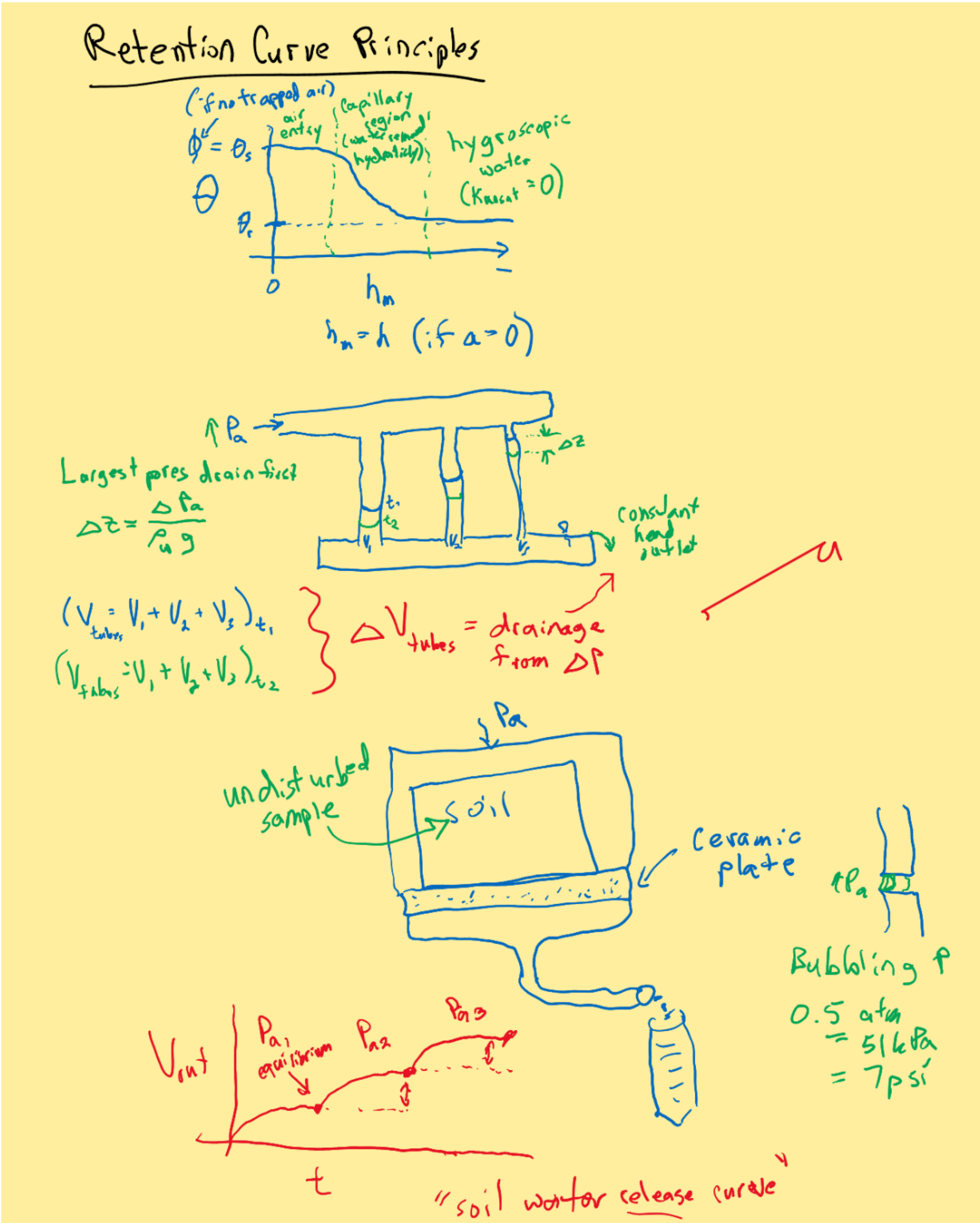
$$H_1 = H_2$$

$$h_1 + \cancel{z_1}^{\,0} = h_2 + \cancel{z_2}^{\,L}$$

$$\boxed{h_1 = h_2 + L}$$

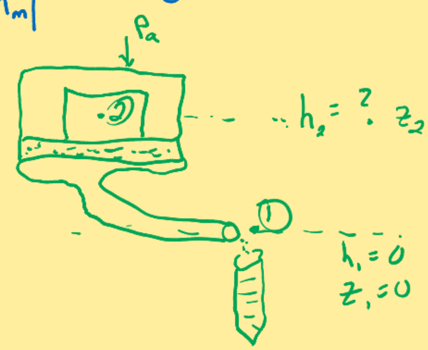
$$h_2 = \frac{-P_{gauge}}{\rho_w g}$$




Retention Curve Principles
(if no trapped air)
air entry
capillary region (water removed hydraulically)
hygroscopic water ($K_{unsat} = 0$)
$\phi = \theta_s$
θ
θ_r
0
h_m
$h_m = h$ (if $a = 0$)
$\uparrow P_a$
Δz
Largest pores drain first
$\Delta z = \frac{\Delta P_a}{\rho_w g}$
t_1
t_2
V_1 V_2 V_3
constant head outlet
$(V_{tubes} = V_1 + V_2 + V_3)_{t_1}$
$(V_{tubes} = V_1 + V_2 + V_3)_{t_2}$
ΔV_{tubes} = drainage from ΔP
P_a
undisturbed sample
soil
ceramic plate
$\uparrow P_a$
Bubbling P
0.5 atm = 51 kPa = 7 psi
V_{out}
P_{a1}
equilibrium
P_{a2}
P_{a3}
t
"soil water release curve"

Retention Curve Hydrostatics

(P_a) particular pressure step



$H_1 = H_2$

$h_1 + z_1 = h_2 + z_2$

$h_2 = -z_2$

next increment in P_a

$h_2 = ?$

$h_2 = -z_2$!

$h_m = h - h_a = h - a$

$H = h + z \qquad \frac{\partial H}{\partial z} \Rightarrow$ flux

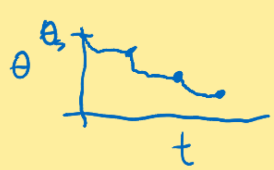
How do we push the water out if h doesn't change?

$h_2 = -z_2$ assumed hydrostatic equilibrium

$\uparrow P_a \Rightarrow \uparrow a \Rightarrow \uparrow h$ temporarily $\Rightarrow \frac{\partial H}{\partial z} \neq 0 \Rightarrow$ removes water

(h_m not change yet

h_m changes enough $\Rightarrow$ new equilibrium



r doesn't change instantly

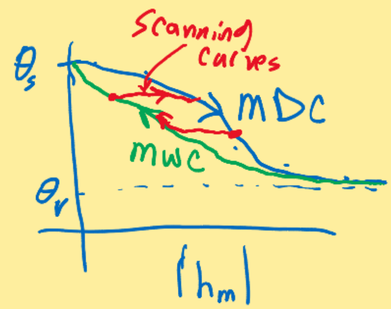
Retention Equations & Parameters

Use MWC if simulating infiltration

Mualem Model

Input MDC

→ estimate MWC & scanning curves



VG (1980)

Effective Saturation = $S_e = \dfrac{\theta - \theta_r}{\theta_s - \theta_r}$ $[0 \le S_e \le 1]$

→ Θ instead of S_e

$$S_e = \frac{1}{\left[1 + (-\alpha h_m)^n\right]^m}$$

Mualem: $m = 1 - \frac{1}{n}$

down to only 2 parameters

VG popular, esp. scientists

BC

h_e = air entry pressure head

(not to be confused w/ ha for air)

– macropores, cracks from structure

$S_e = 1$ $\quad h_m \ge h_e$ less negative (wet)

$S_e = \left(\dfrac{h_e}{h_m}\right)^{\lambda}$ $\quad h_m < h_e$ more neg (drier)

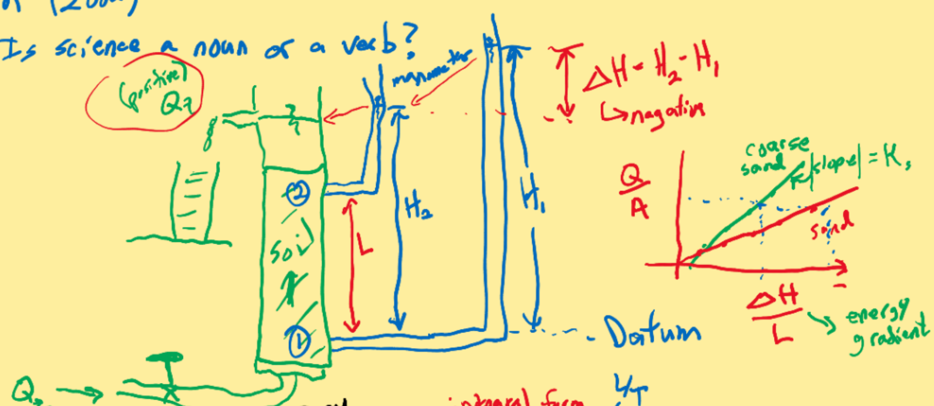
Need 2 parameters

Section 2: Steady Water Flow

Darcy's Law

Brown (2002)

→ Is science a noun or a verb?



$$\frac{L}{T} = \frac{L^3/T}{L^2} [=] \overbrace{\frac{Q}{A}}^{\text{Darcy flux}} = -K_s \overbrace{\frac{\Delta H}{L}}^{\text{integral form}} [=] (?) \frac{L}{L}$$

compare Ohm's Law

cross-sectional area soil

$$\text{Water Flux} = \text{Darcy Flux} = J_w [=] \frac{L}{T}$$

$$\text{Hydraulic gradient} = i = \frac{\Delta H}{L} = \frac{dH}{dz} [=] \frac{L}{L}$$

$$J_{w,z} = -K_s \overbrace{\frac{dH}{dz}}^{\text{differential form}} \hookrightarrow \frac{\partial H}{\partial z}$$

$$\vec{J}_w = -K_s \nabla H = -K_s \left[\frac{\partial H}{\partial x}\hat{i} + \frac{\partial H}{\partial y}\hat{j} + \frac{\partial H}{\partial z}\hat{k}\right]$$

isotropic ↙ ↳ del operator (gradient)

J_w = Darcy flux

$$\text{Mean pore velocity} = \frac{J_w}{\phi}$$

(doesn't account for tortuosity)

Poiseuille Flow

Navier-Stokes

Poiseuille (1842): blood flow in arteries

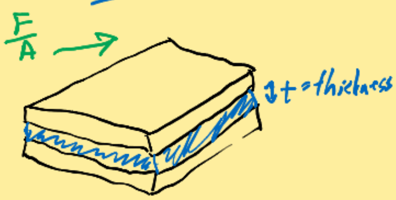
Assumptions:

- Steady flow
- Laminar flow (typical for flow in porous)
  - → no energy loss due to inertial forces
  - → resistance force only due to viscocity
- ρ is constant

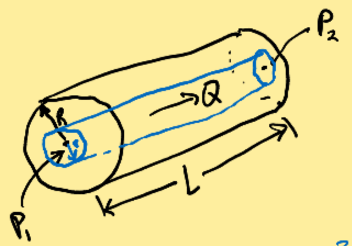
$$\left.\right\} \nabla \vec{V} = 0 \qquad \nabla(\text{fluid inertia}) = 0$$

