NewSolChem
Nouveau solveur pour la chimie à l'équilibre

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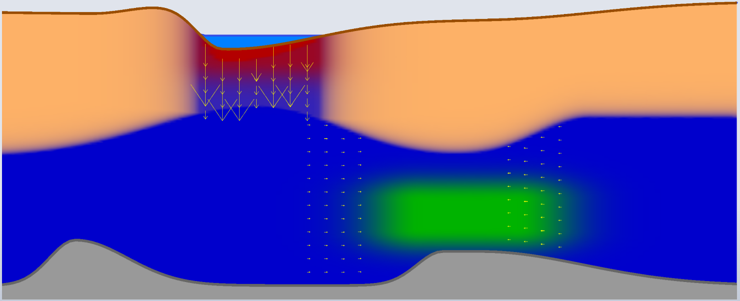
Conférence Needs Clermont-Ferrand

A piece of a global problem

Reactive transport in shallow aquifers



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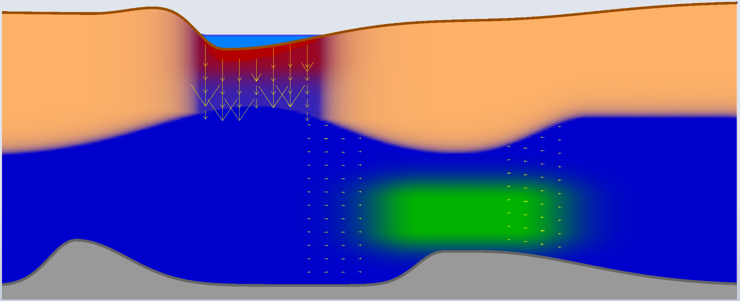

Involved processes

- Unsaturated water flow in porous media
- Transport of chemical species by the water
- Chemical reaction : kinetic or **at the equilibrium**

Difficulties: high numerical cost

Unsaturated water flow in porous media

Classically described by **3d-Richards equations**
$\hookrightarrow$ **non-linear, degenerative, 3d**

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Transport of chemical species by the water

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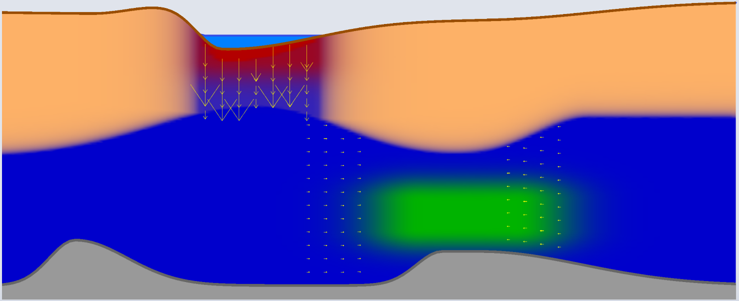
Chemical reactions

- **At the equilibrium: non-linear algebrical system**
  - $\hookrightarrow$ **ill-conditioned**
  - $\hookrightarrow$ **hold at each mesh of the 3d domain**
- **Kinetic:** not yet

How to deal with those dificulties



New strategy to solve the chemical equilibrium

- ↪ avoid the problem “ill-conditioned”
- ↪ reduce the computational time

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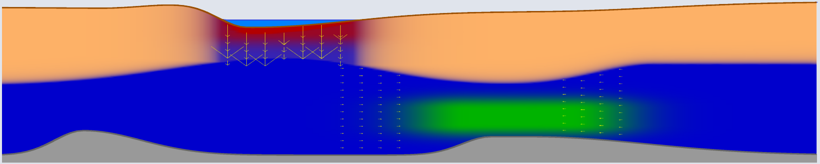


New strategy to solve the chemical equilibrium

↪ avoid the problem "ill-conditioned"

↪ reduce the computational time

Aquifer large and shallow

- For the flow/transport:

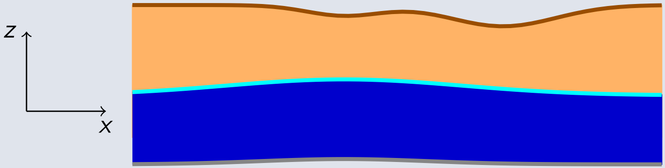
  ↪ more 2d than 3d ?

