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

- **Richards Equation:**
  \[
  \frac{\partial \theta(h, x, y)}{\partial t} = \nabla \cdot [K(h, x, y) \nabla h] + \nabla \cdot K(h, x, y) + Q_s
  \]

- **Transport Equation:**
  \[
  \frac{\partial \theta C}{\partial t} + \nabla \cdot (qC) = \nabla \cdot (\theta D \nabla C)
  \]
3D Richards Equation:

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

With:

- **h**: head water
- **\(\theta\)**: volumetric water content
- **K**: hydraulic conductivity
- **\(Q_s\)**: source term
3D Transport Equation:

\[
\begin{cases}
\frac{\partial \theta C}{\partial t} + \nabla \cdot (qC) = \nabla \cdot (\theta D \nabla C) \\
\theta D = \lambda |q| + \theta D_m \tau
\end{cases}
\]

with:
- \( C \): solute concentration
- \( |q| \): Darcy velocity
- \( \lambda \): longitudinal length pore/solide
- \( \theta \): 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 $\theta$-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: \( D = K \frac{\partial h}{\partial \theta} \) \( [L^2 T^{-1}] \)

Advantages:

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

Inconveniences:

- Limited to unsaturated conditions (In saturation D is infinite !)
- Limited to homogenous soil ($\theta$ 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 heterogeneous soil

Inconveniences:
- Acceptable numerical solutions not always guaranteed
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: \( C(h) = \frac{\partial \theta}{\partial h} \) (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 :

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

K ? C ? \theta ?
The parameters of the physical model:

The Brooks-Corey model:

The Hydraulic conductivity is:

\[
K(h) = \begin{cases} 
  K_s \left[ \frac{\theta h - \theta_r}{\theta_s - \theta_r} \right]^{3+2/n} & \text{If } h < h_d \\
  K_s & \text{If } h \geq h_d 
\end{cases}
\]

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 parameters of the physical model:

The Brooks-Corey model:

The Capillary capacity is taken as followed:

\[
C(h) = \begin{cases} 
  n^{\theta_s - \theta_r} \left( \frac{h_d}{h} \right)^{n+1} & \text{if } h < h_d \\
  0 & \text{if } h \geq h_d 
\end{cases}
\]

NB: The Capillary capacity is always positive!

- $\theta_s$ water content in saturation
- $\theta_r$ residual water content
- $n$ et $m$ parameters linked to the soil structure
The parameters of the physical model:

The Brooks-Corey model:

the volumetric water content is taken as followed:

\[
\begin{align*}
\theta &= \theta_r + (\theta_s - \theta_r)\frac{h_d}{h} \quad \text{if} \quad h < h_d \\
\theta &= \theta_s \quad \text{if} \quad h \geq h_d
\end{align*}
\]

With:

- $\theta_s$ water content in saturation
- $\theta_r$ residual water content
- $n$ et $m$ parameters linked to the soil structure
The van Genuchten Model:

Capillary capacity is taken as followed:

\[
\begin{aligned}
C(h) &= \frac{n \times m \times a \, |h| \, d\theta}{(1 + (a \times |h|)^n)^{1+m}} \quad \text{if } h < 0 \\
C(h) &= 0 \quad \text{if } h \geq 0
\end{aligned}
\]

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 parameters of the physical model:

The van Genuchten Model:

We introduce the saturation $S_e$ as followed:

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

The Hydraulic conductivity is:

$$
\begin{cases}
K(h) = K_s \sqrt{S_e} (1 - \sqrt{1 - S_e^\frac{1}{m}})^m & \text{if } h < 0 \\
K(h) = K_s & \text{if } h \geq 0
\end{cases}
$$

With:

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

NB: Hydraulic conductivity is always positive!
The parameters of the physical model:

The van Genuchten Model:

There is a "relationship" between $\theta$ 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 \( \phi \) 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 Explicit 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:

- \( r = \frac{\Delta t}{\Delta z} \)
- \( \phi \) : numerical flux for \( h \)

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

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

$$\Delta t \leq CFL \frac{\ln C \ast \Delta z^2}{2Maxk}$$
Richards Equation: Numerical scheme

