



MODÉLISATION D'ÉCOULEMENTS DES FLUIDES ET ENVIRONNEMENT

FREE SURFACE AND GROUNDWATER FLOWS MODELING

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By Asymptotic Reduction Methods, we have

- identified small parameter ε and specific asymptotic regime
- expanded the solution in terms of ε
- analyzed the eqs and identified dominant terms as $\varepsilon \rightarrow 0$
- retained leading-order terms to derive the hydrostatic approximation
- vertically averaged these eqs to get the Saint-Venant system with recharge
- this results in a simpler form (loss of one dimension)
- formally justified the two-way coupling

Aims

- Derivation of the Richards' equation (RE) for saturated/unsaturated porous media

- The RE can model the behavior of flows in variably saturated porous media.
- One of the key advantages of RE is its ability to represent the porous medium, incorporating both saturated and unsaturated zones.
- While it doesn't consider the air phase, RE effectively incorporates the effects of gravity and capillarity, enabling the modeling of complex processes across various scales. Notably, RE is a nonlinear parabolic equation that can transform into an elliptic equation under complete saturation conditions.
- The history of RE begins with Darcy's law, formulated experimentally by Darcy in 1856 [6] for saturated porous media.
- This result was later extended to multiphase flows by Buckingham in 1907 [2], resulting in the Darcy-Buckingham law, which serves as the cornerstone for the derivation of RE.
- Richardson first established the equation in 1922 [10], although it was later attributed solely to Richards, who independently published the equation in 1931 [9].
- Initial attempts to numerically solve the RE date back to the late 1960s with the works of Rubin [11] and Cooley [4].
- From the 1980s, RE was extensively studied from both theoretical and numerical perspectives.

LECTURE 2 :

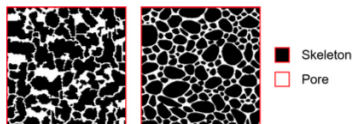
Derivation of the Richards' equation for saturated/unsaturated porous media

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- 3 GOVERNING EQUATION : RICHARDS' EQUATION
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DEFINITIONS

A porous medium is a material constituted of voids filled by fluids, either liquids or gas : The solid portion of material is called the skeleton or matrix (solid phase) while the void portions are called pores (vacuum or fluid phase).



- Lots of natural and artificial structures can be considered as porous media.
- Many processes leading to many concepts for different fields : mechanics, geosciences, biology, material science, or engineering.
- Fluid flow through porous media is a subject of interest

A porous medium is characterized by many variables :

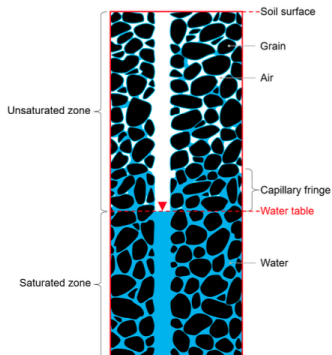
- Porosity $\Phi \in [0, 1]$: pore volume over the total volume
- Saturation S : quantity of water contained in a porous medium. Volume fraction of water compared to the pore volume
- Tortuosity m : path length, characterize the morphological property of porous microstructures.
- Wettability W : contact angle between fluid phases and the solid skeleton
- Permeability p : indicator of the ability for fluids (gas or liquid) to flow
- Granulometry

Grain diameter range	Type name	Common name
> 256 mm	Boulder	Stone
64 mm – 256 mm	Cobble	
4 mm – 64 mm	Pebble	Gravel
2 mm – 4 mm	Granule	
0.5 mm – 2 mm	Coarse sand	Sand
0.25 mm – 0.5 mm	Medium sand	
1/16 mm – 0.25 mm	Fine sand	
1/256 mm – 1/16 mm	Silt	Mud
< 1/256 mm	Clay	

Porous media can have the same porosity but they exhibit different pore connectivity and types of porosity.