Dynamic Viscocity $= \eta \; [=] \; \frac{M}{LT}$

$$V = \frac{\left(\frac{F}{A}\right)t}{\eta}$$



Poiseuille Flow (cylinder)



Free body diagram:

$$\Sigma F = m\cancel{a}^{\,0} = 0$$

steady state → $F_s = F_p$

$$F_p = \pi r^2 (P_2 - P_1) = \pi r^2 \Delta P$$

$$F_s = \underbrace{\tau}_{\text{shear stress}} (2\pi r L)$$

$$\tau(2\cancel{\pi}\cancel{r}L) = \cancel{\pi} r^{\cancel{2}} \Delta P$$

$$\tau = r\frac{\Delta P}{2L}$$

$$\tau = -\eta \frac{dV}{dr}$$

Find: $V(r)$

$$r\frac{\Delta P}{2L} = -\eta\frac{dV}{dr}$$

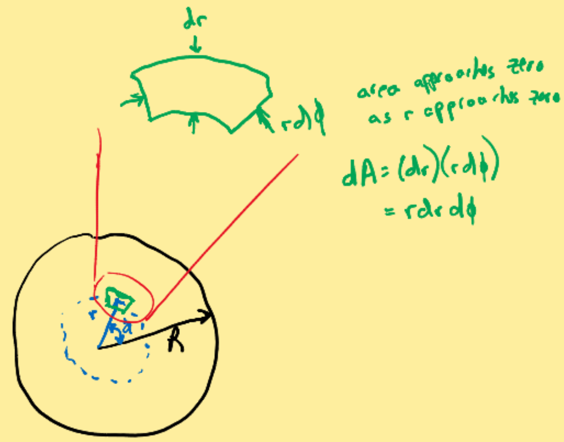
$$r\,dr = -\frac{2L\eta}{\Delta P}dV$$

$$\int_r^R r\,dr = -\frac{2L\eta}{\Delta P}\int_{V(r)}^0 dV$$

$$\left.\frac{r^2}{2}\right|_r^R = -\frac{2L\eta}{\Delta P}\left. V\right|_{V(r)}^0$$

$$\frac{R^2}{2} - \frac{r^2}{2} = 0 + \left(+\frac{2L\eta}{\Delta P}V(r)\right)$$

$$\boxed{V(r) = \frac{\Delta P}{4L\eta}(R^2 - r^2)}$$



$$dA = (dr)(r\,d\phi) = r\,dr\,d\phi$$

Find: $Q \; [=] \; \frac{L^3}{T}$

$$Q = \int V(r)\,dA$$

$$= \int_0^{2\pi}\int_0^R V(r)\,r\,dr\,d\phi$$

$$= \left.\phi\right|_0^{2\pi}\int_0^R V(r)\,r\,dr$$

$$= 2\pi\int_0^R V(r)\,r\,dr \quad \rightarrow V(r) = \frac{\Delta P}{4L\eta}(R^2 - r^2)$$

$$= \frac{\Delta P\pi}{2L\eta}\int_0^R (R^2 - r^2)\,r\,dr$$

$$= \frac{\Delta P\pi}{2L\eta}\left[R^2\int_0^R r\,dr - \int_0^R r^3\,dr\right]$$

$$= \frac{\Delta P\pi}{2L\eta}\left[R^2\left.\frac{r^2}{2}\right|_0^R - \left.\frac{r^4}{4}\right|_0^R\right]$$

$$= \frac{\Delta P\pi}{2L\eta}\left[\frac{R^4}{2} - \frac{R^4}{4}\right]$$

$$\boxed{Q = \frac{\Delta P\pi R^4}{8L\eta}}$$

Poiseuille Applied to Porous Media

Saturated: $Q = \dfrac{\Delta P \pi R^4}{8 L \eta}$

$$\bar{V} = \frac{Q}{A} = \frac{R^2 \Delta P}{8 \eta L}$$

Unsaturated: Flow in a thin film

$$\bar{V} = \frac{b^2 \Delta P}{12 \eta L}$$

$$\text{thickness} = b = \frac{\theta}{\underbrace{(SA)}_{\text{surface area}}(\rho_b)}$$

Can we get to Darcy's Law (K_s) theoretically?

Flow in a capillary tube

$$\bar{V} = \frac{R^2 \Delta P}{8 \eta L} \qquad \text{Convert to units of } H$$

$$\bar{V} = \underbrace{\frac{R^2}{8}}_{\substack{\text{geometry}\\ \text{of pore}\\ \text{space}}} \underbrace{\frac{\rho_w g}{\eta}}_{\substack{\text{fluid}\\ \text{properties}}} \underbrace{\frac{\Delta H}{L}}_{\substack{\text{energy}\\ \text{gradient}}}$$

$$J_w = \bar{V} = -\frac{R^2}{8} \frac{\rho_w g}{\eta} \frac{\partial H}{\partial x}$$

Darcy:

$$J_w = -K_s \frac{\partial H}{\partial z}$$

$$J_w = -\underbrace{k}_{\substack{\text{permeability}\\ \text{geometry of}\\ \text{pore space}}} \underbrace{\left(\frac{\rho_w g}{\eta}\right)}_{\substack{\text{fluid}\\ \text{properties}}} \frac{\partial H}{\partial z}$$

Kozeny Eq: attempt to connect w/ k

Would need to mathematically describe pore space

Too complex to solve PDE

Leap to get k (pore size distribution, tortuosity, dead end pores.... get lumped into k or K_s)

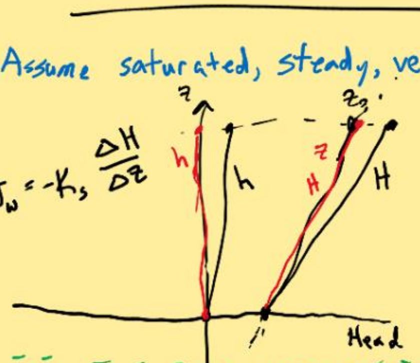
Measure in lab

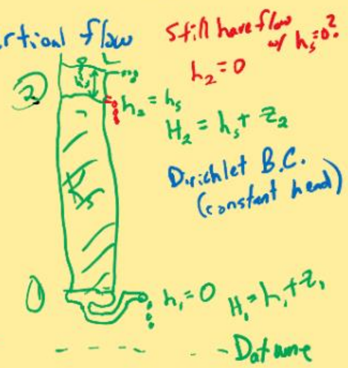
Vertical Flow in Layered Media

Assume saturated, steady, vertical flow

Still have flow w/ $h_s = 0$?

$$J_w = -K_s \frac{\Delta H}{\Delta z}$$





$\frac{\partial H}{\partial z} > 0 \Rightarrow$ still have flow $\Rightarrow J_w < 0$

gravitational flow

unit gradient: $\frac{\partial H}{\partial z} = 1$

How calculate h distribution?

Same BCs

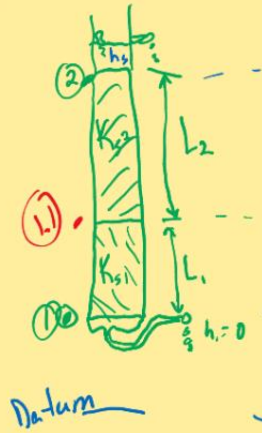
How calc flux?

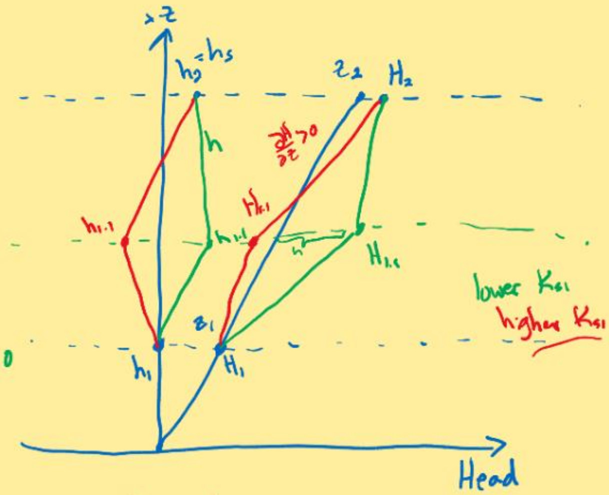
Ohm's Law: series

$R_2 = \frac{1}{C_2}$

$R_1 = \frac{1}{C_1}$

$R_T = R_1 + R_2$





lower K_{s1}

higher K_{s1} $\left.\frac{\partial H}{\partial z}\right|_1 < \left.\frac{\partial H}{\partial z}\right|_2$

Darcy:

$$\frac{K_s}{L} = C_s = \frac{1}{R_s}$$

$$R_s = \frac{L}{K_s} = \frac{L_1 + L_2}{K_{eff}}$$

$$R_T = R_{s1} + R_{s2} = \frac{L_1}{K_{s1}} + \frac{L_2}{K_{s2}}$$

$$K_{eff} = \frac{L_1 + L_2}{R_T} = \frac{L_1 + L_2}{L_1/K_{s1} + \frac{L_2}{K_{s2}}}$$

harmonic mean
length-weighted K_s
small K_s bigger impact

$$J_w = -K_{eff} \frac{\Delta H}{\Delta z}$$

Apply Darcy to a single layer

$$J_w = -K_{s1}\left(\frac{H_{1,1} - H_1}{z_{1,1} - z_1}\right)$$

$$H_{1,1} = \underbrace{\frac{-J_w L_1}{K_{s1}}}_{\text{positive term (since } J_w \text{ is downward)}} + H_1$$

so $H_{1,1} > H_1$

also $H_{1,1} < H_2$

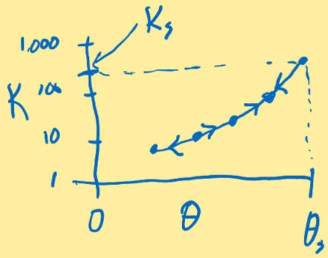
Negative h!
→ unsaturated? No air
→ can h increase along the flow path??
Flow is driven by $\frac{\partial H}{\partial z}$

Unsaturated Hydraulic Conductivity

$J_w = -K_s \frac{dH}{dz}$ Steady saturated flow

$J_w = -\underline{K} \frac{dH}{dz}$ Steady unsaturated flow

$K(\theta)$ negligible hysteresis



$\theta(h_m)$

assumes immiscible fluids ?

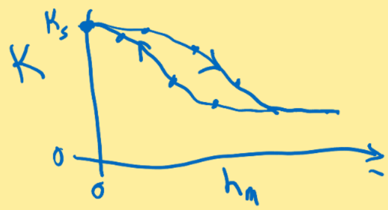
$K(\theta(h_m))$

hysteresis

$K(h_m)$

$h_m = h - \cancel{h_a}^{\,0}$

$K(h)$ unsaturated hydraulic conductivity function



K(h) Equations

VG: $$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

$$K(S_e) = K_s S_e^{\overset{\nearrow \text{as initially}}{\ell}} \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2$$

→ need K_s, retention curve (same parameters)

$m = 1 - \frac{1}{n}$

$$S_e = \left[\frac{1}{1 + (\alpha h)^n}\right]^m$$

$$K_r = \frac{K(S_e)}{K_s}$$

prefer $K(h)$...

$$K_r(h) = \frac{\left\{1 - (\alpha h)^{n-1}\left[1 + (\alpha h)^n\right]^{-m}\right\}^2}{\left[1 + (\alpha h)^n\right]^{m/2}}$$

$\ell = \frac{1}{2}$

BC relate back to
air entry concept

$$K = \begin{cases} K_s, & h \geq h_e \\ K_s\left(\frac{h_e}{h}\right)^{2+3\lambda}, & h < h_e \end{cases}$$

λ reflects pore size distribution

$$K = K_s S_e^{\frac{2+3\lambda}{\lambda}} \qquad (\text{using } \ell = 2)$$

BC parameters ⇒ VG ?

