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Coupling model of underground flow and pollution transport using a Finite volume scheme

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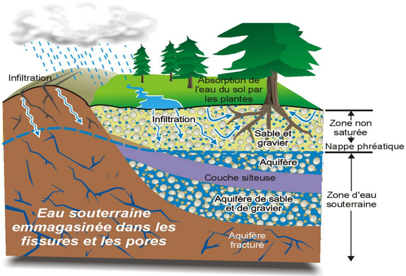
In Nature, It is more complex !



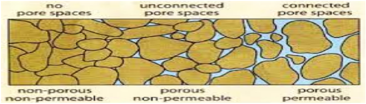


Figure: Porous media

Mathematical Model

The problem is fully descriebed by the following system of equations :

- Richards Equation :

$$\frac{\partial\theta(h,x,y)}{\partial t} = \nabla.[K(h,x,y)\nabla h] + \nabla.K(h,x,y) + Q_s$$

- Transport Equation :

$$\frac{\partial\theta C}{\partial t} + \nabla.(qC) = \nabla.\left(\theta D \nabla C\right)$$

,

3D Richards Equation :

$$\frac{\partial\theta(h,x,y,z)}{\partial t} = \nabla.[K(h,x,y,z)\nabla h] + \nabla.K(h,x,y,z) + Q_s$$

With :

- h : head water
- θ : volumetric water content
- K : hydraulic conductivity
- Q_s :source term

3D Transport Equation :

$$\begin{cases} \frac{\partial \theta C}{\partial t} + \nabla.(qC) = \nabla.\left(\theta D \nabla C\right) \\ \theta D = \lambda |q| + \theta D_m \tau \end{cases}$$

with :

- C : solute concentration
- $|q|$:Darcy velocity
- λ longitudinal lenth pore/solide
- θ : volumetric water content

1D Richards Equation :

The Richards equation takes 3 forms :

- The θ-Form :

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

- The Mixed-Form :

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

- The h-Form :

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

1D Richards Equation :

The θ-Form :

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

With : $D = K\frac{\partial h}{\partial \theta} \quad [L^2 T^{-1}]$

Advantages:

- Conservation form by construction
- Mass balance is improved significantly
- Rapid convergence

Inconvinients:

- limited to unsaturated conditions (In saturation D is infinite !)
- Limited to homogenous soil (θ can be not continuous across interfaces separating the layers !)

1D Richards Equation :

The Mixed-Form :

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

Advantages:

- Mass Conservation / Mass balance
- Applicable to both saturated and unsaturated soil
- Applicable to heterogenous soil

Inconvinients:

- Acceptable numerical solutions not always guarenteed

1D Richards Equation :

The h-Form :

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

With : $C(h) = \dfrac{\partial \theta}{\partial h}$ (C:capillary capacity)

Advantages:

- Applicable to both saturated and unsaturated soil
- Applicable heterogenous soil
- Very close to the physical model
- Less complicated to implement

Inconvinients:

- Poor preservation of mass balance
- Relatively slow convergence

1D-Coupling : We choose the h-Form !

Coupling of h-Form of Richards and Transport equations in 1D :

$$\begin{cases} C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\ \left[K(h)\left(\frac{\partial h}{\partial z} - 1\right)\right] \\ \\ q = -\frac{\partial}{\partial z}\ \left[K(h)\left(\frac{\partial h}{\partial z} - 1\right)\right] \\ \\ \frac{\partial \theta C}{\partial t} = \frac{\partial}{\partial z}\left(\theta D\frac{\partial C}{\partial z}\right) - \frac{\partial q C}{\partial z} \end{cases}$$

K ? C ? θ ?

The Brooks-Corey model:

The Hydraulic conductivity is :

$$\begin{cases} K(h) = K_s[\frac{\theta h - \theta r}{\theta s - \theta r}]^{3+2/n} & If \quad h < h_d \\ K(h) = K_s \quad If & h \geqslant h_d \end{cases}$$

With :

- K_s Hydraulic conductivity in saturation
- h_d is the bubbling or air entry pressure head (L) and is equal to the pressure head to desaturate the largest pores in the medium
- $n = 1 - 1/m$,m parameters linked to the soil structure

The Brooks-Corey model:

The Capillary capacity is taken as followed :

$$\begin{cases} C(h) = n\frac{\theta s - \theta r}{|h_d|}(\frac{h_d}{h})^{n+1} \quad If \ \ h < h_d \\ C(h) = 0 \quad If \quad h \geqslant h_d \end{cases}$$

NB : The Capillary capacity is always positive !