- The porous medium is saturated if water fills fully the pore space, otherwise, is said to be unsaturated.
- Saturated zone (also called phreatic zone)
- Unsaturated zone (also called vadose zone)
- The water table is the surface delimiting these two zones.
- The capillary fringe is generally considered as a part of the unsaturated zone. It is the layer in which water seeps up from water table due to capillary forces. Capillary fringe exhibits a

nearly-saturated state which may extend from few centimetres to several meters. Capillary fringe size depends strongly on local porosity.



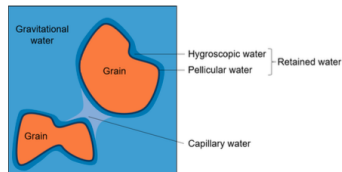
Porous media present a multi-scale structure. Pores may have various sizes and shapes resulting in different flow regimes : fluid flow are mainly driven by two kinds of forces.

- If pores are small enough, then liquid is displaced thanks to intermolecular forces. It is made possible by the combination of cohesive forces within the liquid (surface tension) and adhesive forces between the liquid and the surrounding solid matrix. This is called capillarity.
- Secondly, flow in large pores are subject to gravitational forces. Capillarity effects can be sufficiently strong to elevate fluid such as in plants to move water up or paper towels to absorb liquid.

Water movement in porous media, particularly in soils, has different hydrodynamic regimes according to capillary and gravitational forces.

- When air is present, retained water is attached to the grains, and its thickness depends on molecular forces. It is made of hygroscopic water, which is in direct contact with the grain, immobile, and can only be removed by desiccation or vacuum, and pellicular water, which adheres to hygroscopic water and moves around grains but can be extracted only with centrifugation.
- Retained water cannot be affected by gravity and does not transmit hydrostatic pressure. Capillary water is subject to tension forces at the interface between air and

water. It can be partially extracted by gravity and transmit pressure. Gravitational water can be drained out by gravity and its flow moves under gravity and pressure fields. Capillary water and gravitational water are referred to as free water and they define flow dynamics in unsaturated porous media.



Hydrodynamic regimes :

- The adsorbed regime corresponds to the retained water. At this stage, water can evaporate to make vapor in the air phase.
- In a pendular regime, the flow has no continuous paths so is considered as macroscopically immobile.
- The flow of liquid water is possible from the funicular stage.
- If the amount of water in the system is sufficient, pores can be

filled with water which gives the capillary and saturated regime.

- Capillary regime contains occluded air bubbles and air phase loses its continuity. A saturated regime happens when remaining air is dissolved into water.



From now on, evaporation and dissolution are neglected so we can focus on the funicular, capillary, and saturated regimes.

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- heterogeneous structures at a microscopic scale inducing spatial variability of their hydraulic properties and characteristics such as porosity, permeability, or retention. These micro-structures may influence a larger scale.
- simulating directly such features would require very fine grids resulting in excessive computational cost.
- from an experimental viewpoint, the microscale properties are difficult to reach or not known in much detail. This makes it not purposeful to represent the microscale field if one wants to simulate fields much larger than the pore size.
- A macroscale representation might be assumed to reproduce the system's behavior.

Upscaling approaches try to develop such a model by the mean of averaged values from a volume element representative of a microscale pattern. It can be cast into three main ideas :

- Homogenization [1]
- Volume averaging technique [12]
- Stochastic methods [5]

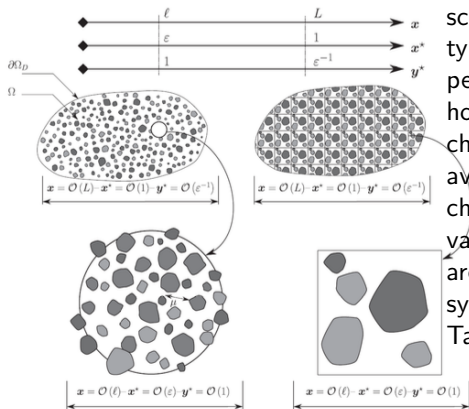
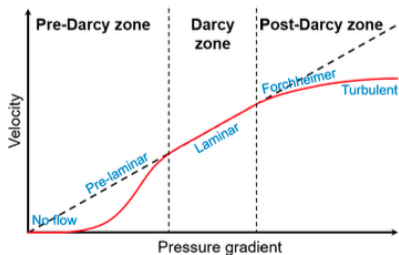