$n = \lambda + 1$
$\alpha = 1/h_e$

some qualifications
read VG...

PTFs (e.g. RETC)

→ retention curve
→ K_s
→ $K(\theta)$
→ $K(h)$

Buckingham-Darcy Equation

Most general form of Darcy:

$$\vec{J}_w = -\hat{K}(\theta)\vec{\nabla}H$$

$\hookrightarrow$ tensor (if anisotropic)

$$\vec{\nabla} = \frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}$$

Assume 1D flow (isotropic)

$$J_w = -K(\theta)\frac{\partial H}{\partial z} \qquad H(z,t)$$

Assume steady flow

By definition: $dH = \underbrace{\frac{\partial H}{\partial z}dz}_{} + \cancel{\frac{\partial H}{\partial t}}^{0}dt$

$$\frac{dH}{dz} = \frac{\partial H}{\partial z}$$

$$J_w = -K(\theta)\frac{dH}{dz}$$

Assume saturated flow:

$$J_w = -K_s\frac{dH}{dz} \quad \text{(differential form)}$$

$$J_w = -K_s\frac{\Delta H}{\Delta z} \quad \text{(integral form, i.e., integrate diff. form)}$$

When can I use this form?

If K is constant in the domain

(then $\frac{dH}{dz}$ is constant in the domain)

Steady Unsaturate Flow:

$$J_w = -K(h)\frac{dH}{dz}$$

$$H = h + z$$

$$\frac{dH}{dz} = \frac{dh}{dz} + 1$$

$$\boxed{J_w = -K(h)\left(\underbrace{\frac{dh}{dz}}_{\text{capillarity}} + \underbrace{1}_{\text{gravity}}\right)} \rightarrow \text{Buckingham-Darcy}$$

$$J_w = -\bar{K}\left(\frac{\Delta H}{\Delta z}\right) \quad ??$$

$\hookrightarrow$ avg of K_1 & K_2

z_2 @ $h_2 = -1{,}000$ cm

$K(h_2) = 0.9 \times 10^{-6}$ cm/hr

30 cm

$\uparrow J_w$

z_1 @ $h_1 = -10$ cm

$K(h_1) = 2 \times 10^{0}$

$= 2$ cm/hr

No!!

$K(h)$ is almost never constant in space

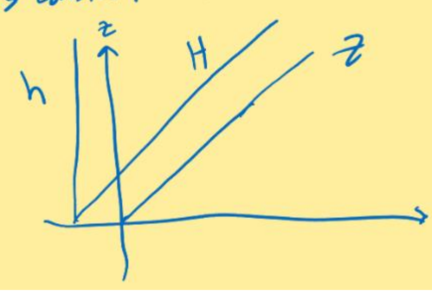
Shape of $K(h)$ is big driver for solution of the problem

Only Exception:

$K(h)$ is constant if unit gradient condition (& steady flow)

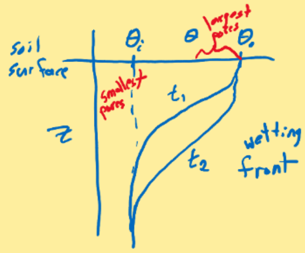
$$1 = \frac{dH}{dz} = \cancel{\frac{dh}{dz}}^{0} + 1 = 1$$

h is constant across domain



Macroscopic Capillary Length (λ_c)

Consider infiltration

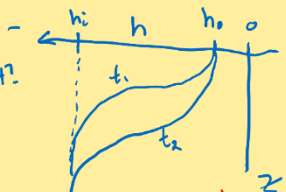


Consider flux....

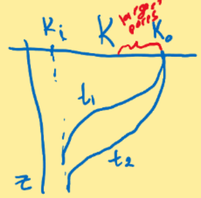
Top boundary: h_o

What is "h" at the wetting front?

λ_c = effective h for unsaturated flow.

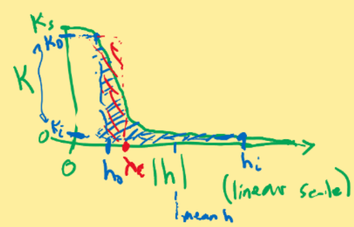


λ_c = K(h)-weighted avg h



how calculate this?

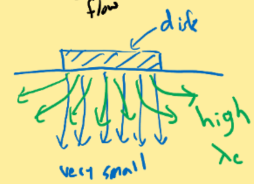
$$\lambda_c = \frac{\int_{h_i}^{h_o} K(h)\,dh}{K(h_o) - K(h_i)}$$



Steady Infiltration from Ring Infiltrometer

Wooding (1968)

$$\underset{\text{infiltration}}{i}_{\underset{\text{steady}}{s}} = \underbrace{K(h_o)\left(1\right.}_{\text{gravity flow}} + \underbrace{\left.\frac{4\lambda_c}{\pi r}\right)}_{\text{effect of capillarity}}$$



$i_s = K(h_o)(1)$

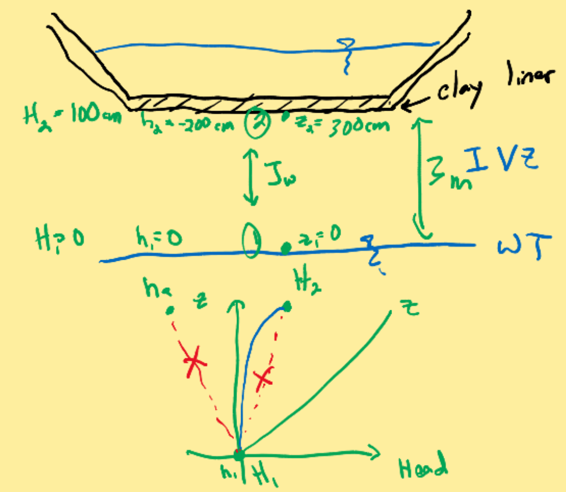
(low clay)

The Integral Solution

Steady flow ($\frac{\partial h}{\partial t}=0$)
1D, vertical flow
Unsaturated flow
Special case: Unit Gradient
→ $\frac{\partial H}{\partial z}=1$ ⇒ $K(h)$ uniform in space

General case: K not constant

wastewater lagoon



Buckingham-Darcy:

$$J_w = -K(h)\left(\frac{\partial h}{\partial z}+1\right)$$

$$-\frac{J_w}{K(h)} = \frac{dh}{dz}+1$$

$$-\left[\frac{J_w}{K(h)}+1\right] = \frac{dh}{dz}$$

$$dz = \frac{-dh}{\frac{J_w}{K(h)}+1}$$

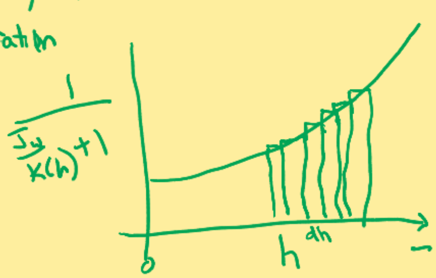
$$\int_{z_1}^{z_2} dz = -\int_{h_1}^{h_2} \frac{1}{\frac{J_w}{K(h)}+1}\,dh$$

$$\boxed{z_2 - z_1 = -\int_{h_1}^{h_2} \frac{1}{\frac{J_w}{K(h)}+1}\,dh}$$

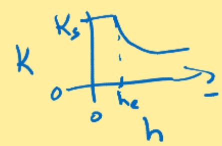
The Integral Solution

Can't solve analytically w/ VG or BC

Numerical Integration
- Excel
- matlab



Iterate w/ J_w
→ initial guess J_w
→ integral ≈ $z_2 - z_1$
→ Excel Solver



$$z_2 - z_1 = -\int_{h_1}^{h_2} \frac{dh}{\frac{J_w}{K(h)}+1}$$

If $h_1 > h_e$, integrate by parts:

$$z_2 - z_1 = -\int_{h_1}^{h_e} \frac{dh}{\frac{J_w}{K(h)}+1} - \underbrace{\int_{h_e}^{h_2} \frac{dh}{\frac{J_w}{K_s}+1}}_{\text{analytical soln}}$$

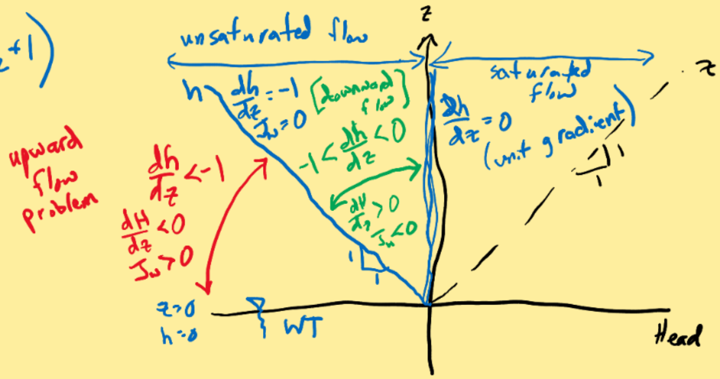
h_e defines capillary fringe

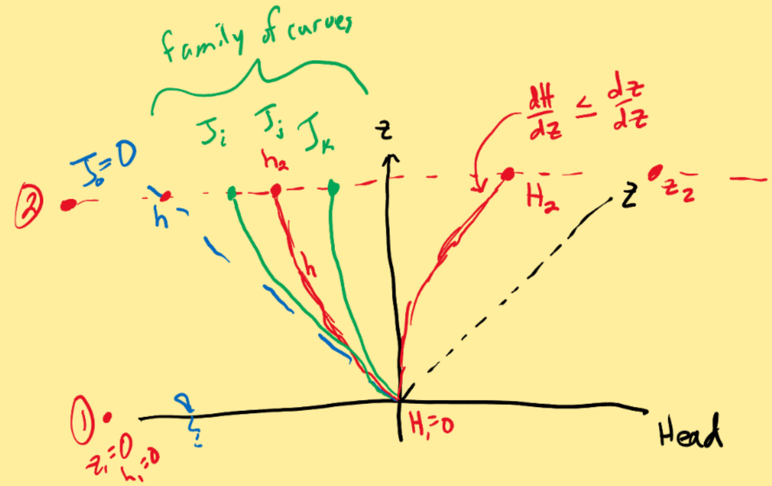
$$= -\int_{h_1}^{h_e} \frac{dh}{\frac{J_w}{K(h)}+1} - \frac{h_2 - h_e}{\frac{J_w}{K_s}+1}$$

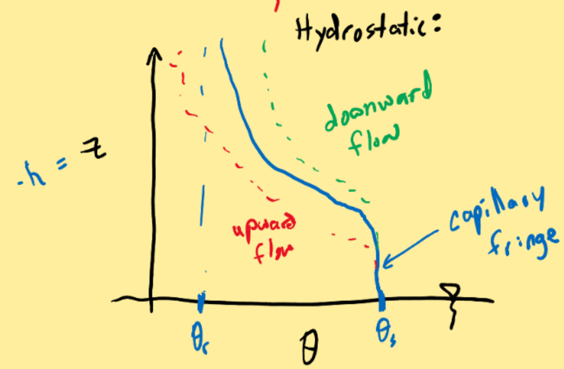
Determine J_w
Then $h(z)$

Vertical Flow Above a Water Table

$J_w = -K\left(\frac{dh}{dz}+1\right)$







$K_1 = K_s,\quad K_2 = K(h_2) \Rightarrow K_2 < K_1$

$J_{w,1} = J_{w,2}$ which is greater?