- θs water content in saturation
- θr residual water content
- n et m parameters linked to the soil structure

The Brooks-Corey model:

the volumetric water content is taken as followed :

$$\begin{cases} \theta = \theta_r + (\theta_s - \theta_r)\frac{h_d}{h} \quad If \quad h < h_d \\ \theta = \theta_s \quad If \quad h \geqslant h_d \end{cases}$$

With :

- θs water content in saturation
- θr residual water content
- n et m parameters linked to the soil structure

The van Genuchten Model:

Capillary capacity is taken as followed :

$$\begin{cases} C(h) = \frac{n*m*a \ |h| \ d\theta}{(1+(a*|h|)^n)^{1+m}} \quad If \quad h < 0 \\ C(h) = 0 \quad If \quad h \geqslant 0 \end{cases}$$

NB : The Capillary capacity is always positive !
With:

- $d\theta = \theta s - \theta r$
- S^* The specific volumetric storativity
- a,n et m parameters linked to the soil structure

The van Genuchten Model:

We introduice the saturation S_e as followed :

$$S_e = \frac{1}{(1 + a^n \left|h\right|^n)^m}$$

The Hydraulic conductivity is :

$$\begin{cases} K(h) = K_s \sqrt{S_e}(1 - \sqrt{1 - S_e^{\frac{1}{m}}})^m & \mathit{If} \quad h < 0 \\ K(h) = K_s \quad \mathit{If} & h \geqslant 0 \end{cases}$$

With:

- K_s Hydraulic conductivity in saturation
- a,n et m parameters linked to the soil structure

NB : Hydraulic conductivity is always positive !

The van Genuchten Model:

There is a "relationship" between θ and S_e , and it's formulated this way :

In saturation case :

$$S_e = \frac{\theta - \theta r}{\theta s - \theta r}$$

In non saturation case :

$$S_e = 1$$

Finite Volumes Scheme : General form

we use the following FV-schemes :

- Explicite :

$$h_j^{n+1} = h_j^n - r[\phi(h_j^n, h_{j+1}^n) - \phi(h_j^n, h_{j-1}^n)]$$

- Implicite :

$$h_j^{n+1} = h_j^n - r[\phi(h_j^{n+1}, h_{j+1}^{n+1}) - \phi(h_j^{n+1}, h_{j-1}^{n+1})]$$

with ϕ the numerical flux (In our case, we consider 2 numerical flux adequate to our study :flux of ROE or Lax-Frederick)

Richards Equation :Numerical scheme

The Explicite Finite volume scheme :

$$h_j^{n+1} = h_j^n + \frac{r}{C(h_j^n)}(\phi_{j+1/2}^n - \phi_{j-1/2}^n)$$

with :

- $r = \frac{\Delta t}{\Delta z}$
- ϕ : numerical flux for h

$$\phi_{j+1/2}^n = -\frac{K(h_{j+1/2}^n)}{\theta(h_{j+1/2}^n)}(\frac{h_{j+1}^n - h_j^n}{\Delta z} - 1)$$

For the explicit version of our model The stability condition is :

$$\Delta t \leq CFL \frac{InfC * \Delta z^2}{2Maxk}$$

Richards Equation :Numerical scheme

The implicite Finite volume scheme :

$$h_j^{n+1} = h_j^n + \frac{r}{C(h_j^{n+1})}(\phi_{j+1/2}^{n+1} - \phi_{j-1/2}^{n+1})$$

with :

- $r = \frac{\Delta t}{\Delta z}$
- ϕ : numerical flux for h

$$\phi_{j+1/2}^{n+1} = -\frac{K(h_{j+1/2}^{n+1})}{\theta(h_{j+1/2}^{n+1})}(\frac{h_{j+1}^{n+1} - h_j^{n+1}}{\Delta z} - 1)$$

Transport Equation :Numerical scheme

We use an upwind scheme (1st order) :

$$C_j^{n+1} = C_j^{n+1} - r * V * (fluxS_j^n - fluxS_{j-1}^n) + r * \frac{2}{\theta_j^n + \theta_{j+1}^n} * (DiffS_j^n - DiffS_{j-1}^n)$$

With :

- $V = \frac{qS_j^n + qS_{j+1}^n}{2}$
- $qS_j^n = \frac{q_j^n}{\theta_j^n}$
- $\begin{cases} fluxS_j^n = C_j^n & If \quad q \geqslant 0 \\ fluxS_j^n = C_{j+1}^n & If \qquad q < 0 \end{cases}$
- $DiffS_j^n = \frac{dz * |q_j^n|}{Pe} * (C_{j+1}^n - C_j^n)/dz$