Diagram of coordinate systems and scale hierarchy for non-periodic media typical of volume averaging (left) and periodic media typical of homogenization (right). μ is pore-scale characteristic length, l is the size of averaging volume, L is a macroscale characteristic length, x is a spatial variable coordinate system, x^* and y^* are nondimensionalized coordinate systems with L and l respectively. Taken from [7].

The volume average method is a more intuitive approach for Darcy's law derivation. It uses control volume (CV) in which physical quantities are averaged. These averaged quantities are reorganized and some are disregarded according to assumptions. The average velocity is obtained and corresponds to Darcy's velocity :

$$q = -\frac{k}{\mu} \nabla p$$

where q is the flow of a fluid [$L \cdot T^{-1}$] of viscosity μ [$L \cdot L^{-1} \cdot T^{-1}$] through a porous medium of permeability k [L^2] and ∇p [$M \cdot L^{-2} \cdot T^{-2}$].

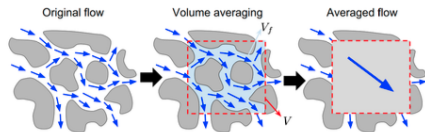


Range of validity of Darcy's law. Darcy zone delimits the linear approximation of the flow-pressure gradient relation. Outside, nonlinear deviations are observed.

VOLUME AVERAGING METHOD : REV

Volume averaging method consists in averaging equations of porous medium over the Representative Elementary Volume (REV). In other words, it is a filtering of small space scales. The general approach aims to average equations to obtain terms which are estimated against each other. Then, given hypotheses at disposal, some of the terms are disregarded. The closure of the problem allows to model of non-local terms and so, the rising average velocity is assimilated to the Darcy velocity.

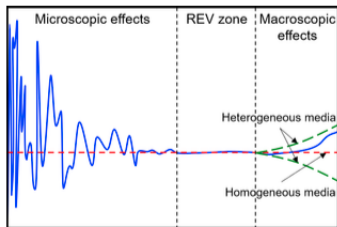
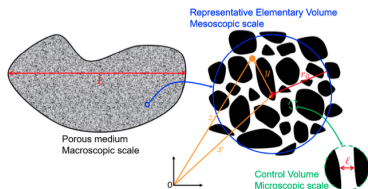
Volume averaging procedure to get an equivalent homogeneous macroscale medium from the heterogeneous micro-structure. The red square stands for the representative elementary volume.



- Fluid phase is F and Solid one is S
- Assume that $l \leq r_0 \ll L$ with L macroscopic length scale, r_0 mesoscopic and l microscopic one
- $x \in \Omega \subset \mathbb{R}^3$: global space variable
- y : local space variable for the REV of center x which can associated to

$$\forall x \in \Omega, V = B(x, r_0) = V_F + V_S = \text{cst}$$

- REV size is crucial !



X stands for S or F . Inside the REV, assume that

- $\exists r_X(x); \text{Vol}(V_X) = \text{Vol}(B(x, r_X(x)))$
- $\exists s_X(x); \text{Surf}(V_X) = \text{Vol}(B(x, s_X(x)))$
- define $\Phi(x) = \frac{V_{\text{poral}}(x)}{V_{\text{total}}(x)} = \frac{r_F^3(x)}{r_0^3}$: porosity
- One can define the following classification of a porous medium :
 - $l \approx r_0 \ll L$: ordered (Homogenization tech. are suitable)
 - $l \ll r_0 \ll L$: disordered (REV tech. are suitable)
 - $\nabla\Phi \ll I_d$: homogenous
 - $\nabla\Phi \gg I_d$: heterogeneous
- define fluid phase indicator function : $1_F(x+y) = 1$ if $|y| < r_F(x)$
- define phase average : $\langle f \rangle(x) = \frac{1}{r_0^3} \int_{B(0, r_0)} 1_F(y) f(x+y) dy$
- define intrinsic average : $\bar{f}(x) = \frac{1}{r_F^3} \int_{B(0, r_0)} 1_F(y) f(x+y) dy$
 - yielding to $\langle f \rangle(x) = \Phi(x) \bar{f}(x)$
 - yielding to $\langle 1_F \rangle(x) = \Phi(x)$