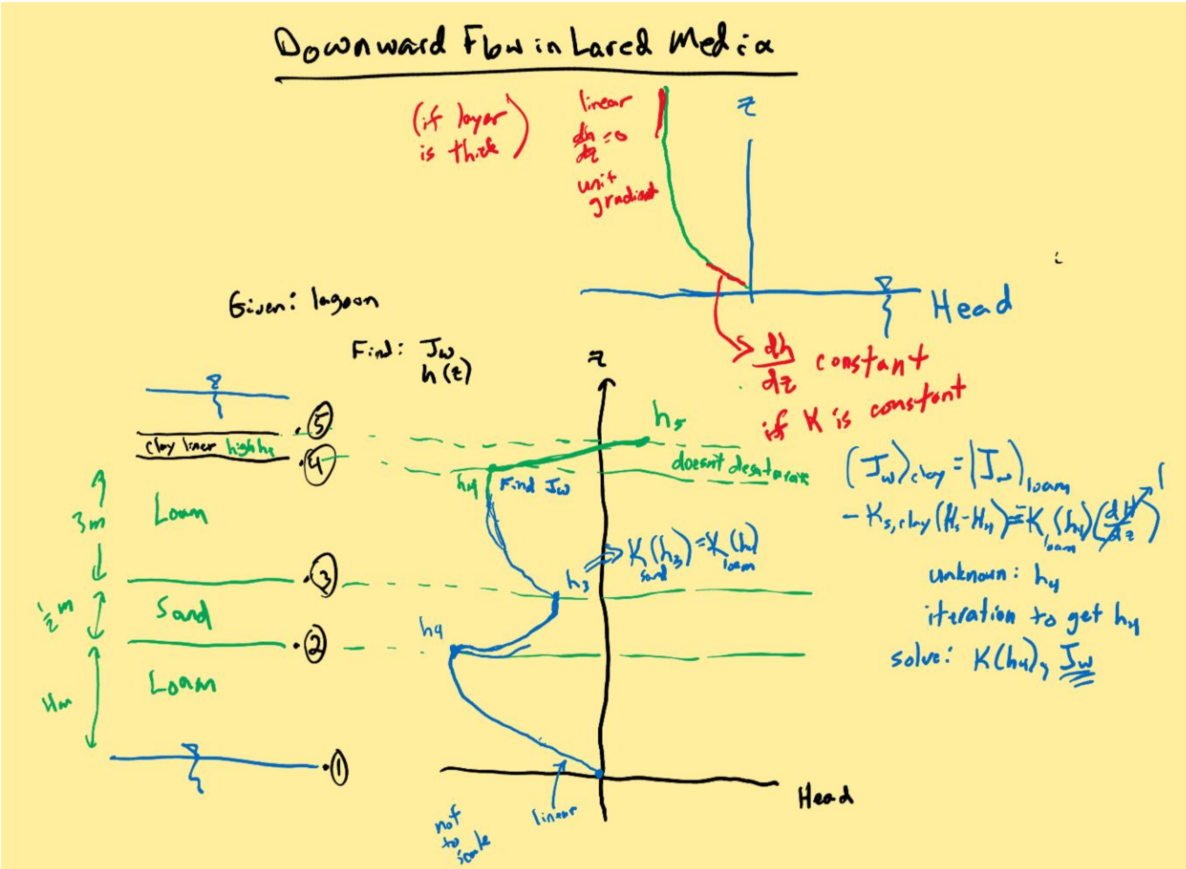
↳ b/c steady flow

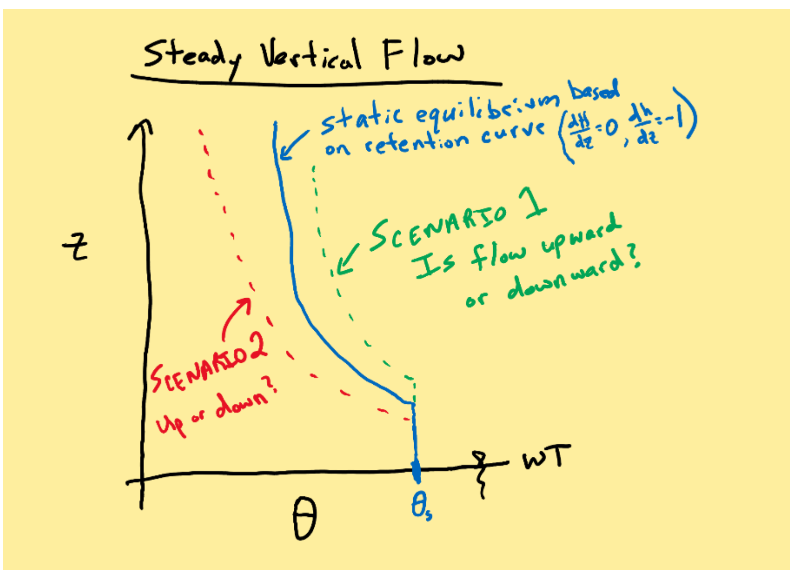
$\left(\frac{dH}{dz}\right)_2 > \left(\frac{dH}{dz}\right)_1$

↳ close to zero, little friction loss

↳ close to 1 much friction loss

$|J_k| > |J_j| > |J_i| > 0$


Downward Flow in Layered Media
(if layer is thick)
linear
$\frac{dh}{dz}=0$
unit gradient
z
Head
$\frac{dh}{dz}$ constant if K is constant
Given: lagoon
Find: J_w, $h(z)$
clay liner high h_s
Loam
3m
Sand
½ m
Loam
H_m
⑤
④
③
②
①
h_s
doesn't desaturate
h_4
Find J_w
$K(h_3)_{sand}=K(h_4)_{loam}$
h_3
h_4
not to scale
linear
Head
$(J_w)_{clay}=(J_w)_{loam}$
$-K_{s,clay}(H_s-H_4)=K_{loam}(h_4)\left(\frac{dH}{dz}\right)$
unknown: h_4
iteration to get h_4
solve: $K(h_4)$, J_w


Steady Vertical Flow
static equilibrium based on retention curve $\left(\frac{dH}{dz}=0, \frac{dh}{dz}=-1\right)$
z
SCENARIO 1
Is flow upward or downward?
SCENARIO 2
Up or down?
WT
θ
θ_s

Introduction to Richards Eq.

So far: Steady flow, $\frac{\partial h}{\partial t} = 0$

Now: Transient flow, $\frac{\partial h}{\partial t} \neq 0$, $\frac{d\theta}{dt} \neq 0$ $\Rightarrow$ changes in storage

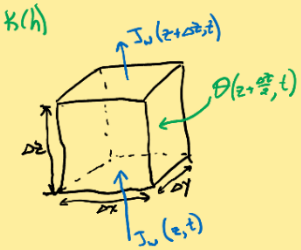
Conservation of Energy

Buckingham-Darcy: $J_w = -K(\theta)\frac{\partial H}{\partial z}$

$$J_w = -K(h)\left(\frac{\partial h}{\partial z} + 1\right)$$

$$J_w = -K(h)\frac{\partial h}{\partial z} - K(h)$$

Conservation of Mass (Continuity Eq.)
- assume fluid density is constant
- consider a small REV
- consider 1D vertical flow (upward)
- consider flow over a time interval from t to $t+\Delta t$



Initial volume of water: $\theta(z+\frac{\Delta z}{2}, t)\Delta x \Delta y \Delta z$ [=] L^3

Final volume: $\theta(z+\frac{\Delta z}{2}, t+\Delta t)\Delta x \Delta y \Delta z$

Total volume across bottom face: $J_w(z, t+\frac{\Delta t}{2})\Delta x \Delta y \Delta t$ [=] L^3

Total volume exiting the top face: $J_w(z+\frac{\Delta z}{2}, t+\frac{\Delta t}{2})\Delta x \Delta y \Delta t$

Conservation of mass:

Δ storage = in − out

$$\theta(z+\tfrac{\Delta z}{2}, t+\Delta t)\Delta x\Delta y\Delta z - \theta(z+\tfrac{\Delta z}{2}, t)\Delta x\Delta y\Delta z = J_w(z, t+\tfrac{\Delta t}{2})\Delta x\Delta y\Delta t - J_w(z+\Delta z, t+\tfrac{\Delta t}{2})\Delta x\Delta y\Delta t$$

divide through by $\Delta x \Delta y \Delta z \Delta t$

$$\frac{\theta(z+\frac{\Delta z}{2}, t+\Delta t) - \theta(z+\frac{\Delta z}{2}, t)}{\Delta t} = \frac{J_w(z, t+\frac{\Delta t}{2}) - J_w(z+\Delta z, t+\frac{\Delta t}{2})}{\Delta z} \; [=] \; \frac{1}{T}$$

By definition:

$$\frac{\partial J_w}{\partial z} = \lim_{\Delta z \to 0}\left[\frac{J_w(z+\Delta z, t) - J_w(z,t)}{\Delta z}\right]$$

↗ order opposite

$$\frac{\partial \theta}{\partial t} = \lim_{\Delta t \to 0}\left[\frac{\theta(z, t+\Delta t) - \theta(z,t)}{\Delta t}\right]$$

Reduce REV to infitesimal
- assumption of continuum mechanics
- continuous mass (not discrete particles)

$$\frac{\partial \theta}{\partial t} = -\frac{\partial J_w}{\partial z}$$

Add a term for sources/sinks (root water uptake)

$$\frac{\partial \theta}{\partial t} = -\frac{\partial J_w}{\partial z} - S(h)$$

Substitute J_w w/ Buckingham-Darcy:

$$\frac{\partial \theta(h)}{\partial t} = -\frac{\partial}{\partial z}\left[-K(h)\left(\frac{\partial h}{\partial z} + 1\right)\right] - S(h)$$

$$= \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} + 1\right)\right] - S(h)$$

$$\boxed{\underbrace{\frac{\partial \theta(h)}{\partial t}}_{\text{storage term}} = \underbrace{\frac{\partial}{\partial z}\left(K(h)\frac{\partial h}{\partial z}\right)}_{\text{capillarity effect}} + \underbrace{\frac{\partial K(h)}{\partial z}}_{\text{gravity effect}} - \underbrace{S(h)}_{\text{sink}}}$$

Richards Equation
Richards (1931)
"Mixed Form"

Transient, vertical 1D flow, variably saturated
Independent variables: t, z
2^{nd} order PDE
Dependent variables: θ, h ("mixed form")
Variable Coefficient: $K(h)$
Usually can't solve analytically
Use numerical methods
Assumed: ρ is constant, media rigid

Goal: reduce eq. to one dependant variable

Chain rule

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial \theta(h)}{dh}\frac{\partial h}{\partial t} = C_w(h)\frac{\partial h}{\partial t}$$

$C_w(h)$ = soil water capacity $= \frac{d\theta(h)}{dh}$

$$\boxed{C_w(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left(K(h)\frac{\partial h}{\partial z}\right) + \frac{\partial K(h)}{\partial z} - S(h)}$$

"pressure head form"
"capacitance form" of RE

Eliminated θ!
h is the only dependant variable

Water Content Form of RE

RE: $\frac{\partial\theta(h)}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]$

$D(\theta)$ = soil water diffusivity

$D(\theta) = K(\theta)\left(\frac{dh}{d\theta}\right)$

Buckingham-Darcy

$$J_w = -K(h)\frac{dh}{dz} - K(h)$$

Some noticed that water appears to move from wet to dry soil...