The implicit 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:

- \( r = \frac{\Delta t}{\Delta z} \)
- \( \phi : \) numerical flux for \( h \)

\[ \phi_{j+1/2}^{n+1} = -\frac{K(h_{j+1/2}^{n+1})}{\theta(h_{j+1/2}^{n+1})} \left( \frac{h_{j+1}^{n+1} - h_{j}^{n+1}}{\Delta z} - 1 \right) \]
We use an upwind scheme (1st order):

\[ C_j^{n+1} = C_j^{n+1} - r \times V \times (\text{flux}S_j^n - \text{flux}S_{j-1}^n) + r \times \frac{2}{\theta_j^n + \theta_{j+1}^n} \times (\text{Diff}S_j^n - \text{Diff}S_{j-1}^n) \]

With:
- \( V = \frac{qS_j^n + qS_{j+1}^n}{2} \)
- \( qS_j^n = \frac{q_j^n}{\theta_j^n} \)
- \( \text{flux}S_j^n = C_j^n \quad \text{If} \quad q \geq 0 \)
- \( \text{flux}S_j^n = C_{j+1}^n \quad \text{If} \quad q < 0 \)
- \( \text{Diff}S_j^n = \frac{dz \times |q_j^n|}{Pe} \times (C_{j+1}^n - C_j^n) / dz \)
Numerical results

Soil parameters for our test case:

![Diagram of soil layers](image)

**Figure:** The soil
Numerical resultats

Soil parameters for our test case:

<table>
<thead>
<tr>
<th>case Sand</th>
<th>Infiltration through homogenous parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domaine lenth</td>
<td></td>
</tr>
<tr>
<td>Parameters</td>
<td></td>
</tr>
<tr>
<td>case 1</td>
<td></td>
</tr>
<tr>
<td>$K_s = 0.00922 cm/s$, $\theta_s = 0.368$, $\theta_r = 0.102$, $a = 0.0335 cm^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\Delta z = 0.2 cm$, $Pe = 0.2$</td>
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</tr>
<tr>
<td>$\Delta z = 2 cm$, $Pe = 20$</td>
<td></td>
</tr>
<tr>
<td>$\Delta z = 2 cm$, $Pe = 200$</td>
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</tr>
<tr>
<td>case 2</td>
<td></td>
</tr>
<tr>
<td>$K_s = 0.000151 cm/s$, $\theta_s = 0.4686$, $\theta_r = 0.106$, $a = 0.03104 cm^{-1}$</td>
<td></td>
</tr>
<tr>
<td>Domaine lenth</td>
<td></td>
</tr>
<tr>
<td>Parameters (Clay)</td>
<td></td>
</tr>
<tr>
<td>case 3</td>
<td></td>
</tr>
</tbody>
</table>
Numerical results

Head water in 5 and 10 days:

Figure: Head water in 5 and 10 days

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Numerical resultats : Solute concentration

Solute concentration in 5 and 10 days:
Numerical results: Hydraulic conductivity

Hydraulic conductivity in 5 and 10 days:

![Graph showing hydraulic conductivity over time and depth for 5 and 10 days. The graphs display the change in hydraulic conductivity (K) with depth (z) and time in days.]
Numerical results: Water content

Volumetric Water content in 5 and 10 days:

![Graphs showing volumetric water content over time and depth for 5 and 10 days.]
In the first test case, we consider the following equation:

\[ -\nabla \cdot (|\nabla u|^{p-2} \nabla u) = f \]

Taking:
- \( \Omega := (0, 1) \ast (0, 1) \).
- \( f(x, y) = 2 \).
- Boundaries conditions and exact solution:
  \[ u(x, y) = -\frac{p-1}{p} |(x, y) - (0.5, 0.5)|^{\frac{p-1}{p}} + \frac{p-1}{p} \left( \frac{1}{2} \right)^{\frac{p-1}{p}} \]
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