Case disordered porous medium $l \ll r_0 \ll L^a$

- $0 < r(x) \leq r_0 \Rightarrow \varepsilon_l = \frac{l}{L} \ll \varepsilon_0 = \frac{r_0}{L} \ll 1$ with $\varepsilon(x) = \frac{r(x)}{L}$
- Spatial averaging theorem :

$$\langle f \rangle(x) = \bar{f}(x) + \frac{1}{r_0^3} \int_{\Sigma(0, s(x))} 1_F(y) f(x+y) ds$$

where $\Sigma(0, s(x)) = \text{Surf}(B(0, s(x)))$

- assume that inertial forces are small compared to viscous forces in the medium : Stokes Equations :

$$\begin{aligned} -\mu \Delta u + \nabla p - \rho g &= 0 \\ u \cdot n &= 0 \end{aligned}$$

a. subscript F is omitted

- Pressure terms :

$$\langle \nabla p \rangle(x) = \Phi(x) \nabla \bar{p}(x) + \bar{p}(x) \nabla \Phi(x) + \frac{1}{r_0^3} \int_{\Sigma(0,s(x))} 1_F(y) p(x+y) ds$$

- Viscous terms :

$$\langle -\mu \Delta u \rangle(x) = -\mu (\Phi(x) \Delta \bar{u}(x) + \bar{u}(x) \Delta \Phi(x) + 2 \nabla \Phi(x) \nabla \bar{u}(x))$$

$$-\frac{\mu}{r_0^3} \int_{\Sigma(0,s(x))} 1_F(y) (\nabla u \cdot n)(x+y) ds$$

- Gravity terms :

$$\langle -\rho g \rangle(x) = -\rho g \langle 1_F \rangle(x) = -\rho g \Phi(x)$$

- Pressure terms :

$$\begin{aligned} \langle \nabla p \rangle(x) &= \Phi(x) \nabla \bar{p}(x) + \bar{p}(x) \nabla \Phi(x) + \frac{1}{r_0^3} \int_{\Sigma(0,s(x))} 1_F(y) \bar{p}(x+y) ds \\ &\quad + \frac{1}{r_0^3} \int_{\Sigma(0,s(x))} 1_F(y) \tilde{p}(x+y) ds \end{aligned}$$

- Viscous terms :

$$\begin{aligned} \langle -\mu \Delta u \rangle(x) &= -\mu (\Phi(x) \Delta \bar{u}(x) + \bar{u}(x) \Delta \Phi(x) + 2 \nabla \Phi(x) \nabla \bar{u}(x)) \\ &\quad - \frac{\mu}{r_0^3} \int_{\Sigma(0,s(x))} 1_F(y) (\nabla \bar{u} \cdot n)(x+y) ds \\ &\quad - \frac{\mu}{r_0^3} \int_{\Sigma(0,s(x))} 1_F(y) (\nabla \tilde{u} \cdot n)(x+y) ds \end{aligned}$$

- Gravity terms :

$$\langle -\rho g \rangle(x) = -\rho g \langle 1_F \rangle(x) = -\rho g \Phi(x)$$

- define nondimensional numbers

$$\rightarrow Re = \frac{\rho L \bar{U}}{\mu} \text{ (Reynolds)}$$

$$\rightarrow Ma = \bar{U} \sqrt{\frac{\rho}{\bar{P}}} \text{ (Mach)}$$

$$\rightarrow Fr = \frac{\bar{U}}{\sqrt{gL}} \text{ (Froude)}$$

- define nondimensional variables for $X = \bar{u}^*$ or $X = \bar{p}^*$ or $X = \tilde{u}^*$, $\bar{x}^* = \frac{x}{L}$ and $\bar{y}^* = \frac{y}{r_0}$ and

$$v = \frac{\tilde{U}}{\bar{U}}, \quad \Psi = \frac{\tilde{P}}{\bar{P}}, \quad \text{and} \quad \eta(x) = \frac{s^2(x)}{r_0^2}$$