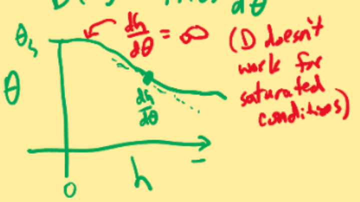
$$\frac{\partial h}{\partial z} = \frac{\partial \theta}{\partial z}\frac{dh}{d\theta}$$

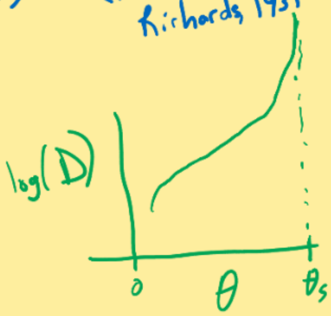
$$J_w = -K(\theta)\frac{\partial\theta}{\partial z}\frac{dh}{d\theta} - K(\theta)$$

$$J_w = -D(\theta)\frac{\partial\theta}{\partial z} - K(\theta)$$

(introduced by Richards 1931)

$$D(\theta) = K(\theta)\frac{dh}{d\theta}$$





Conservation of Mass

$$\frac{\partial\theta}{\partial t} = -\frac{\partial J_w}{\partial z}$$

$$\boxed{\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta)\frac{\partial\theta}{\partial z} + K(\theta)\right]}$$

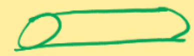
"water content form" of RE

only one dependent variable: θ

two variable coefficients: $K(\theta)$, $D(\theta)$

Special Case I: Horizontal Infiltration (Imbibition)

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left[D(\theta)\frac{\partial\theta}{\partial x}\right]$$



Diffusion equation!

Convenient mathematical form (not direct physical meaning)

→ existing solutions! (parallel Theis)

$D(\theta)$ does not exhibit hysteresis

$D(\theta)$ less nonlinear than $K(\theta)$ and $K(h)$

→ easier to do numerical solutions

Special Case II: surface evaporation

soil becomes dry → $\frac{\partial h}{\partial z} \gg \frac{\partial z}{\partial z}$

gravity term becomes negligible

RE takes the same form:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta)\frac{\partial\theta}{\partial z}\right]$$

How does $D(\theta)$ relate to $C(h)$?

$$D(\theta) = K\frac{dh}{d\theta} = \frac{K}{d\theta/dh} = \frac{K}{C}$$

Domain, ICs, and BCs

Governing Eq: RE

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]$$

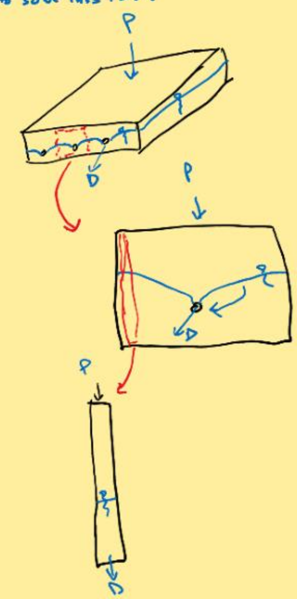
What would it take to solve this PDE?

Domain:

Example: drainage
3D (real life)

Simplify to 2D
- assume homogeneity

Simplify to 1D
- natural drainage only



Initial Conditions (IC):

Example: infiltration

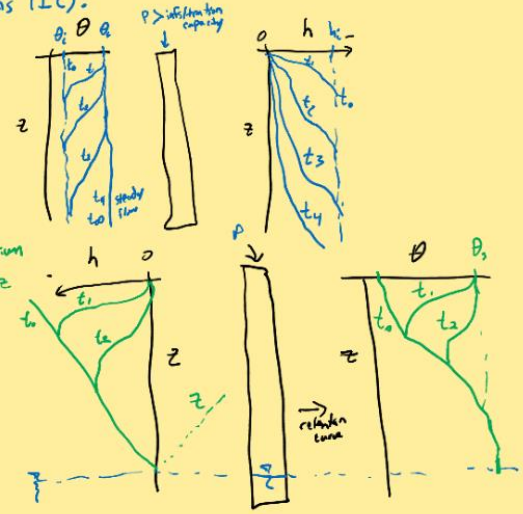
$\theta(z,0) = \theta_i$

prefer pressure head

$h(z,0) = h_i$

Hydrostatic Equilibrium

$h(z,0) = h_i(z) = -z$



Boundary Conditions (BC):

System-independent BCs

"Dirichlet" or Type 1 BC

Upper BC

$h(z_2,t) = h_2$

Lower BC

$h(z_1,t) = h_1$

i.e., constant pressure head

"Neumann" or Type 2 BC

i.e., constant flux

Example: irrigation

$I <$ infiltration capacity

solid set: I is constant

$J_w(z_2,t) = J_0 = -I$

Gradient-type BC

$i(z_1,t) = \frac{\partial h}{\partial z} + 1$

special case: unit gradient

$i(z_1,t) = 1$

"free drainage"

System-dependent BCs

"seepage face" BC

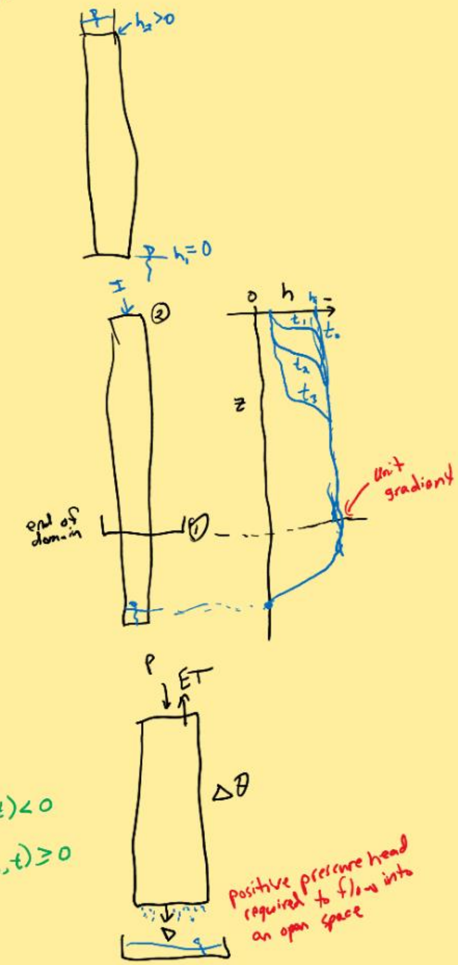
Example: lysimeter

unsaturated:

$J_w(z_1,t) = 0 \quad h(z_1,t) < 0$

saturated:

$h(z_1,t) = 0 \quad h(z_1,t) \geq 0$



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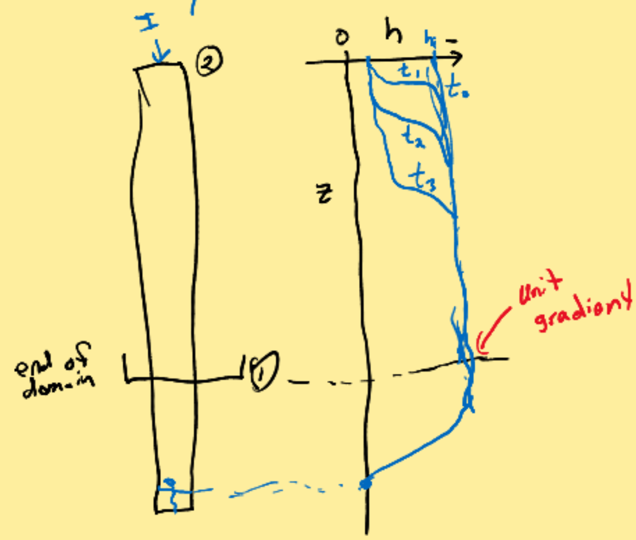
$I <$ infiltration capacity

solid set: I is constant

$$J_w(z_2, t) = J_0 = -I$$



Gradient-type BC

$$i(z_1, t) = \frac{\partial h}{\partial z} + 1$$

special case: unit gradient

$$i(z_1, t) = 1$$

"free drainage"

System-dependent BCs

"seepage face" BC

Example: lysimeter

unsaturated:

$$J_w(z_1, t) = 0 \qquad h(z_1, t) < 0$$

saturated:

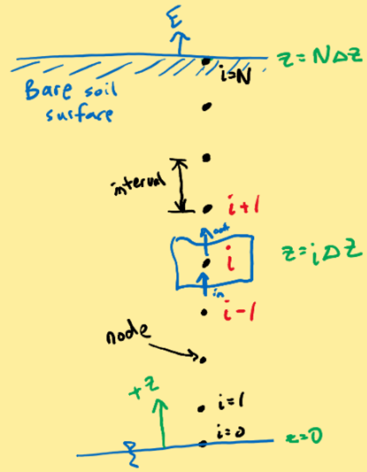
$$h(z_1, t) = 0 \qquad h(z_1, t) \geq 0$$

RE Discretization

RE (pressure head form)

$$C_w(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]$$

Example: upward flux from a shallow WT for E



Discretize into N intervals

$i = 0 \ldots N$ nodes

\# of nodes = N+1

Discretize in time: Δt

$j = 0 \ldots m$

m time steps

m+1 points in time

time at point j:

$$t_j = j\Delta t$$

Assume Δz and Δt are constant in space and time

Buckingham-Darcy

$$K_{i-\frac{1}{2}} = K\left(\frac{h_i - h_{i-1}}{2}\right)$$

In: $J_{i-\frac{1}{2}} = -K_{i-\frac{1}{2}}\left(\frac{\partial h}{\partial z}+1\right) = -K_{i-\frac{1}{2}}\left(\frac{h_i-h_{i-1}}{z_i-z_{i-1}}+1\right) = -K_{i-\frac{1}{2}}\left(\frac{h_i-h_{i-1}}{\Delta z}+1\right)$

Out: $J_{i+\frac{1}{2}} = -K_{i+\frac{1}{2}}\left(\frac{h_{i+1}-h_i}{\Delta z}+1\right)$

