Flow and Reactive transport in shallow aquifer

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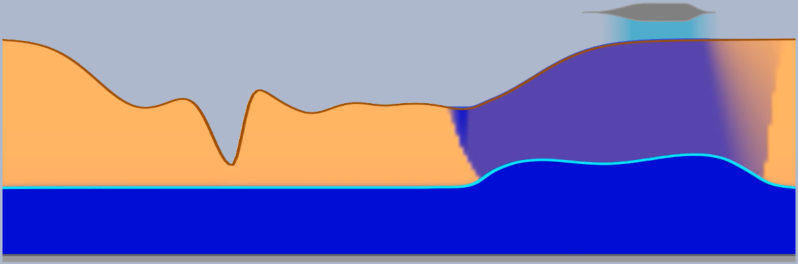
Journées transport réactif, LMPA Calais

Objective and outline



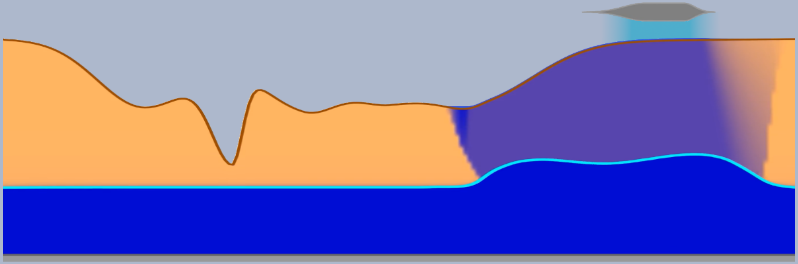
Context

Describe **efficiently** pollutant transport in **shallow aquifers**.

↪ **Typically** nitrates pollution of the watertable due to agriculture

↪ **Modelling**: Flow + Transport + Chemical reaction

Objective and outline



Context

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↪ **Modelling**: **Flow** + **Transport** + **Chemical reaction**

Objective and outline

Dificulties in the flow description

- Flow in porous media: **3d-Richards model**

  $\hookrightarrow$ **non-linear + 3d = Difficult** (mathematically and numerically)

- **Lagre geometry**

  $\hookrightarrow$ long time scale seems important

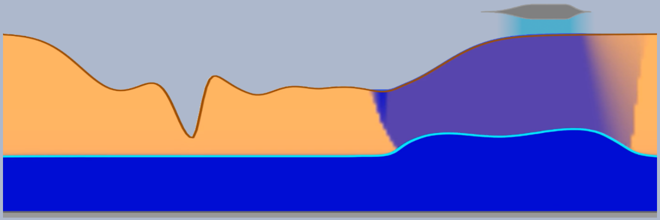
- Chemical reactions may occur **above the water table**

  $\hookrightarrow$ short time scale seems important

Objective: Propose simplified models to describe the **flow** and the **reactive transport**

Strategy: use the shallow geometry to simplify the flow modelling

Outline

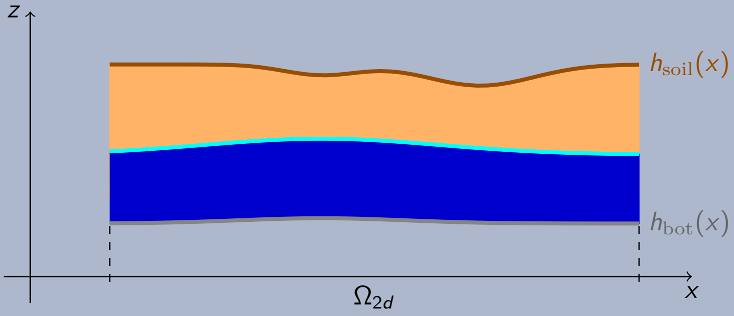


1. **Geometry and 3d-Richards equations**
2. **Dominant componants of the flow: effective problems**
3. **A coupled model coupling dominant componants**
4. **Numerical scheme**
5. **Considering reactive transport**
6. **Reactive transport: Dominant componant and coupled model**
7. **Numerical scheme**

Plan

1. **Geometry and 3d-Richards equations**
2. Dominant componants of the flow: effective problems
3. A coupled model coupling dominant componants
4. Numerical scheme
5. Considering reactive transport
6. Reactive transport: Dominant componant and coupled model
7. Numerical scheme

Notations and Geometry



- Ω_{2d} : horizontal domain
- x : horizontal variable
- z : vertical variable

- e_3 : unitary vertical vector
- $h_{\mathrm{bot}}(x)$: level of the bottom
- $h_{\mathrm{soil}}(x)$: level of the soil

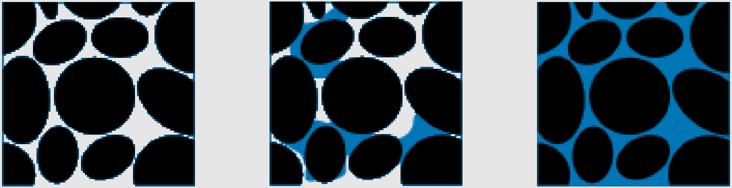
$$\Omega_{3d} := \left\{ (x,z) \mid x \in \Omega_{2d} \ , z \in \left] h_{\mathrm{bot}}(x), h_{\mathrm{soil}}(x) \right[\right\}$$