  ↪ what for the recharge ?

- For the chemical part:

  ↪ reduce the number of mesh ?

Unsaturated flow in porous media: Richards equation

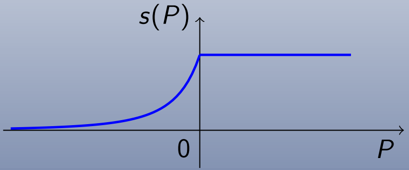


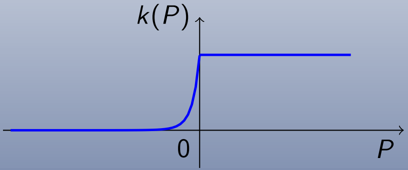
Richards Equation in $]0, T[\times\Omega_{3d}$

$$\frac{\partial s(P)}{\partial t} - \operatorname{div}\left(k(P)\,\nabla H\right) = 0, \qquad + \text{ Boundary conditions,}$$

P: **pressure**, $H = P - z$: **hydraulic head**

$s(P)$: water saturation, $k(P)$: hydraulic conductivity.





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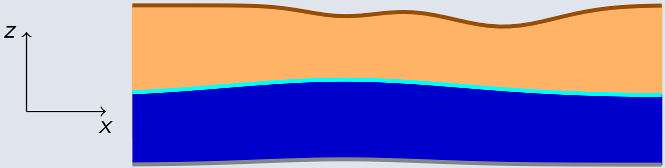

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Objective: Propose a simplified model for shallow aquifers

- With the same **dominant components** than 3d-Richards flow
- For a large range of **time scale**

Dominant components of the flow

Short-time scale: 1d vertical Richards problem

$$\frac{\partial s(\overline{P}_0)}{\partial \overline{t}} - \frac{\partial}{\partial \overline{z}} \left(\overline{k}(\overline{P}_0) \frac{\partial \overline{H}_0}{\partial \overline{z}} \right) = 0 \qquad (1)$$

No time for the water to have a significant horizontal displacement.

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Long-time scale: 2d horizontal "Dupuit's problem"

$$\begin{cases} \overline{H}_0(\overline{t},\overline{x},\overline{z}) = \overline{H}_0(\overline{t},\overline{x}) \\ +\ \text{2d problem characterizing } \overline{H}_0 \end{cases} \tag{2}$$

Vertical flow seems instantaneous: stationary state is reached.

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Conclusion: **3d-Richards problem** $\longrightarrow$ **effective equations** (1)-(2).

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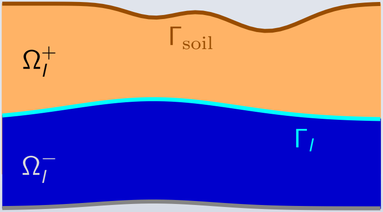
Idea:

Propose a **simplier problem $\longrightarrow$ effective equations** (1)-(2).

Coupled model in physical variables

I = **interface saturated/unsaturated**

Flow in Ω_I^+:



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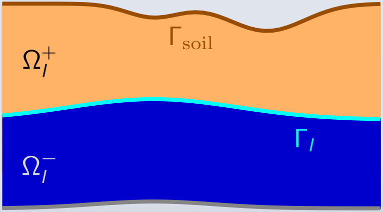

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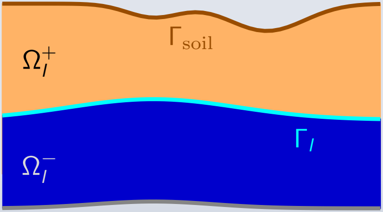