Conservation of Mass (in − out = Δθ)

$$\left.\frac{\partial J}{\partial z}\right|_i = \frac{J_{i-\frac{1}{2}} - J_{i+\frac{1}{2}}}{z_{i+\frac{1}{2}} - z_{i-\frac{1}{2}}} = -\frac{J_{i+\frac{1}{2}} - J_{i-\frac{1}{2}}}{\Delta z}$$

$$\left.\begin{aligned} &= + \frac{\left[+K_{i+\frac{1}{2}}\left(\frac{h_{i+1}-h_i}{\Delta z}+1\right)\right] - \left[+K_{i-\frac{1}{2}}\left(\frac{h_i-h_{i-1}}{\Delta z}+1\right)\right]}{\Delta z}\end{aligned}\right\} \text{RHS}$$

$$\overset{\frac{d\theta}{dh}}{C_w}(h)\frac{\partial h}{\partial t}$$

notation: h_i^j — $j \to$ time coordinate, $i \to$ space coordinate

Consider time step Δt from t_j to t_{j+1}

→ evaluate at midpoint in time

node i

$$\left.C\frac{\partial h}{\partial t}\right|_i^{j+\frac{1}{2}} = \underbrace{C_i^{j+\frac{1}{2}}\left(\frac{h_i^{j+1}-h_i^{j}}{\Delta t}\right)}_{LHS}$$

$$C = C(h) = C\left(h_i^{j+\frac{1}{2}}\right)$$

5

$$RE: \; C\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K\left(\frac{\partial h}{\partial z}+1\right)\right]$$

$$C_i^{j+\frac{1}{2}}\left(\frac{h_i^{j+1}-h_i^{j}}{\Delta t}\right) = \frac{K_{i+\frac{1}{2}}\left(\frac{h_{i+1}-h_i}{\Delta z}+1\right)-K_{i-\frac{1}{2}}\left(\frac{h_i-h_{i-1}}{\Delta z}+\cancel{1}^{\frac{\Delta z}{\Delta z}}\right)}{\Delta z}$$

$$= \frac{K_{i+\frac{1}{2}}\left(\frac{h_{i+1}-h_i+\Delta z}{\Delta z}\right)-K_{i-\frac{1}{2}}\left(\frac{h_i-h_{i-1}+\Delta z}{\Delta z}\right)}{\Delta z}$$

$$\boxed{C_i^{j+\frac{1}{2}}\left(\frac{h_i^{j+1}-h_i^{j-1}}{\Delta t}\right) = K_{i+\frac{1}{2}}\frac{h_{i+1}-h_i+\Delta z}{(\Delta z)^2} - K_{i-\frac{1}{2}}\frac{h_i-h_{i-1}+\Delta z}{(\Delta z)^2}}$$

Note: on RHS, we don't have a time index

Goal: solve for state variable h

Options: Explicit method $t = t^j$

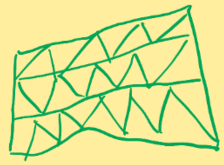
Fully implicit method $t = t^{j+1}$

Crank-Nicolson implicit method $t = t^{j+\frac{1}{2}}$

Practical Guidelines for Numerical Methods

Finite Difference
- rectangles

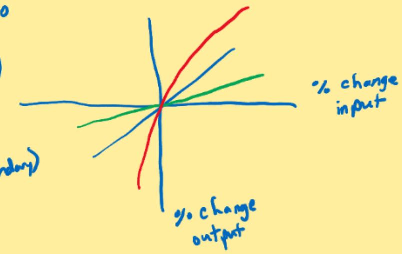
Finite Element
- triangles or other shapes
- complex geometry
- solve at nodes
- shape function
  - h
  - ⇒ distribution of state variable across an element
  - → common to do a linear interpolation



HYDRUS
- finite element in space
- finite difference in time

Quality Control:
- convergence
- mass balance error
- numerical stability

Sensitivity Analysis:
- choose a baseline scenario
- change an input (K_s)
- change in output (cumulative flux across bottom boundary)



Numerical Stability

Explicit Method
- easier calculations
- less stable → need very small time steps

Implicit Method
- need matrix algebra
- more stable → larger time steps → less computational time

Quantify Numerical Stability:

for RE: instability $\approx \dfrac{\Delta t K}{(\Delta z)^2 C}$

$\uparrow K \Rightarrow \uparrow$ flow $\Rightarrow \uparrow$ instability

stability criterion: $\dfrac{\Delta t K}{(\Delta z)^2 C} \leq 0.5$ so that error doesn't grow

$\rightarrow = |a_i|, |c_i|$

$b_i = 1 - a_i - c_i$

if $a_i > 0.5$ and $c_i > 0.5$

then b_i becomes a negative term

→ becomes unstable

Imbibition: Bruce-Klute Lab Test

Imbibition: displacement of one fluid by another immiscible fluid

→ "wicking"

→ capillarity

1D, Homogenous, semi-infinite domain, w/ step change in BC

IC: $\theta(x, t=0) = \theta_i$

BC: $\theta(0, t) = \theta_0$

$\theta(\infty, t) = \theta_i$ stop experiment w/ at least one ring still at θ_i (same in HYDRUS)

Observe:

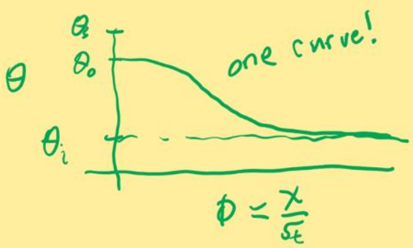
$J_{w,x} \propto \frac{1}{\sqrt{t}}$

Use Boltzman transform:

$$\phi = \frac{x}{\sqrt{t}} \quad (\text{sometimes } \eta \text{ or } \lambda)$$

Now: one indepnt variable

$\theta(x,t) = \theta(\phi)$



Applications

Simpler form of the water content form of RE

Can measure $D(\theta)$ in the lab

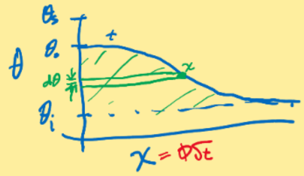
Can measure sorptivity (s)

Mathematically characterize horizontal infiltration

Sorptivity

Cumulative infiltration amount:

$$I(t) = \int_0^\infty \underbrace{(\theta-\theta_i)}_{\text{volume of water}}\, dx$$



Consider alternate perspective.

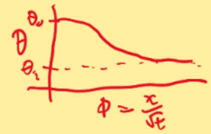
$$I(t) = \int_{\theta_i}^{\theta_0} x\, d\theta'$$

↳ dummy variable of integration

$$= \int_{\theta_i}^{\theta_0} \phi\sqrt{t}\, d\theta'$$

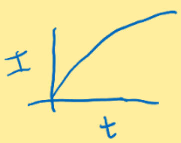
$$I(t) = \sqrt{t}\,\underbrace{\int_{\theta_i}^{\theta_0} \phi\, d\theta'}_{\text{Sorptivity} = S}$$

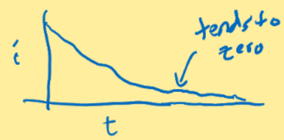
Boltzman Transform



$$S = S(\theta_0, \theta_i) = \int_{\theta_i}^{\theta_0} \phi\, d\theta' \; [=] \; \frac{L}{\sqrt{T}}\,\frac{L^3}{L^3} = \frac{L}{\sqrt{T}}$$

$$\left.\begin{aligned} I &= S\sqrt{t} = S t^{1/2} \\ J_w &= i = \frac{dI}{dt} = \frac{1}{2} S t^{-1/2} \end{aligned}\right\} \text{Philip}$$





Applications

- Horizontal infiltration
- Vertical infiltration if $\frac{\partial h}{\partial z} \gg 1$
- S appears in some equations in capillarity term

Approximation:

$$S \cong \sqrt{1.818\, K_s \lambda_c \Delta\theta}$$

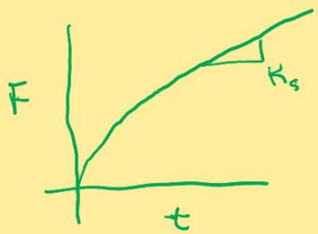
$$D(\theta) = -\frac{1}{2}\frac{d\phi}{d\theta} S(\theta, \theta_i)$$

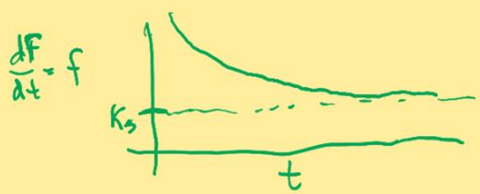
Green & Ampt

f = infiltration rate
F = cumulative infiltration
i = rainfall intensity

} positive values

uniform soil





Approximate w/ piston wetting front

$$J_w = -K_s\left(\frac{h_2 - h_1}{z_2 - z_1} + 1\right)$$

$$= -K_s\left(\frac{h_p - ?}{L} + 1\right)$$

h_f = wetting front suction

h_f is positive

$$h_1 = -h_f$$

$$J_w = -K_s\left(\frac{h_p + h_f}{L} + 1\right)$$

$$f = -J_w$$

$$f = K_s\left(\frac{h_p + h_f}{L} + 1\right)$$

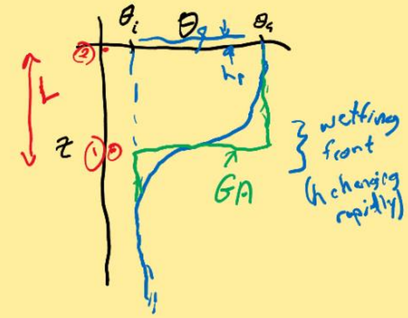
$$F = \Delta\theta L$$

$$L = \frac{F}{\Delta\theta}$$

$$f = K_s\left(\frac{\Delta\theta(h_p + h_f)}{F} + 1\right)$$

C_d = capillary drive function

f is a function of F
(not necessarily time)



$$f = K\left[\frac{C_d}{F} + 1\right]$$

$$\frac{dF}{dt} = K\left[\frac{C_d}{F} + 1\right]$$

$$K\,dt = \frac{dF}{\left[\frac{C_d}{F} + 1\right]}$$

$$K\int_0^t dt = \int_0^F \frac{dF}{\frac{C_d}{F} + 1}$$

$$K_s t = F - C_d \ln\left[1 + \frac{F}{C_d}\right]$$

can't simply find F for a given t

$$t = \frac{F - C_d \ln\left(1 + \frac{F}{C_d}\right)}{K_s}$$

$$K_s t = F - C_d \ln\left[\frac{C_d + F}{C_d}\right]$$

$$f = K_s\left(\frac{C_d}{F} + 1\right)$$

Mein & Larson

Green & Ampt (1911)
Mein & Larson (1973)

$$K_s t = F - C_d \ln\left[1 + \frac{F}{C_d}\right]$$
$$f = K_s\left(\frac{C_d}{F} + 1\right)$$

instantaneous ponding

Constant Flux

$i < K_s$ ⇒ never ponding ⇒ $f = i$

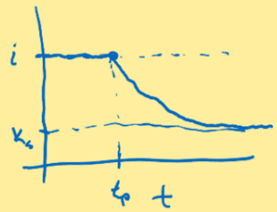
$i > K_s$ ⇒ ponding will start at $t = t_p$

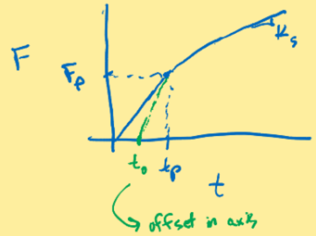
$F = it$ $\quad t < t_p$

$F_p = it_p$ $\quad t = t_p$

2. $\quad t > t_p$

$$f = \frac{dF}{dt}$$





1) $K_s(t_p - t_o) = F_p - C_d \ln\left[1 + \frac{F_p}{C_d}\right]$

2) $K_s(t - t_o) = F - C_d \ln\left[1 + \frac{F}{C_d}\right]$

Subtract Eq. 1) from Eq. 2)

$$\boxed{\begin{array}{ll} K_s(t - t_p) = F - F_p - C_d \ln\left[\frac{C_d + F}{C_d + F_p}\right] & t > t_p \\ F = it & t < t_p \end{array}}$$

implicit

Find t_p:

when $t = t_p$:

$$i = f = K_s\left[\frac{C_d}{F_p} + 1\right]$$
$$i = K_s\left[\frac{C_d}{it_p} + 1\right]$$
$$\boxed{t_p = \frac{K_s C_d}{i(i - K_s)}} \quad i > K_s$$

$$\boxed{\begin{array}{ll} f = i & t \le t_p \\ f = K_s\left(\frac{C_d}{F} + 1\right) & t > t_p \end{array}}$$

HYDRUS

$i < K_s$ ⇒ Neuman BC

$i > K_s$ → expect ponding

System-Dependent BC

constant flux

once reach t_p, changes to constant head BC

What happens to rain that doesn't infiltrate?