Physical quantities and Richards equation

- P : **Pressure head**
- H : **Hydraulic head**
- $\boldsymbol{v}^f$: Fluid velocity
- θ : Water saturation
- k : Hydraulic conductivity

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

$$\begin{cases} \dfrac{\partial\theta}{\partial t} + \operatorname{div} \boldsymbol{v}^f = 0 \\ \boldsymbol{v}^f = -k\nabla H \\ H = P + z \end{cases}$$



$\theta \simeq 0$ $\quad 0 < \theta < 1$ $\quad \theta = 1$

Physical quantities and Richards equation

- P : **Pressure head**
- H : **Hydraulic head**
- $\boldsymbol{v}^f$: Fluid velocity

- $\theta(P)$: Water saturation
- $k(P)$: Hydraulic conductivity

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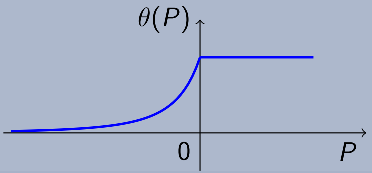
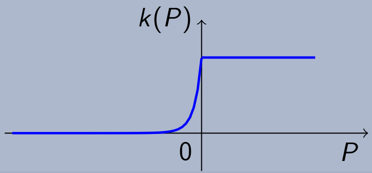
Hypothesis:

- $\theta = \theta(P), \quad k = k(P)$
- $\theta(P) = 1 \iff P \geq 0$

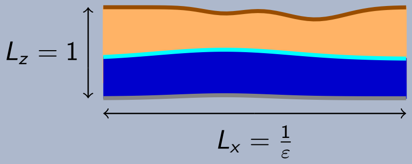




Plan

Dominant components of the flow

- **Objective:**
  exhibits dominant component of the flow when the aquifer is very large
- **Strategy:**
  - Aquifer large and shallow: $L_x = \frac{1}{\varepsilon}$, $L_z = 1$ then make $\varepsilon \to 0$



Physical variables (x, z)

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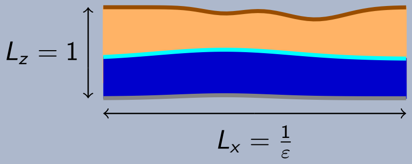
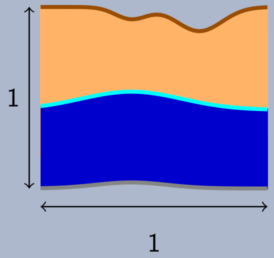
- **Strategy:**
  - Aquifer large and shallow: $L_x = \frac{1}{\varepsilon}$, $L_z = 1$ then make $\varepsilon \to 0$
  - Change of variable

$$\overline{x} = \frac{x}{L_x} = \varepsilon x, \qquad \overline{z} = \frac{z}{L_z} = z$$



Physical variables (x, z)



Dimensionless variables $(\overline{x}, \overline{z})$

Rescaled Richards equation

Richards Equation

$$\frac{\partial\theta(P)}{\partial t} - \mathrm{div}_x\left(k(P)\,\nabla_x H\right) - \frac{\partial}{\partial z}\left(k(P)\frac{\partial H}{\partial z}\right) = 0$$

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Richards Equation

$$\frac{\partial \theta(P)}{\partial t} - \mathrm{div}_x\,(k(P)\,\nabla_x H) - \frac{\partial}{\partial z}\left(k(P)\frac{\partial H}{\partial z}\right) = 0$$

- $L_x = \frac{1}{\varepsilon}$ characteristic size of Ω_{2d} $\Rightarrow$ $\bar{x} = \dfrac{x}{L_x}$
- $L_z = 1$ characteristic vertical size of Ω_{3d} $\Rightarrow$ $\bar{z} = \dfrac{z}{L_z}$
- T characteristic time $\Rightarrow$ $\bar{t} = \dfrac{t}{T}$

Rescaled Richards equation

Richards Equation

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Dimensionless Richards Equation

$$\frac{1}{T}\frac{\partial \theta(\overline{P})}{\partial \overline{t}} - \varepsilon^2 \operatorname{div}_{\overline{x}} \left(k(\overline{P})\, \nabla_{\overline{x}} \overline{H}\right) - \frac{\partial}{\partial \overline{z}}\left(k(\overline{P})\frac{\partial \overline{H}}{\partial \overline{z}}\right) = 0$$

What for the time ?

$$\frac{1}{T}\frac{\partial\theta(\overline{P})}{\partial\overline{t}} - \varepsilon^2\,\mathrm{div}_{\overline{x}}\left(k(\overline{P})\,\nabla_{\overline{x}}\overline{H}\right) - \frac{\partial}{\partial\overline{z}}\left(k(\overline{P})\frac{\partial\overline{H}}{\partial\overline{z}}\right) = 0$$

Time consideration

- Short time scale: $T = 1$

$$\frac{\partial\theta(\overline{P})}{\partial\overline{t}} - \varepsilon^2\,\mathrm{div}_{\overline{x}}\left(k(\overline{P})\,\nabla_{\overline{x}}\overline{H}\right) - \frac{\partial}{\partial\overline{z}}\left(k(\overline{P})\frac{\partial\overline{H}}{\partial\overline{z}}\right) = 0$$