Flow in Ω_I^-: Dupuit-type model

$$\begin{cases} H(t,x,z) = H(t,x) \\ + \text{ 2d problem characterizing } H \end{cases}$$

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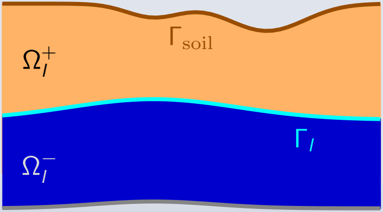

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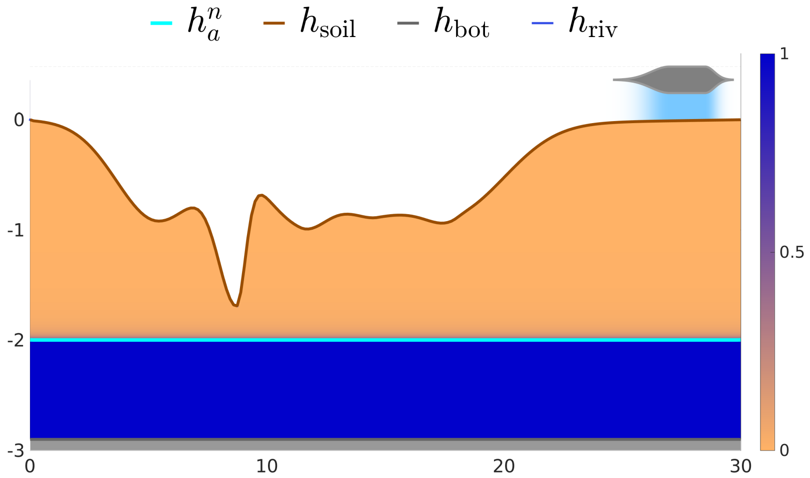
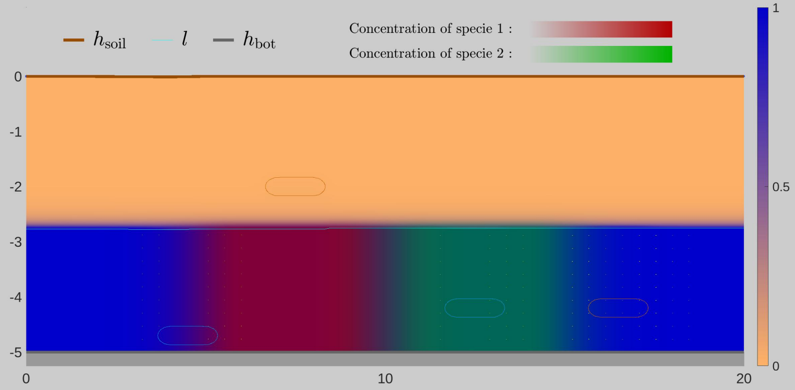
Coupled problem $\longrightarrow$ effective equations (1)-(2).

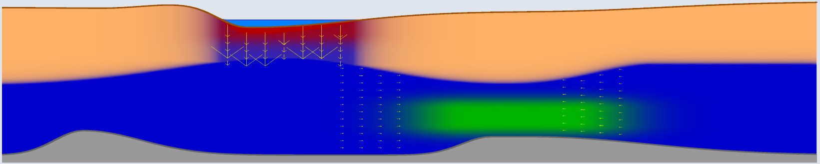
With some rain and infiltration



The same kind of model coupled with transport



Improvements



Aquifer large and shallow: Coupled Dupuit-Richards problem

- For the flow/transport:
  - ↪ Coupling 2d with 1ds (instead of 3d)
  - ↪ Good approximation at every time scale,
- For the chemical part:

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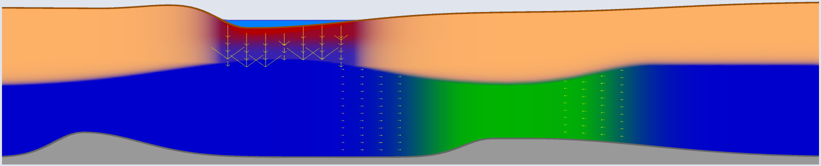

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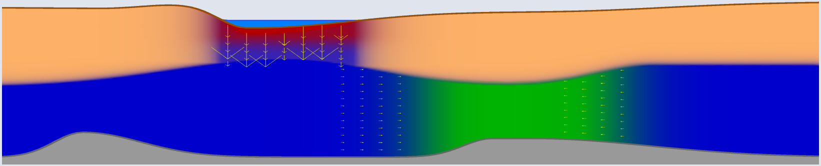

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New strategy to solve the chemical equilibrium

↪ avoid the problem "ill-conditioned"

Equilibrium reactions :

$$\sum_{j=1}^{n_p} \mu_{ij}\, \chi_j \rightleftharpoons \mathcal{C}_i \qquad\qquad i = 1, ..., n_s$$

χ_j: components (of cardinal n_p)
$\mathcal{C}_i$: secondary species (of cardinal n_s)
μ: stoichiometric matrix

Mathematical model

Law of mass action

$$\mathcal{C}_i = K_i \prod_{k=1}^{n_p} {\chi_k}^{\mu_{ik}}$$

K: equilibrium constant

Mass conservation

$$T_j = \sum_{i=1}^{n_s} \mu_{ij} \, \mathcal{C}_i$$

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Non-linear system of equations:

We search $\chi \in \mathbb{R}^{n_p}$ such that

$$\sum_{i=1}^{n_s} \mu_{ij} (K_i \prod_{k=1}^{n_p} {\chi_k}^{\mu_{ik}}) - T_j = 0$$

for all $j \in \{1, \ldots, n_p\}$

Mathematical model

Non-lineair problem

We search $\chi \in \mathbb{R}^{n_p}$ such that

$$F(\chi) = 0,$$

with $F : \mathbb{R}^{n_p} \rightarrow \mathbb{R}^{n_p}$ (non-linear)

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Strategies:

- Classical method : **Newton method**

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  - Problem : high computational time, even non convergence
- Alternative : **Positive continuous fraction method (PCF)**

Positive continuous fraction method (PCF)

Problem reformulation:

$$T_j = \sum_{i=1}^{n_s} \mu_{ij}\,\mathcal{C}_i = \sum_{\mu_{ij}>0} \mu_{ij}\,\mathcal{C}_i + \sum_{\mu_{ij}<0} \mu_{ij}\,\mathcal{C}_i$$

$$\Longleftrightarrow$$

$$SR_j(\chi) = SP_j(\chi)$$

Sum of reactants: $SR_j = \begin{cases} \sum_{\mu_{ij}>0} \mu_{ij}\,\mathcal{C}_i & T_j \geq 0 \\ |T_j| + \sum_{\mu_{ij}>0} \mu_{ij}\,\mathcal{C}_i & T_j < 0 \end{cases}$

Sum of products: $SP_j = \begin{cases} T_j + \sum_{\mu_{ij}<0} |\mu_{ij}|\,\mathcal{C}_i & T_j \geq 0 \\ \sum_{\mu_{ij}<0} |\mu_{ij}|\,\mathcal{C}_i & T_j < 0 \end{cases}$

Fix-point problem

We build a sequence χ_j^n such that

$$\chi_j^{n+1} = \chi_j^n \left(\frac{SP_j(\chi^n)}{SR_j(\chi^n)} \right)^{\frac{1}{\mu_{i_0 j}}}$$

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- **Advantage**: no Jacobian matrix needed
- **Problem**: high computational time, even non convergence
- **Strategy**:
  coupling with methods of acceleration of the convergence rate
  - Anderson acceleration
  - Minimale polynomiale extrapolation
  - Reduced rank extrapolation