→ runoff (Atmospheric BC with surface runoff)

→ pond to accumulate water (Atmospheric BC w/ surface layer)

"Time Variable" BC

Dual Porosity

Macropores – mobile

Matrix – immobile

$$\frac{\partial \theta_{mo}}{\partial t} = \frac{\partial}{\partial z}\left[K(h_m)\left(\frac{\partial h_{mo}}{\partial z}+1\right)\right] - \Gamma_w$$

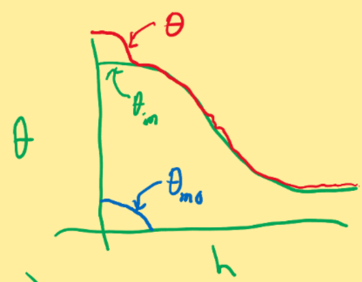
transfer rate

water

$$\frac{\partial \theta_{im}(h_{in})}{\partial t} = + \Gamma_w$$

$$\Gamma_w = \alpha_w \underbrace{(h_{mo} - h_{im})}_{\text{actual driving force}}$$

more parameters



$$\Gamma_w = \omega\left[S_e^{mo} - S_e^{im}\right]$$

(like "diffusivity")

more stable

Preferential Flow Models

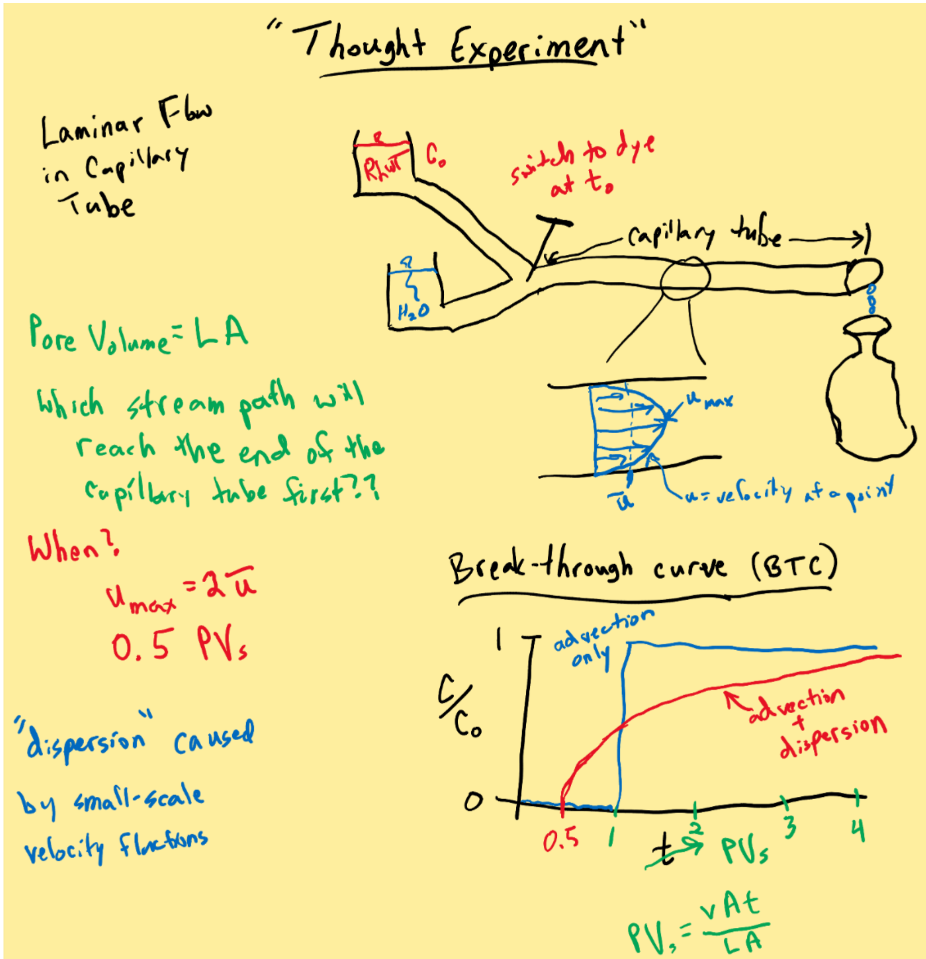
Dual porosity } HYDRUS

Dual permeability } Simunek et al. (2003)

Move away from RE? Beven & Germann (2013)

Source Responsive Model Nimmo (2010)

Section 4: Solute Transport



Advection-Dispersion Equation

$$\underbrace{\frac{\partial(\theta c)}{\partial t}}_{\text{storage term}} = \underbrace{\frac{\partial}{\partial z}\left[\theta D_e \frac{\partial c}{\partial z}\right]}_{\text{dispersion/ diffusion term}} - \underbrace{\frac{\partial(J_w c)}{\partial z}}_{\text{advection term}}$$

Example: N Leaching

No N in initial soil water: $c(z,0)=0$

Saturated soil: $\theta = \phi \rightarrow$ steady flow
$\hookrightarrow \phi = 0.5$

No sorption

Fertilizer event $\rightarrow$ spike input

Worst-case scenario: two large consecutive storms
avg. 2 cm/hr for 12 hr

Assume macropore flow is negligible

Negligible plant uptake in short time frame

Governing PDE:

$$\frac{\partial(\theta c)}{\partial t} = D_e \frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z}$$

$$v = \frac{J_w}{\phi} = \frac{-2\ cm/hr}{0.5} = 4\ cm/hr$$

Analytical Sol'n

$$c(z,t) = \frac{m_a}{2\phi\sqrt{\pi D_e t}} \exp\left[\frac{-(z-vt)^2}{4 D_e t}\right]$$

$$[=] \frac{M/L^2}{\sqrt{\frac{L^2}{T}T}} = \frac{M/L^2}{L} = \frac{M}{L^3}$$

m_a = mass per unit area

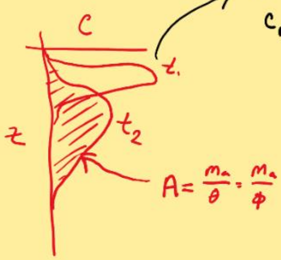
$= 100\ lb/ac = 1{,}120\ \frac{\mu g}{cm^2}$

$$C [=] \frac{M}{L^3} = \frac{\mu g}{cm^3} = \frac{mg}{L} = ppm$$

$D_e = \lambda v$
$\hookrightarrow$ = 10% of length scale
1m root zone

$\lambda = 0.1 * 1m = 10\ cm$

$D_e = (10cm)(4\ cm/hr) = 40\ cm^2/hr$



where is the peak?
$C_{peak} \Rightarrow \exp = 1$
$\Rightarrow$ numerator $= 0$
$\Rightarrow z = vt$

$m_a = \int(\theta c)dz$
$= \theta\int c\,dz$
$= \theta A$

Find: concentration profile
at 3 hr and 10 hr

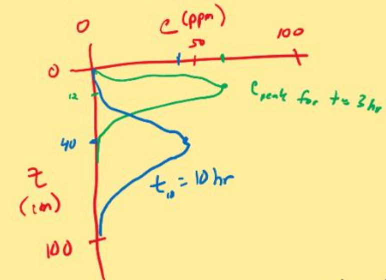
t	3hr	10 hr
z_{peak}	12 cm	40 cm
C_{peak}	58 ppm	32 ppm

$z_{peak} = vt = 4\ cm/hr\ (3hr) = 12\ cm$

$$C_{peak} = C(3hr, 12cm) = \frac{m_a}{2\phi\sqrt{\pi D_e t}} \quad (1)$$

$$= \frac{1{,}120\ \mu g/cm^2}{2(0.5)\sqrt{\pi(40\ cm^2/hr)(3hr)}} = 58\ \frac{\mu g}{cm^3} = 58\ ppm$$

Hand sketch



Last Step: plot in Excel

N leaching problem

April, 2021

100	lb/ac
43560	ft2/ac
0.002296	lb/ft2
30.48	cm/ft
2.47105E-06	lb/cm2
453.6	g/lb
0.0011	g/cm2
1.1209	mg/cm2
1121	μg/cm2 = m_a = total mass of solute per unit area of land surface
2242	μg/cm2 = m_a/ϕ = total mass of solute per (horizontal) unit area of water

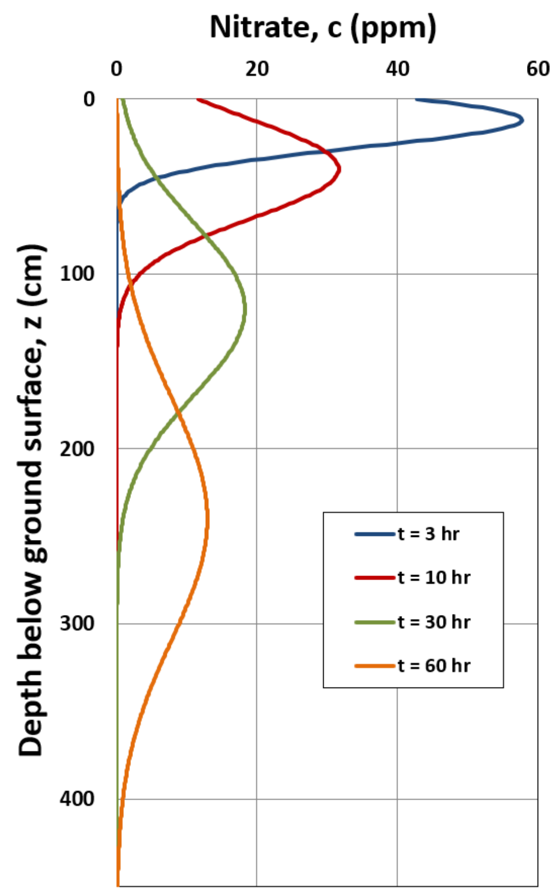
100	cm, length of problem
10	λ, dispersivity (cm)
2	Jw, water flux (cm/hr) = precipitation rate
0.5	ϕ
4	v, average pore water velocity (cm/hr)
40	D_e, dispersian coefficient (cm2/hr)

Table:

t (hr)	3	10	30	60
z_{peak} (cm)	12	40	120	240
Cmax (μg/cm3)	57.7	31.6	18.3	12.9

Profiles: Concentration, c (μg/cm3 = mg/L = ppm)

z (cm)	c(z,3)	c(z,10)	c(z,30)	c(z,60)
0	42.8	11.6	0.9	0.0
1	44.9	12.2	1.0	0.0
2	46.9	12.8	1.0	0.0
3	48.8	13.4	1.1	0.0
4	50.5	14.1	1.1	0.0
5	52.1	14.7	1.2	0.0
6	53.6	15.4	1.2	0.0