- Long time scale: $T = \frac{1}{\varepsilon^2}$

$$\varepsilon^2\frac{\partial\theta(\overline{P})}{\partial\overline{t}} - \varepsilon^2\,\mathrm{div}_{\overline{x}}\left(k(\overline{P})\,\nabla_{\overline{x}}\overline{H}\right) - \frac{\partial}{\partial\overline{z}}\left(k(\overline{P})\frac{\partial\overline{H}}{\partial\overline{z}}\right) = 0$$

Effective problems: short-time scale

Asymptotic expansion

Formally:

$$\overline{P}_\varepsilon = \overline{P}_0 + \varepsilon \overline{P}_1 + \varepsilon^2 \overline{P}_2 + \dots \qquad \overline{H}_\varepsilon = \overline{H}_0 + \varepsilon \overline{H}_1 + \varepsilon^2 \overline{H}_2 + \dots$$

$$\frac{\partial \theta(\overline{P}_\varepsilon)}{\partial t} - \varepsilon^2 \operatorname{div}_{\overline{x}} \left(\overline{k}(\overline{P}_\varepsilon) \nabla_{\overline{x}} \overline{H}_\varepsilon \right) - \frac{\partial}{\partial \overline{z}} \left(k(P_\varepsilon) \frac{\partial \overline{H}_\varepsilon}{\partial \overline{z}} \right) = 0$$

1d-Richards problem

$$\phi \frac{\partial \theta(\overline{P}_0)}{\partial \overline{t}} - \frac{\partial}{\partial \overline{z}} \left(\overline{k}(\overline{P}_0) \frac{\partial \overline{H}_0}{\partial \overline{z}} \right) = 0 \qquad \text{in } \Omega_{3d}$$

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

$$\varepsilon^2 \frac{\partial \theta(\overline{P}_\varepsilon)}{\partial t} - \varepsilon^2 \, \mathrm{div}_{\overline{x}} \left(\overline{k}(\overline{P}_\varepsilon) \, \nabla_{\overline{x}} \overline{H}_\varepsilon \right) - \frac{\partial}{\partial \overline{z}} \left(\overline{k}(\overline{P}_\varepsilon) \frac{\partial \overline{H}_\varepsilon}{\partial \overline{z}} \right) = 0$$

Dupuit-like problem

$$\begin{cases} \overline{H}_0(t, x, z) = \overline{H}_0(t, x) \\ \\ \\ \end{cases}$$

Effective problems: long-time scale

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$$\begin{cases} \overline{H}_0(t,x,z) = \overline{H}_0(t,x) \\ \dfrac{\partial}{\partial \overline{t}} \displaystyle\int_{\overline{h}_{\mathrm{bot}}}^{\overline{h}_{\mathrm{soil}}} \theta(\overline{P}_0)\, d\overline{z} - \mathrm{div}_{\overline{x}} \left(\tilde{k}(\overline{H}_0) \nabla \overline{H}_0 \right) = 0 \\ \tilde{k}(\overline{H}_0) = \displaystyle\int_{\overline{h}_{\mathrm{bot}}}^{\overline{h}_{\mathrm{soil}}} \overline{k}(\overline{P}_0)\, d\overline{z} \end{cases}$$

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Vertical flow seems instantaneous: stationary state is reached.

Conclusion of asymptotic analysis

Short-time scale: 1d vertical Richards problem

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

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

$$\begin{cases} \overline{H}_0(\overline{t}, \overline{x}, \overline{z}) = \overline{H}_0(\overline{t}, \overline{x}) \\ \dfrac{\partial}{\partial \overline{t}} \displaystyle\int_{\overline{h}_{\mathrm{bot}}}^{\overline{h}_{\mathrm{soil}}} \theta(\overline{P}_0)\, d\overline{z} - \mathrm{div}_{\overline{x}} \left(\tilde{k}(\overline{H}_0) \nabla_{\overline{x}} \overline{H}_0 \right) = 0 \end{cases}$$

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Conclusion: 3d-Richards problem $\longrightarrow$ effective equations

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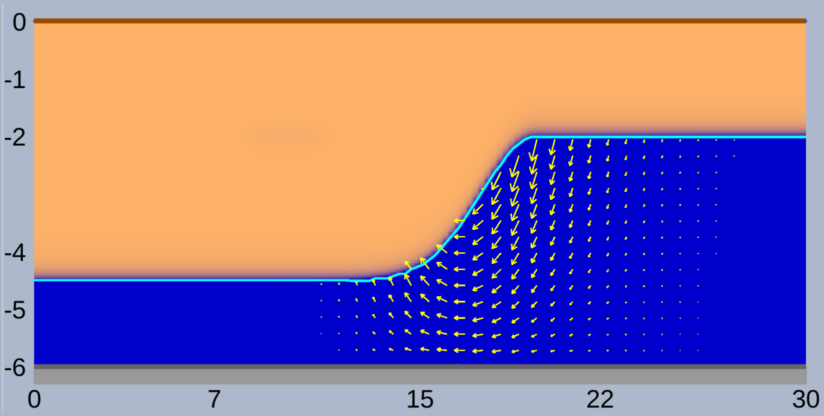
Conclusion: 3d-Richards problem $\longrightarrow$ effective equations