Numerical resultats

Soil parameters for our test case :

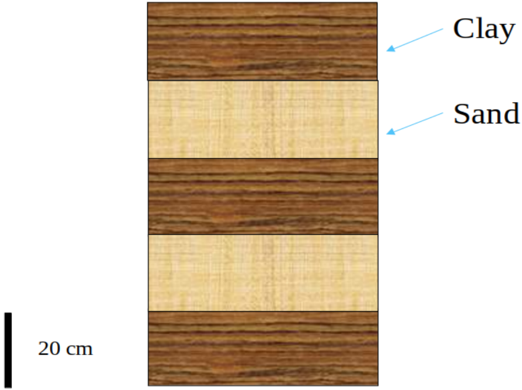


Figure: The soil

Numerical resultats

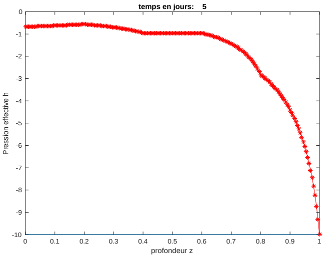
Soil parameters for our test case :

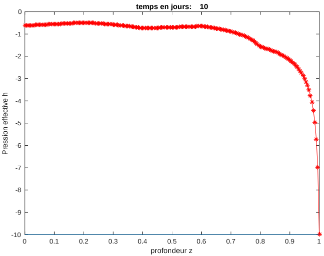
case Sand	Infiltration through homogenous
Domaine lenth	L=100 cm
Parameters	$K_s = 0.00922 cm/s$,$\theta_s = 0.368$,$\theta_r = 0.102$, $a = 0.0335 cm^{-1}$
case 1	$\Delta z = 0.2cm$, $Pe = 0.2$
case 2	$\Delta z = 2cm$, $Pe = 20$
case 3	$\Delta z = 2cm$, $Pe = 200$

case 2	Infiltration Through hetergenous soil
Domaine lenth	L=100 cm
Parameters (Clay)	$K_s = 0.000151 cm/s$,$\theta_s = 0.4686$,$\theta_r = 0.106$, $a = 0.03104 cm^{-}$

Numerical resultats

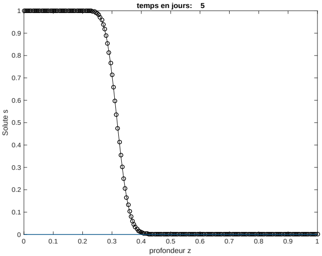
Head water in 5 and 10 days :

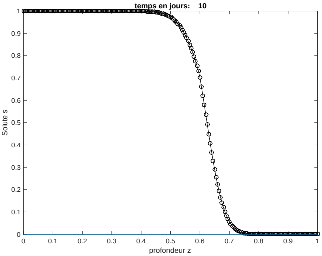




Numerical resultats : Solute concentration

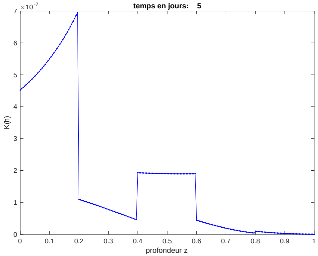
Solute concentration in 5 and 10 days :

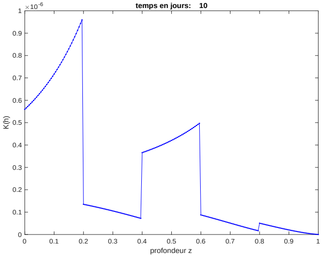




Numerical resultats :Hydraulic conductivity

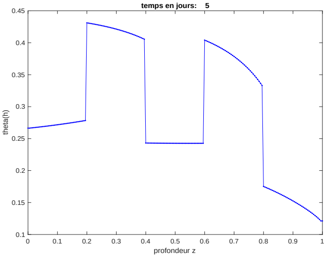
Hydraulic conductivity in 5 and 10 days:

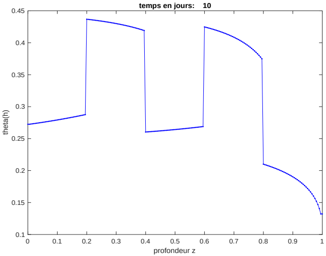




Numerical resultats :Water content

Volumetric Water content in 5 and 10 days:





Darcy Non-Linear – Cas test1 :