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Min</th>
<th>Max</th>
<th>$\epsilon_1$</th>
<th>$\epsilon_2$</th>
<th>$\epsilon_{\infty}$</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>10*10</td>
<td>-0.1607</td>
<td>0.2229</td>
<td>3.2634e-04</td>
<td>5.5239e-04</td>
<td>0.0019</td>
<td>0.750136</td>
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<td>20*20</td>
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</tbody>
</table>
Numerical results - test case 2

In the second case, we consider the following equation:

\[-\nabla.(u\nabla u) = f\]

With:

- \(\Omega := (0, 1) \times (0, 1)\).
- \(f(x, y) = -8(x^2 + y^2)\).
- 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

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Min</th>
<th>Max</th>
<th>$\epsilon_1$</th>
<th>$\epsilon_2$</th>
<th>$\epsilon_{\infty}$</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.1772</td>
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<td>20*20</td>
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<td>2</td>
<td>0.0538</td>
<td>0.0502</td>
<td>0.1085</td>
<td>5.136513</td>
</tr>
<tr>
<td>30*30</td>
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<td>0.0274</td>
<td>0.0724</td>
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<tr>
<td>50*20</td>
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<td>0.2331</td>
<td>0.0062</td>
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<tr>
<td>50*50</td>
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<tr>
<td>100*100</td>
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<td>2</td>
<td>0.0032</td>
<td>0.0046</td>
<td>0.0217</td>
<td>848.066829</td>
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</tbody>
</table>
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 structured mesh and we obtain the following system:

\[
\frac{h_{k}^{n+1} - h_{k}^{n}}{dt} = - \frac{K_{12}^{k,k+1} + K_{21}^{k,k+n}}{4\Delta x \Delta y} h_{k+n+1}
\]

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

\[
+ \frac{K_{12}^{k,k-1} + K_{21}^{k,k+n}}{4\Delta x \Delta y} h_{k+n-1}
\]
Richards 2D : FV Diamant

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

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

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

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

\[ - \frac{K_{12}^{k,k-1} + K_{21}^{k,k-n}}{4\Delta x\Delta y} h_{k-n-1} \]
Richards Linear: test case 1

For the 2D model we take :

**The boundaries conditions:** $h = Hex$ everywhere.

**The exact solution** :

$$Hex(x, z, t) = \exp(-B \times t) \sin\left(\frac{p2\pi x}{a}\right) \sin\left(\frac{q2\pi z}{b}\right)$$

with $B, p, q, a$ and $b$ are parameters to be defined.

**The initial solution** is

$$Hex(x, z, 0) = \sin\left(\frac{p2\pi x}{a}\right) \sin\left(\frac{q2\pi z}{b}\right)$$
Linear Richards: test case 1 (Explicit/Implicit)

Figure: Numerical and exact solution
Linear Richards: test case 2

For the 2D model we take:

**The boundaries conditions:** \( h = Hex \) everywhere.

**The exact solution:**

\[
Hex(x, z, t) = \sum \sum \frac{200}{\pi^2} \times (1 + (-1)^{k+l} \times \frac{1 - \cos(l \times \pi/2)}{k \times l} \times \sin(t \times \pi/2 \times x) \times \sin(l \times \pi/2 \times z) \times \exp((-\pi^2 \times (l^2 + k^2) \times t/36))
\]

**The initial solution** is

\[
Hex(x, z, 0) = \sum \sum \frac{200}{\pi^2} \times (1 + (-1)^{k+l} \times \frac{1 - \cos(l \times \pi/2)}{k \times l} \times \sin(t \times \pi/2 \times x) \times \sin(l \times \pi/2 \times z)
\]
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 $n \times m = 100 \times 100$
Richards Non-Linear : test case 3

the error for $n \times m = 20 \times 20$
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

- Mohamed Hayek. An exact explicit solution for one-dimensional, transient, nonlinear Richards’ equation for modeling infiltration with special hydraulic functions.
- Mohammad Sayful Islam. IMPLEMENTATION AND TESTING OF TECHNIQUES FOR IMPROVING THE PERFORMANCE OF RICHARDS EQUATION SOLVERS AND THE HANDLING OF HETEROGENEOUS SOILS.
THANK you for your Attention!