Strategy: Simplier coupled problem $\longrightarrow$ effective equations

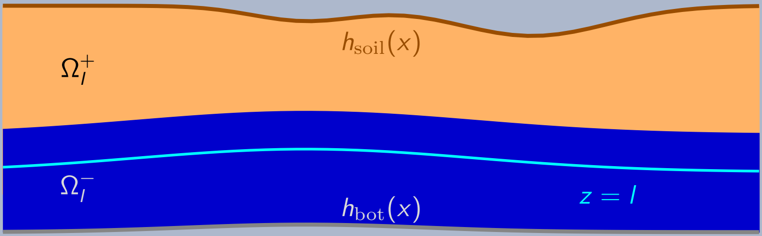
Numerical experiment

Flow described by the 3d-Richards model



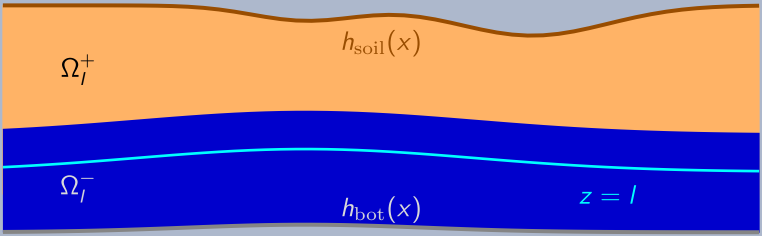
Plan

Coupled model in physical variables



Flow in short time scale

$$\frac{\partial \theta(P)}{\partial t} - \frac{\partial}{\partial z}\left(k(P)\frac{\partial H}{\partial z}\right) = 0 \quad \text{in }]h_{\mathrm{bot}}, h_{\mathrm{soil}}[$$

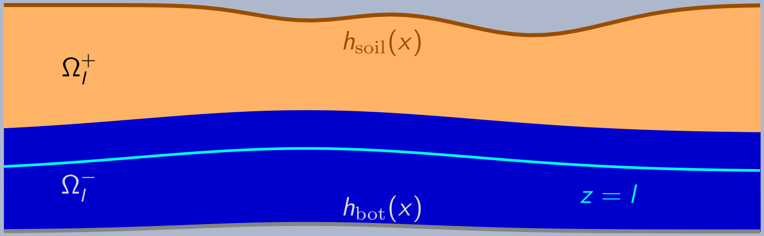


Flow in short time scale

$$\frac{\partial \theta(P)}{\partial t} - \frac{\partial}{\partial z}\left(k(P)\frac{\partial H}{\partial z}\right) = 0 \quad \text{in } \Omega_l^+$$

$$\underbrace{\frac{\partial \theta(P)}{\partial t}}_{=0} - \frac{\partial}{\partial z}\left(\underbrace{k(P)}_{=1}\frac{\partial H}{\partial z}\right) = 0 \quad \text{in } \Omega_l^-$$

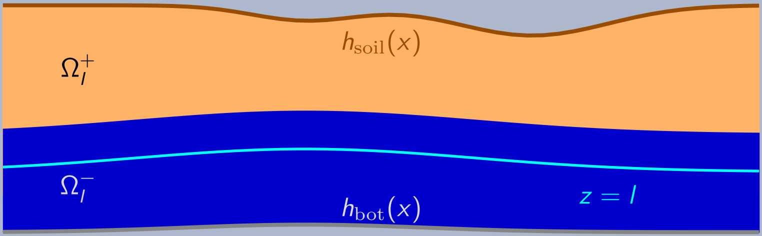
Coupled model in physical variables



Flow in short time scale

$$\frac{\partial \theta(P)}{\partial t} - \frac{\partial}{\partial z}\left(k(P)\frac{\partial H}{\partial z}\right) = 0 \quad \text{in } \Omega_l^+$$

$$-\frac{\partial^2 H}{\partial z^2} = 0 \quad \text{in } \Omega_l^-$$



Flow in short time scale

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$$H(t,x,z) = H(t,x) \quad \text{in } \Omega_l^-$$

Coupled model in physical variables

Flow in short time scale

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$$H(t,x,z) = H(t,x) \quad \text{in } \Omega_l^-$$

Long time problem

$$\begin{cases} H(t,x,z) = H(t,x) \\ \dfrac{\partial}{\partial t}\displaystyle\int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}} \theta(P)\,dz - \mathrm{div}_x\left(\tilde{k}(\tilde{H})\nabla_x H\right) = 0 \end{cases}$$

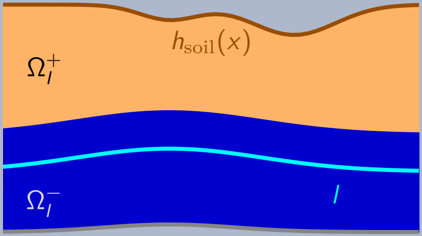
Coupled model in physical variables

Flow in Ω_l^+: 1d-Richards

$$\left\{ \right.$$

Flow in Ω_l^-:

$$H(t,x,z) = \tilde{H}(t,x)$$



Evolution of Hydraulic head:

Evolution of interface: 2 choices

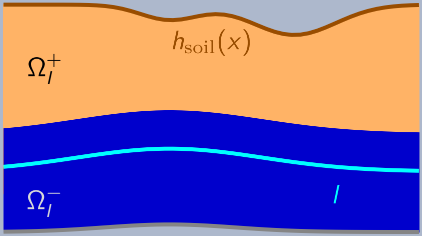
Coupled model in physical variables

Flow in Ω_l^+: 1d-Richards

$$\begin{cases} \dfrac{\partial \theta(P)}{\partial t} + \dfrac{\partial u}{\partial z} = 0 \\ u = -k(P)\dfrac{\partial H}{\partial z} \\ H = \tilde{H} \qquad \text{on} \quad \Gamma_l \end{cases}$$

Flow in Ω_l^-:

$$H(t,x,z) = \tilde{H}(t,x)$$



Evolution of Hydraulic head:

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Coupled model in physical variables

Flow in Ω_l^+: 1d-Richards

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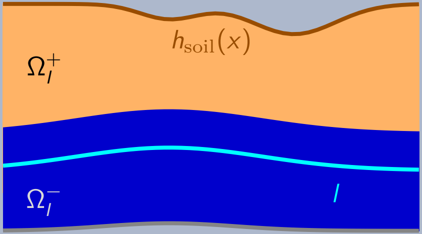

Evolution of Hydraulic head:

$$\frac{\partial}{\partial t}\left(\int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}} \theta(P)\, dz\right) - \mathrm{div}_x\left(\tilde{k}(\tilde{H})\nabla_x \tilde{H}\right) = 0$$

Evolution of interface: 2 choices

Coupled model in physical variables

Flow in Ω_I^+: 1d-Richards

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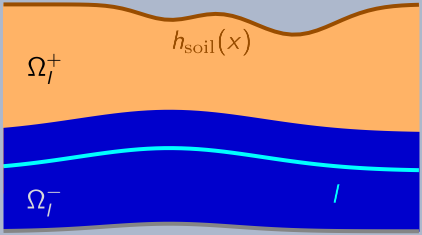
Flow in Ω_I^-:

$$H(t,x,z) = \tilde{H}(t,x)$$



Evolution of Hydraulic head:

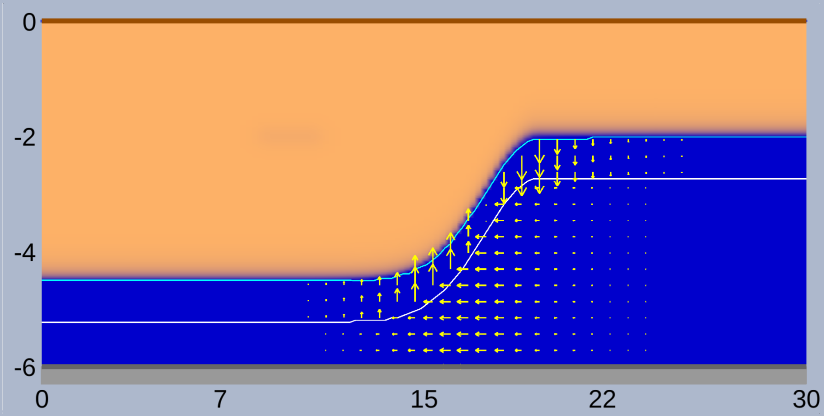
$$\frac{\partial}{\partial t}\left(\int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}} \theta(P)\, dz \right) - \mathrm{div}_x \left(\tilde{k}(\tilde{H}) \nabla_x \tilde{H} \right) = 0$$

Evolution of interface: 2 choices

- I is given a priori.
- I depends on the other variables

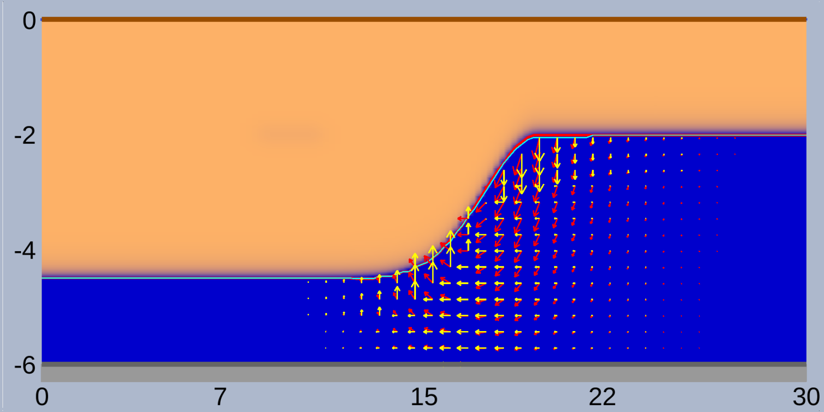
Numerical experiment

Flow described by the "Dupuit-Richards" model



Numerical experiment

Comparison between the two models



Summary of the coupled model for Richards

Geometrical coupling of dominant behavior

- Domain splitted **into too parts**
- **Upper part:** vertical Richards (fast componant)
- **Lower part:** horizontal flow (slow componant)

Advantages

- Coupled model and 3d-Richards models: **same effective behaviors**
  ↪ at each time scale
- **Numerically efficient**
  ↪ 2d problem coupled with many 1d problems
  ↪ mass-conservative
- **Can be tuned** thanks to l

Drawbacks

- Bad description of water fluxes
  ↪ jump from vertical to horizontal at level l.