- multiply the previous phase averaged Stokes equation by $\frac{L}{\rho \bar{U}^2}$ and omit the star in superscript

- Pressure terms :

$$\begin{aligned}
 \langle \nabla p \rangle(x) &= \frac{1}{Ma^2} \Phi(x) \nabla \bar{p}(x) + \frac{1}{Ma^2} \bar{p}(x) \nabla \Phi(x) \\
 &+ \underbrace{\frac{\eta(x)}{\varepsilon_0 Ma^2} \int_{\Sigma(0,1)} 1_F(y) \bar{p}(x + s(x)y) ds}_{\text{non-local term}} \\
 &+ \frac{\Psi \eta(x)}{\varepsilon_0^3 Ma^2} \int_{\Sigma(0,1)} 1_F(y) \tilde{p}(x + s(x)y) ds
 \end{aligned}$$

- Viscous terms :

$$\langle -\mu \Delta u \rangle(x) = -\underbrace{\mu (\Phi(x) \Delta \bar{u}(x) + \bar{u}(x) \Delta \Phi(x) + 2 \nabla \Phi(x) \nabla \bar{u}(x))}_{\text{Brinkman's correction}}$$

$$-\underbrace{\frac{\mu}{r_0^3} \int_{\Sigma(0,s(x))} 1_F(y) (\nabla \bar{u} \cdot n)(x+y) ds}_{\text{non-local term}}$$

$$-\frac{\mu}{r_0^3} \int_{\Sigma(0,s(x))} 1_F(y) (\nabla \tilde{u} \cdot n)(x+y) ds$$

- Gravity terms :

$$\langle -\rho g \rangle(x) = -\rho g \langle 1_F \rangle(x) = -\frac{1}{Fr^2} \Phi(x)$$

- Red terms are the basis of the derivation of the Darcy's law : fundamental to derive the Richards' equation ^a

$$q = -\frac{k}{\mu} \nabla p$$

a. works is still in progress, open problem

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- Mass conservation principles for two-phase flow :

$$X \in \{\text{air, water}\}, \begin{cases} \partial_t(\rho_X \Phi S_X) + \nabla \cdot (\rho_X q_X) & = 0 \\ q_X & = -\frac{k(S_X)}{\mu_X} \nabla(p_X + \rho_X g z) \end{cases}$$

where ρ_X is the density [$M \cdot L^{-3}$], Φ is the porosity [-], S_X is the saturation [-], q_X is the Darcy velocity [$M \cdot L^{-1}$], μ_X is the dynamic viscosity [$M \cdot L^{-1} \cdot T^{-1}$], p_X is the pressure [$M \cdot L^{-1} \cdot T^{-2}$], t is the time [T], z is the elevation [L], g is the gravity constant [$L \cdot T^{-2}$].

- $S_{\text{air}} + S_{\text{water}} = 1$
- $p_{\text{air}} - p_{\text{water}} = P_c(S_{\text{water}})$ with P_c [$M \cdot L^{-1} \cdot T^{-2}$] = capillary pressure^a

a. invertible function deduced from experiment

- Neglect air phase
 - the air phase is assumed to be connected continuously to the atmosphere air
 - no trapped air pocket
- air viscosity is 50 times smaller than the water viscosity
 - the pressure gradients balance much faster in air : $\nabla(p_{\text{air}} + \rho_{\text{air}}) = 0$, i.e.
 $p_{\text{air}} = p_0 - \rho_{\text{air}}g$ where p_0 is the atmospheric pressure.
- With these assumptions, one can solely consider only the water phase :

$$\partial_t(\rho\Phi S) - \nabla \cdot \left(\frac{\rho}{\mu} k(S) \nabla(p + \rho g z) \right) = 0$$