ADE Discretization

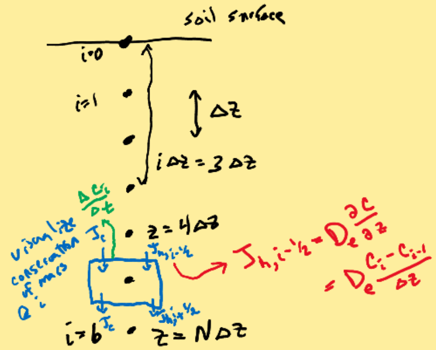
$$\frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z}\left[\theta D_e \frac{\partial c}{\partial z}\right] - \frac{\partial (J_w c)}{\partial z}$$

Assume steady & uniform θ

$$\frac{\theta}{\theta}\frac{\partial c}{\partial t} = \frac{\theta D_e}{\theta}\frac{\partial^2 c}{\partial z^2} - \frac{J_w}{\theta}\frac{\partial c}{\partial z}$$

$$\boxed{\frac{\partial c}{\partial t} = D_e \frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z}}$$

e.g. unit gradient



Space: $i = 0 \ldots N$

$N = 6 \Rightarrow$ 6 intervals, 7 nodes

$z = i\Delta z$

Time: $j = 0 \ldots M$

interval $= \Delta t$

$t = j\Delta t$

Notation: C_i^j

ADE:

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = D_e\left[\frac{\left.\frac{\partial c}{\partial z}\right|_{i+1/2} - \left.\frac{\partial c}{\partial z}\right|_{i-1/2}}{\Delta z}\right] - v\left.\frac{\partial c}{\partial z}\right|_i$$

$$= D_e\left[\frac{\frac{C_{i+1}-C_i}{\Delta z} - \frac{C_i - C_{i-1}}{\Delta z}}{\Delta z}\right] - v\left(\frac{C_{i+1}-C_{i-1}}{2\Delta z}\right)$$

$\rightarrow$ easier than interpolating

$$= D_e\left[\frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta z^2}\right] - v\left(\frac{C_{i+1}-C_{i-1}}{2\Delta z}\right)$$

Need to assign a time to RHS

Explicit Method: RHS is at the known time (t_j)

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = D_e\left(\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{\Delta z^2}\right) - v\left(\frac{C_{i+1}^j - C_{i-1}^j}{2\Delta z}\right)$$

Only one unknown: C_i^{j+1}

$$\boxed{C_i^{j+1} = C_{i-1}^j \underbrace{\left(\frac{\Delta t v}{2\Delta z} + \frac{\Delta t D_e}{\Delta z^2}\right)}_{\text{constants}} + C_i^j\left(1 - \frac{2\Delta t D_e}{\Delta z^2}\right) + C_{i+1}^j\left(-\frac{\Delta t v}{2\Delta z} + \frac{\Delta t D_e}{\Delta z^2}\right)}$$

Practical Guidelines

Oscillations / stability

Numerical dispersion

Caused primarily by advection term

- sharp concentration fronts
- if transport is dominated by advection

"grid" Peclet number (P_e)

$P_e \leq 5$

Choose a space discretization

Courant number (C_r)

$C_r \leq 1$

Chose time step

Simultaneous Models

Flow & transport

Can have transient transport but steady flow

both transient (more difficult)

"Linked" models

Output from flow model is input for transport model

HYDRUS

"Coupled" models

Accounts for effects of each model on the other

E.g. heat transport, temp effect on ρ & K_s

Very difficult

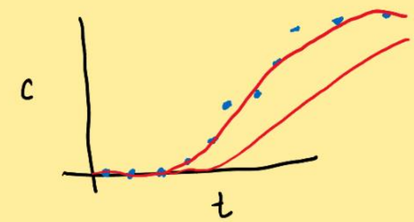
Inverse Modeling (backwards problem)

Soil Column Exp.

Find D_e (or λ) that best fits data

Parameter Optimization (e.g. K_s & λ)

BTC



Adsorption Isotherms

Conservative solute: stays in solution

Non-conservative solutes:

- adsorption
- decay
- chemical reaction

Adsorption

Assume adsorption is instantaneous ("equilibrium")
(contrast kinetic/nonequilibrium sorption)

Linear Adsorption Isotherm

$s \; [=] \; \frac{\text{mg sorbate}}{\text{kg soil}}$

$s = K_d C$ → linear sorption coefficient

$\frac{mg}{kg} = \frac{L}{kg}\,\frac{mg}{L}$

Most applicable to dilute, inorganic solutes

Organic solutes:

K_{oc} = organic C partitioning coefficient

f_{oc} = fraction of organic carbon in soil (≈ 60% om)

$K_d = K_{oc} f_{oc}$

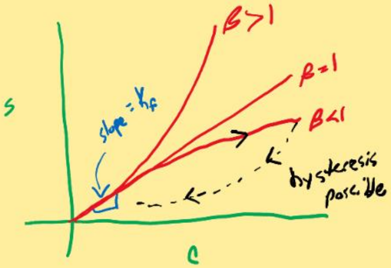
pesticide adsorption proportional to soil om

Freundlich

most common isotherm

$s = K_f c^{\beta}$

Note: no maximum s



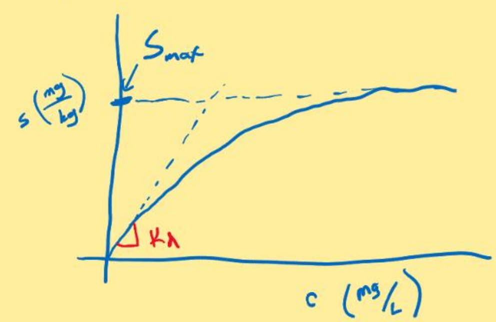
Langmuir Isotherm

$$s = \frac{K_d c}{1 + \eta c}$$

$$s = \frac{\eta K_d c}{\eta (1 + \eta c)}$$

$$s = S_{max}\left(\frac{\eta c}{1 + \eta c}\right)$$

Note: $\eta \to 0 \Rightarrow$ becomes linear



Terminology:

"sorption" general term

"adsorption" molecule attaches to solid surface

"precipitation" form new mineral

ADE with Adsorption

$$\frac{\partial(\theta c + \rho_b \overbrace{s}^{\text{solid phase}})}{\partial t} = -\frac{\partial}{\partial z}\left(J_w c - \theta D_e \frac{\partial c}{\partial z}\right)$$

Assume steady & uniform flow: $\theta(z,t) = \theta$

Divide by θ

$$\frac{\partial c}{\partial t} + \frac{\rho_b}{\theta}\frac{\partial s}{\partial t} = D_e \frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z}$$

Have 2 dependent variables: c, s

Assumptions: linear isotherm (no hysteresis)
chemical equilibrium (instantaneous sorption)

$$s = K_d c$$

$$\frac{\partial c}{\partial t} + \frac{\rho_b}{\theta}\frac{\partial (K_d c)}{\partial t} = D_e \frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z}$$

$$\underbrace{\left[1 + \frac{\rho_b K_d}{\theta}\right]}_{= R = \text{retardation factor } (R \geq 1)}\frac{\partial c}{\partial t} = D_e \frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z}$$

$$R\frac{\partial c}{\partial t} = D_e \frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z}$$

$$\frac{\partial c}{\partial t} = \frac{D_e}{R}\frac{\partial^2 c}{\partial z^2} - \frac{v}{R}\frac{\partial c}{\partial z}$$

dispersion is "slowed down"

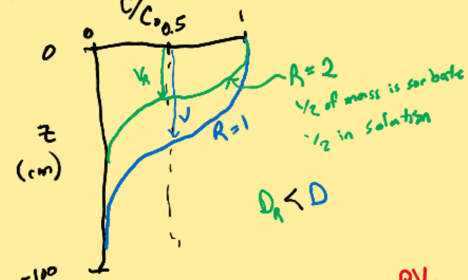
adsorption is slowing down advection

$$\boxed{\frac{\partial c}{\partial t} = D_R \frac{\partial^2 c}{\partial z^2} - v_R \frac{\partial c}{\partial z}}$$

ADE w/ linear sorption

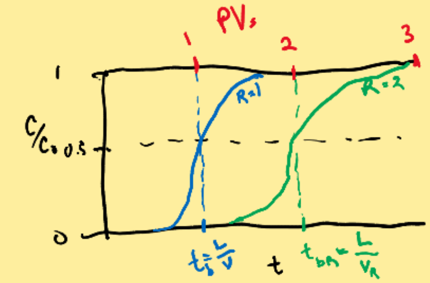
Can apply same analytical solutions!

Solute Front:



$D_R < D$

BTC:



Physical Nonequilibrium

Consider two porosities (mo, im)

Consider slow transport between the two porosities (nonequilibrium)

Mass Balance:

$$C_T = \theta_{mo} c_{mo} + f \rho_b s_{mo} + \theta_{im} c_{im} + (1-f) \rho_b s_{im}$$

f = fraction of sorption sites in mo zone

sometimes assume:

$f = \frac{\theta_{mo}}{\theta}$ (sorption sites distributed uniformly)

probably higher density of sorption sites in im zone

$$f < \frac{\theta_{mo}}{\theta}$$

ADE:

$$\frac{\partial}{\partial t}(\theta_{mo} c_{mo}) + \frac{\partial}{\partial t}(f \rho_b K_d c_{mo}) =$$

$$\frac{\partial}{\partial z}\left(\theta_{mo} D_{mo} \frac{\partial c_{mo}}{\partial z}\right) - \frac{\partial (J_w c_{mo})}{\partial z} - \Gamma_s$$

assuming all vertical flow is in mo zone

$v_{mo} = \frac{J_w}{\theta_{mo}}$ $\quad v_{mo} > v$

$$\frac{\partial}{\partial t}(\theta_{im} c_{im}) + \frac{\partial}{\partial t}\left[(1-f)\rho_b K_d c_{im}\right] = \Gamma_s$$

Γ_s → solute exchange rate

$$\Gamma_s = \underbrace{\alpha_s (c_{mo} - c_{im})}_{\text{apparent diffusion}} + \underbrace{\Gamma_w c^*}_{\text{advection term}}$$

Γ_w → water exchange rate

α_s = exchange rate coefficient $[=] \frac{1}{T}$

$c^* = c_{mo}$ $\quad \Gamma_w > 0$ $\quad$ (flow mo → im)

$c^* = c_{im}$ $\quad \Gamma_w < 0$ $\quad$ (flow im → mo)

no advection $\quad \Gamma_w = 0$

"Uniform Flow"

Flow: single porosity

Transport: equilibrium

"Mobile-Immobile"

Flow: single porosity $\quad \Gamma_w = 0$

Transport: nonequilibrium $\quad \Gamma_w c^* = 0$ (no advection between zones)

popular for transport

works especially well for steady flow problems

"Dual Porosity"

Flow: dual porosity

Transport: nonequilibrium

important for transient flow

if small Γ_w, then most solute flux is staying in macropore, and most flow staying in macropore

⇒ velocity of solute front >> v in uniform flow

so, flow parameters ($\theta_{mo,s}$ and ω) make a big difference