Plan

Implicit time scheme

$(t_n)_n$: **discretization of** $[0, T]$**,** δ_t: **time step.**

$$P^n(x,z) \simeq P(t_n,x,z)\ , \quad H^n(x) \simeq H(t_n,x).$$

Evolution of Hydraulic head:

$$\frac{1}{\delta_t}\Big(\int_{h_{\rm bot}}^{h_{\rm soil}} \theta(P^n)\,dz - \int_{h_{\rm bot}}^{h_{\rm soil}} \theta(P^{n-1})\,dz\Big) - \mathrm{div}_x\left(\tilde{k}(\tilde{H}^n)\nabla_x \tilde{H}^n\right) = 0$$

1d-Richards

$$\begin{cases} \dfrac{\theta(P^n)-\theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^n}{\partial z} = 0 & \text{in} \quad]I^n, h_{\rm soil}[\\ u^n = -k(P^n)\dfrac{\partial H^n}{\partial z} & \text{in} \quad]I^n, h_{\rm soil}[\\ H^n = \tilde{H}^n & \text{on} \quad \Gamma_{I^n} \end{cases}$$

Implicit time scheme

$(t_n)_n$: **discretization of** $[0, T]$**,** δ_t: **time step.**

$$P^n(x,z) \simeq P(t_n,x,z)\ , \quad H^n(x) \simeq H(t_n,x).$$

Evolution of Hydraulic head:

$$\frac{1}{\delta_t}\Big(\int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}}\theta(P^n)\,dz - \int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}}\theta(P^{n-1})\,dz\Big) - \mathrm{div}_x\left(\tilde{k}(\tilde{H}^n)\nabla_x\tilde{H}^n\right) = 0$$

1d-Richards

$$\begin{cases} \dfrac{\theta(P^n)-\theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^n}{\partial z} = 0 & \text{in } \ ]I^n, h_{\mathrm{soil}}[\\ u^n = -k(P^n)\dfrac{\partial H^n}{\partial z} & \text{in } \ ]I^n, h_{\mathrm{soil}}[\\ H^n = \tilde{H}^n & \text{on } \ \Gamma_{I^n} \end{cases}$$

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Evolution of Hydraulic head:

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1d-Richards: Solved to compute Λ

$$\begin{cases} \dfrac{\theta(P^n)-\theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^n}{\partial z} = 0 & \text{in } \ ]I^n, h_{\mathrm{soil}}[\\ u^n = -k(P^n)\dfrac{\partial H^n}{\partial z} & \text{in } \ ]I^n, h_{\mathrm{soil}}[\\ H^n = \tilde{H}^n & \text{on } \ \Gamma_{I^n} \end{cases}$$

Implicit time scheme

$(t_n)_n$: discretization of $[0, T]$, $\quad$ **δ_t: time step.**

$$P^n(x,z) \simeq P(t_n,x,z)\ , \quad H^n(x) \simeq H(t_n,x).$$

Evolution of Hydraulic head:

$$\Lambda(\tilde{H}^n) - \mathrm{div}_x\left(\tilde{k}(H^n)\nabla_x \tilde{H}^n\right) = 0$$

1d-Richards: Solved to compute Λ

$$\begin{cases} \dfrac{\theta(P^n)-\theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^n}{\partial z} = 0 & \text{in } \;]l^n, h_{\mathrm{soil}}[\\ u^n = -k(P^n)\dfrac{\partial H^n}{\partial z} & \text{in } \;]l^n, h_{\mathrm{soil}}[\\ H^n = \tilde{H}^n & \text{on } \; \Gamma_{l^n} \end{cases}$$

Picard's fix-point strategy

$$A^{n_0} = A^{n-1}, \quad A^{n_k} \to A^n \quad \text{for} \quad A = P, H, h, u \; .$$

Evolution of Hydraulic head :

$$\Lambda(\tilde{H}^{n_k}) - \mathrm{div}_x \left(\tilde{k}(\tilde{H}^{n_k}) \nabla_x \tilde{H}^{n_k} \right) = 0$$

1d-Richards: used to compute Λ

$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in } \;]I^n, h_{\text{soil}}[\\ u^{n_k} = -k(P^{n_k}) \dfrac{\partial H^{n_k}}{\partial z} & \text{in } \;]I^n, h_{\text{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on } \; \Gamma_{I^n} \end{cases}$$

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$$A^{n_0} = A^{n-1}, \quad A^{n_k} \to A^n \quad \text{for} \quad A = P, H, h, u \ .$$

Evolution of Hydraulic head :

$$\underbrace{\Lambda(\tilde{H}^{n_k})}_{\simeq \Lambda(\tilde{H}^{n_k - 1})} - \mathrm{div}_x \left(\underbrace{\tilde{k}(H^{n_k})}_{\simeq \tilde{k}(\tilde{H}^{n_k - 1})} \nabla_x \tilde{H}^{n_k} \right) = 0$$