- Additional simplifications :
 - water density homogenous : $\nabla\rho = 0$
 - water is incompressible : $\partial_t\rho$
 - solid skeleton is not deformable : $\partial_t\Phi$
 - air density is about 820 times smaller than water density at 15°C :

$$\nabla \left(\frac{p}{\rho g} \right) = \nabla \left(\frac{p_{\text{air}} - P_c}{\rho g} \right) = -\nabla \left(\frac{P_c}{\rho g} \right)$$

- Define
 - $\theta(S) = \Phi S$: water content
 - $K(S) = \frac{\rho g}{\mu} k(S)$: hydraulic conductivity
 - $\psi = \frac{p}{\rho g}$: pressure head
 - $S = P_c(p) = P_c(\rho g \psi)$: retention curve (= soil moisture)
- Richards' equation (hydraulic head formulation, see [3] for other formulation) :

$$\partial_t \theta(\psi) - \nabla \cdot (K(\psi) \nabla(\psi + z)) = 0$$

$$\iff$$

$$\partial_t \theta(h - z) - \nabla \cdot (K(h - z) \nabla h) = 0 \text{ widely used in hydrology}$$

where $h = \psi + z$

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- Generally, k (permeability tensor) and K (hydraulic conductivity) are supposed to react identically in each space direction :

$$k(\psi) = k_s k_r(\psi) \text{ and } K(\psi) = K_s K_r(\psi)$$

where k_s [L^2] permeability tensor at saturation, k_r [-], relative permeability, K_s [$L \cdot T^{-1}$] hydraulic conductivity at saturation and K_r relative hydraulic conductivity.

- Water content is often given as a function of the effective saturation S_e [-] :

$$S_e = \frac{\theta(\psi) - \theta_r}{\theta_s - \theta_r}$$

where θ_s water content at saturation, θ_r residual water content corresponding to the maximal and minimal saturations, resp.

- Air entry pressure ψ_e [L] (generally set to 0) :

$$\text{porous medium's zone : } \begin{cases} \text{unsaturated zone} & \text{if } \psi < \psi_e \\ \text{water table} & \text{if } \psi = \psi_e \\ \text{saturated zone} & \text{if } \psi > \psi_e \end{cases}$$

- Capillary fringe (water is raised due to capillary forces) $\in \{\psi_e^l < \psi < \psi_e\}$ where ψ_e^l depends on the grains, flow regime, etc.
- Hydraulic properties are defined as follows (empirical laws or closure) :

$$S_e(\psi) = \begin{cases} 1 & \text{if } \psi \geq \psi_e \\ S_e^*(\psi) & \text{otherwise} \end{cases}$$

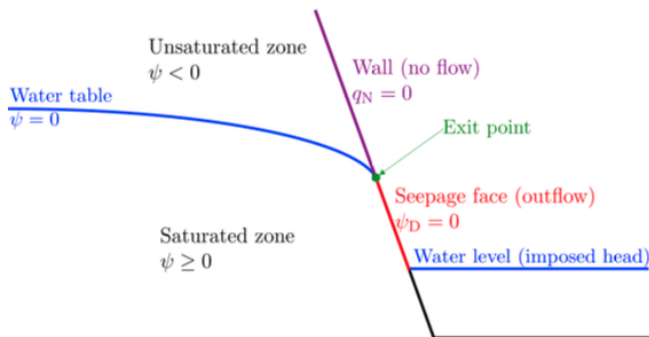
and

$$K_r(\psi) = \begin{cases} 1 & \text{if } \psi \geq \psi_e \\ K_r^*(\psi) & \text{otherwise} \end{cases}$$