In the first test case, we consider the following equation :

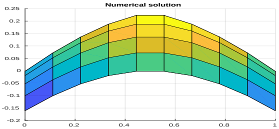
$$-\nabla.(|\nabla u|^{p-2}\nabla u) = f$$

Taking :

- $\Omega := (0,1) * (0,1)$.
- $f(x,y) = 2$.
- Boundries conditions and exact solution : $u(x,y) = -\frac{p-1}{p}|(x,y) - (0.5, 0.5)|^{\frac{p-1}{p}} + \frac{p-1}{p}(\frac{1}{2})^{\frac{p-1}{p}}$

Résultats numériques – Cas test1 :

Maillage 10*10



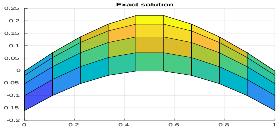
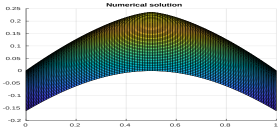


Figure: Numerical (left) and Exact solution (right)

Numerical results – Cas test1 :

Maillage 100*100



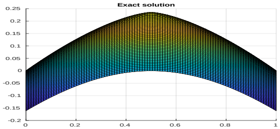


Figure: Numerical (left) and Exact solution (right)

Darcy Non linear:

Table: Comparaison of the different meshes . CPU time in seconds

	Cas test2					
Mesh	Min	Max	ϵ_1	ϵ_2	$\epsilon_{infinity}$	CPU
10*10	-0.1607	0.2229	3.2634e-04	5.5239e-04	0.0019	0.750136
20*20	-0.1607	0.2317	7.5575e-05	1.3516e-04	7.3847e-04	7.261438
30*30	-0.1607	0.2336	3.2654e-05	5.9558e-05	4.1908e-04	18.881606
50*50	-0.1607	0.2347	1.1482e-05	2.1288e-05	2.0302e-04	106.678507
100*100	-0.1607	0.2354	2.8183e-06	5.2933e-06	7.4894e-05	1722.546010

Numerical results -test case 2

In the seconde case, we consider the following equation :

$$-\nabla.(u\nabla u) = f$$

With :

- $\Omega := (0,1) * (0,1)$.
- $f(x,y) = -8(x^2 + y^2)$.
- Boundary conditions and exact solution : $u(x,y) = x^2 + y^2$

Darcy Non linear

Maillage 100*100

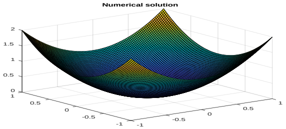


Figure: Numerical (left) and Exact solution (right)

Darcy Non linear

Table: Comparaison of the different meshes . CPU time in seconds

			test Cas 2			
Mesh	Min	Max	ϵ_1	ϵ_2	$\epsilon_{infinity}$	CPU
10*10	0.2389	2	0.1772	0.1426	0.2142	0.77791
20*20	0.1140	2	0.0538	0.0502	0.1085	5.136513
30*30	0.0748	2	0.0266	0.0274	0.0724	19.165506
50*20	-0.1607	0.2331	0.0062	0.0024	0.0030	24.463862
50*50	0.0443	2	0.0109	0.0128	0.0435	113.689984
100*100	0.0219	2	0.0032	0.0046	0.0217	848.066829

Richards 2D : FV Diamant

The 2-D model :
We consider this simplified version of Richards equation :

$$\frac{\partial h}{\partial t} = \nabla.[K\nabla h] + \nabla.K$$

We use a Diamant finite volumes scheme in a structred mesh and we obtain the following sytem :

$$\frac{h_k^{n+1} - h_k^n}{dt} =$$

$$-\frac{K_{12}^{k,k+1} + K_{21}^{k,k+n}}{4\Delta x\Delta y} h_{k+n+1}$$

$$-(\frac{K_{12}^{k,k+1} - K_{12}^{k,k-1}}{4\Delta x\Delta y} + \frac{K_{22}^{k,k+1}}{\Delta y^2}) h_{k+n}$$

$$+\frac{K_{12}^{k,k-1} + K_{21}^{k,k+n}}{4\Delta x\Delta y} h_{k+n-1}$$

Richards 2D : FV Diamant

$$+\left(\frac{K_{11}^{k,k+1}+K_{11}^{k,k-1}}{\Delta x^2}+\frac{K_{22}^{k,k+n}+K_{22}^{k,k-n}}{\Delta y^2}\right)h_k$$