1d-Richards: used to compute Λ

$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ u^{n_k} = -k(P^{n_k}) \dfrac{\partial H^{n_k}}{\partial z} & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on} \quad \Gamma_{I^n} \end{cases}$$

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Picard's fix-point strategy

$$A^{n_0} = A^{n-1}, \quad A^{n_k} \to A^n \quad \text{for} \quad A = P, H, h, u\ .$$

Evolution of Hydraulic head :

$$\Lambda(\tilde{H}^{n_{k-1}}) - \mathrm{div}_x\left(\tilde{k}(\tilde{H}^{n_{k-1}})\nabla_x \tilde{H}^{n_k}\right) = 0$$

1d-Richards: used to compute Λ

$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ u^{n_k} = -k(P^{n_k})\dfrac{\partial H^{n_k}}{\partial z} & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on} \quad \Gamma_{I^n} \end{cases}$$

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Picard's fix-point strategy

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Evolution of Hydraulic head :

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$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in} \quad]l^n, h_{\text{soil}}[\\ u^{n_k} = -k(P^{n_k}) \dfrac{\partial H^{n_k}}{\partial z} & \text{in} \quad]l^n, h_{\text{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on} \quad \Gamma_{l^n} \end{cases}$$

- **Good point**: if $(H^{n_k})_k$ converges, the limit is H^n !
-

Picard's fix-point strategy

$$A^{n_0} = A^{n-1}, \quad A^{n_k} \to A^n \quad \text{for} \quad A = P, H, h, u \ .$$

Evolution of Hydraulic head :

$$\Lambda(\tilde{H}^{n_{k-1}}) - \mathrm{div}_x \left(\tilde{k}(\tilde{H}^{n_{k-1}}) \nabla_x \tilde{H}^{n_k} \right) = 0$$

1d-Richards: used to compute Λ

$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ u^{n_k} = -k(P^{n_k}) \dfrac{\partial H^{n_k}}{\partial z} & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on} \quad \Gamma_{I^n} \end{cases}$$

- **Good point**: if $(H^{n_k})_k$ converges, the limit is H^n !
- **Bad point**: it does not converges...

Pseudo-Newton strategy

$$A^{n_0} = A^{n-1}, \quad A^{n_k} \to A^n \quad \text{for} \quad A = P, H, h, u \ .$$

Evolution of Hydraulic head :

$$\Lambda(\tilde{H}^{n_k}) - \mathrm{div}_x \left(\tilde{k}(\tilde{H}^{n_k}) \nabla_x \tilde{H}^{n_k} \right) = 0$$

1d-Richards: used to compute Λ

$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in} \quad]l^n, h_{\mathrm{soil}}[\\ u^{n_k} = -k(P^{n_k}) \dfrac{\partial H^{n_k}}{\partial z} & \text{in} \quad]l^n, h_{\mathrm{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on} \quad \Gamma_{l^n} \end{cases}$$

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$$A^{n_0} = A^{n-1}, \quad A^{n_k} \to A^n \quad \text{for} \quad A = P, H, h, u \ .$$

Evolution of Hydraulic head :

$$\underbrace{\Lambda(\tilde{H}^{n_k})}_{\simeq \Lambda(\tilde{H}^{n_k-1}) + \Lambda'(\tilde{H}^{n_k-1})(\tilde{H}^{n_k} - \tilde{H}^{n_k-1})} - \mathrm{div}_x \left(\underbrace{\tilde{k}(H^{n_k})}_{\simeq \tilde{k}(\tilde{H}^{n_k-1})} \nabla_x \tilde{H}^{n_k} \right) = 0$$

1d-Richards: used to compute Λ

$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ u^{n_k} = -k(P^{n_k}) \dfrac{\partial H^{n_k}}{\partial z} & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on} \quad \Gamma_{I^n} \end{cases}$$

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Pseudo-Newton strategy

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Evolution of Hydraulic head :

$$\Lambda(\tilde{H}^{n_{k-1}}) + \Lambda'(\tilde{H}^{n_{k-1}})(\tilde{H}^{n_k} - \tilde{H}^{n_{k-1}}) - \mathrm{div}_x \left(\tilde{k}(\tilde{H}^{n_{k-1}}) \nabla_x \tilde{H}^{n_k} \right) = 0$$

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$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ u^{n_k} = -k(P^{n_k}) \dfrac{\partial H^{n_k}}{\partial z} & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on} \quad \Gamma_{I^n} \end{cases}$$

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Pseudo-Newton strategy

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$$\Lambda(\tilde{H}^{n_{k-1}}) + \Lambda'(\tilde{H}^{n_{k-1}})(\tilde{H}^{n_k} - \tilde{H}^{n_{k-1}}) - \mathrm{div}_x \left(\tilde{k}(\tilde{H}^{n_{k-1}}) \nabla_x \tilde{H}^{n_k} \right) = 0$$