Name	Expression	Parameters
Gardner-Irmay relations (1958) [72, 73]	$S_e^*(\psi) = e^{\frac{\alpha\psi}{m}}$ $K_r^*(\psi) = e^{\alpha\psi}$	α : pore-size distribution [-] m : tortuosity [-]
Vachaud's relations (1971) [74]	$S_e^*(\psi) = \frac{C}{C + \psi ^D}$ $K_r^*(\psi) = \frac{A}{A + \psi ^B}$	A, C : empirical shape parameters [$L^{B,D}$] B, D : empirical shape parameters [-]
Van Genuchten-Mualem relations (1980) [75, 76]	$S_e^*(\psi) = (1 + (\alpha \psi)^n)^{-m}$ $K_r^*(\psi) = S_e^{*l}(\psi) \left(1 - \left(1 - S_e^{*\frac{1}{m}}(\psi)\right)^m\right)^2$	$l = \begin{cases} 0.5 & \text{for Mualem [75]} \\ 1 & \text{for Burdine [77]} \end{cases}$: pore connectivity [-] α : parameter linked to air entry pressure inverse [L^{-1}] $n > 1$: pore-size distribution [-] $m = 1 - \frac{1}{n}$: pore-size distribution [-]
Modified Van Genuchten-Mualem relations (2001) [78]	$S_e^*(\psi) = (1 + (\alpha \psi)^n)^{-m}$ $K_r^*(\psi) = \left(\frac{S_e^*(\psi)}{S_*}\right)^l \left(\frac{1 - \left(1 - S_e^{*\frac{1}{m}}(\psi)\right)^m}{1 - \left(1 - S_*^{\frac{1}{m}}\right)^m}\right)^2$	$S_* = (1 + (-\alpha\psi_s)^n)^{-m}$ [-] with $\psi_s \leq \psi_e = 0$ [-] $l = \begin{cases} 0.5 & \text{for Mualem [75]} \\ 1 & \text{for Burdine [77]} \end{cases}$: pore connectivity [-] α : parameter linked to air entry pressure inverse [L^{-1}] $n > 1$: pore-size distribution [-] $m = 1 - \frac{1}{n}$: pore-size distribution [-]

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$$\begin{cases} h_D = z & \text{if } h \geq z \text{ and } -\mathbb{K}(h - z)\nabla h \cdot \mathbf{n} > 0, \\ q_N = -\mathbb{K}(h - z)\nabla h \cdot \mathbf{n} = 0 & \text{otherwise.} \end{cases}$$



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- under complete saturation, hydraulic properties become constant and Richards' equation degenerates into an elliptic equation characterized by fast
- under almost complete unsaturation, hydraulic properties get very near-zero values which stop diffusion and may be inconvenient
- for a particular set of parameters, when $\psi \rightarrow 0^-$, constitutive laws may exhibit very steep gradients and even a numerical singularity. Nevertheless, these gradient values can be large but are bounded in practice.
- Other difficulties
 - Wetting front is a moving dynamic front and can be extremely sharp according to the hydraulic properties. This is mainly due to the nonlinear diffusivity.
 - The same holds for drying fronts.
 - Heterogeneity and anisotropy : the interface between two materials of different hydraulic properties can lead to a sudden change of saturation states=internal layer.

All of these may generate spurious oscillations, and instabilities and make hard the convergence of numerical solver [8].

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We have presented

- the (formal) derivation of the Richards' equation by upscaling approaches
- the hydraulic properties (or closure)

To do,

- Introduction to the Discontinuous Galerkin (DG) method for conservation laws (hyperbolic, c.f. M. Parisot's lectures for the Finite Volume approach)
- Introduction to the DG method for parabolic-elliptic equation
- Application of the DG method for a convection-diffusion equation

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- 2 MODEL REDUCTION : UPSCALING APPROACHES
- 3 GOVERNING EQUATION : RICHARDS' EQUATION
- 4 HYDRAULIC PROPERTIES
- 5 SEEPAGE AND DYNAMIC FORCING BOUNDARY CONDITIONS
- 6 NUMERICAL CHALLENGES OF RICHARDS' EQUATION
- 7 CONCLUSIONS AND PERSPECTIVES
- 8 REFERENCES

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