$$+\left(\frac{K_{21}^{k,k+n}-K_{21}^{k,k-n}}{4\Delta x\Delta y}-\frac{K_{11}^{k,k-1}}{\Delta x^2}\right)h_{k-1}$$

$$+\frac{K_{12}^{k,k+1}+K_{21}^{k,k-n}}{4\Delta x\Delta y}h_{k-n+1}$$

$$+\left(\frac{K_{12}^{k,k+1}-K_{12}^{k,k-1}}{4\Delta x\Delta y}+\frac{K_{22}^{k,k-n}}{\Delta y^2}\right)h_{k-n}$$

$$-\frac{K_{12}^{k,k-1}+K_{21}^{k,k-n}}{4\Delta x\Delta y}h_{k-n-1}$$

Richards Linear: test case 1

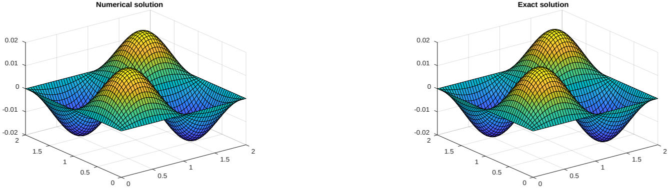
For the 2D model we take :
The boundaries conditions: $h = Hex$ everywhere.
The exact solution :

$$Hex(x, z, t) = exp(-B * t) sin(p2\pi xx/a) sin(q2\pi z/b)$$

with B,p,q,a and b are parameters to be defined.
The initial solution is

$$Hex(x, z, 0) = sin(p2\pi xx/a) sin(q2\pi z/b)$$

Linear Richards: test case 1 (Explicite/Implicite)



Linear Richards: test case 2

For the 2D model we take :

The boundaries conditions: $h = Hex$ everywhere.

The exact solution :

$$Hex(x,z,t) =$$

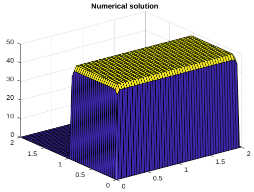
$$\Sigma\Sigma\frac{200}{\pi^2} * (1 + (-1)^{k+l} * \frac{1 - cos(l * \pi/2)}{k * l} * sin(t * \pi/2 * x) * sin(l * \pi/2 * z)$$

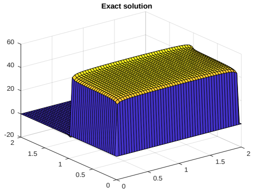
$$* exp((-\pi^2 * (l^2 + k^2) * t/36))$$

The initial solution is

$$Hex(x,z,0) = \Sigma\Sigma\frac{200}{\pi^2} * (1 + (-1)^{k+l} * \frac{1 - cos(l * \pi/2)}{k * l} * sin(t * \pi/2 * x) * sin(l * \pi/2 * z)$$

Richards Lineair:test case 2 (Explicite/Implicite)





Linear Non-Richards: test case 3

For the 2D model we take :

$$\frac{\partial h}{\partial t} = \nabla.[h\nabla h] + Q_s$$

The source term :

$$Q_s = -\alpha * (x + y) * exp(-\alpha * t)$$

The boundaries conditions: $h = Hex$ everywhere
The exact solution :

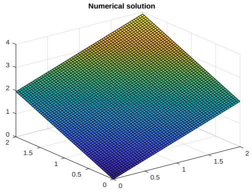
$$Hex(x, z, t) = (x + z) * \exp(-\alpha * t)$$

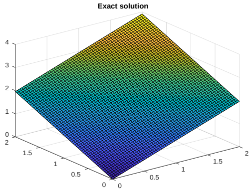
The initial solution is

$$Hex(x, z, 0) = x + z$$

RichardsNon-Linear : test case 3

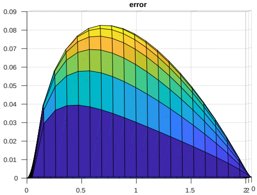
The Numerical and exact solution for $n * m = 100 * 100$

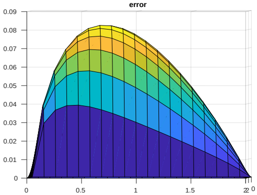




Richards Non-Linear :test case 3

the error for $n * m = 20 * 20$





Conclusion and Outlooks

Goinh on :

- Full Richards non lineair using Picard and Newton method

Next steps :

- Coupling of Richards, Transport and Saint-Venant Equations in 2D

If I am to be optimist :)

- Irregular mesh
- The MULTPHASE model

References

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THANK you for your Attention !