1d-Richards: used to compute Λ

$$\begin{cases} \dfrac{\theta(P^{n_k}) - \theta(P^{n-1})}{\delta_t} + \dfrac{\partial u^{n_k}}{\partial z} = 0 & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ u^{n_k} = -k(P^{n_k}) \dfrac{\partial H^{n_k}}{\partial z} & \text{in} \quad]I^n, h_{\mathrm{soil}}[\\ H^{n_k} = \tilde{H}^{n_k} & \text{on} \quad \Gamma_{I^n} \end{cases}$$

- **Good point**: if $(H^{n_k})_k$ converges, the limit is H^n !
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Pseudo-Newton strategy

$$A^{n_0} = A^{n-1}, \quad A^{n_k} \to A^n \quad \text{for} \quad A = P, H, h, u \ .$$

Evolution of Hydraulic head :

$$\Lambda(\tilde{H}^{n_{k-1}}) + \Lambda'(\tilde{H}^{n_{k-1}})(\tilde{H}^{n_k} - \tilde{H}^{n_{k-1}}) - \mathrm{div}_x \left(\tilde{k}(\tilde{H}^{n_{k-1}}) \nabla_x \tilde{H}^{n_k} \right) = 0$$

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- **Good point**: if $(H^{n_k})_k$ converges, the limit is H^n !
- **Bad point**: none !

Plan

Chemical equilibrium: example of nitrate creation

Morel table (mobile/fixed)

	Primary Species			Secondary Species				
	H^+	NH_4^+	$SoilH$	OH^-	NH_3	$Soil^-$	$SoilH_2^+$	$SoilNH_4$
H^+	**1**			-1	-1	-1	1	-1
NH_4^+		**1**			1			1
$SoilH$			**1**			1	1	1
$\boldsymbol{K}$				10^{-9}	10^{-14}	10^{-7}	10^2	0.4

Chemical equilibrium: example of nitrate creation

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NH_4^+		**1**			1			1
$SoilH$			**1**			1	1	1
K				10^{-9}	10^{-14}	10^{-7}	10^2	0.4

Unkwnowns

- **Concentration** of species
  $[H^+]$, $[NH_4^+]$, $[SoilH]$ . . . . (Primary)
  $[OH^-]$, $[NH_3]$, $[Soil^-]$, $[SoilH_2^+]$, $[SoilNH_4]$ . . . . (Secondary)
-
-

Chemical equilibrium: example of nitrate creation

Morel table (mobile/fixed)

	Primary Species			Secondary Species				
	H^+	NH_4^+	$SoilH$	OH^-	NH_3	$Soil^-$	$SoilH_2^+$	$SoilNH_4$
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- **Concentration** of species
  $[H^+]$, $[NH_4^+]$, $[SoilH]$ . . . . (Primary)
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- Total of each **component**: T_{H^+}, $T_{NH_4^+}$, T_{SoilH}

Chemical equilibrium: example of nitrate creation

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	Primary Species			Secondary Species				
	H^+	NH_4^+	$SoilH$	OH^-	NH_3	$Soil^-$	$SoilH_2^+$	$SoilNH_4$
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Unkwnowns

- **Concentration** of species
  $[H^+]$, $[NH_4^+]$, $[SoilH]$ . . . . (Primary)
  $[OH^-]$, $[NH_3]$, $[Soil^-]$, $[SoilH_2^+]$, $[SoilNH_4]$ . . . . (Secondary)
- Total of each **component**: T_{H^+}, $T_{NH_4^+}$, T_{SoilH}
- **mobile** and **fixed** contrib.: $T^m_{H^+}$, $T^m_{NH_4^+}$, T^m_{SoilH}, $T^f_{H^+}$, $T^f_{NH_4^+}$, T^f_{SoilH}

Chemical equilibrium: example of nitrate creation

Morel table (mobile/fixed)

	Primary Species			Secondary Species				
	H^+	NH_4^+	$SoilH$	OH^-	NH_3	$Soil^-$	$SoilH_2^+$	$SoilNH_4$
H^+	**1**			-1	-1	-1	1	-1
NH_4^+		**1**			1			1
$SoilH$			**1**			1	1	1
K				10^{-9}	10^{-14}	10^{-7}	10^2	0.4

Unkwnowns

- **Concentration** of species

  $\boldsymbol{a} = (\boldsymbol{a}^m, \boldsymbol{a}^f) = ([H^+], [NH_4^+], [SoilH])$ .... (Primary)

  $\boldsymbol{b} = (\boldsymbol{b}^m, \boldsymbol{b}^f) = ([OH^-], [NH_3], [Soil^-], [SoilH_2^+], [SoilNH_4])$ ..... (Sec.)

- Total of each **component**: $\boldsymbol{T} = (T_{H^+}, T_{NH_4^+}, T_{SoilH})$
- **mobile** and **fixed** contrib.: $\boldsymbol{T}^m = (T^m_{H^+}, T^m_{NH_4^+}, T^m_{SoilH})$, $\boldsymbol{T}^f = (T^f_{H^+}, T^f_{NH_4^+}, T^f_{SoilH})$

Chemical Equilibrium: example of nitrate creation

Morel Table $\Longrightarrow$ $\begin{cases} \text{Stoechiometry matrix } \begin{pmatrix} \boldsymbol{I}_d & \boldsymbol{M} \end{pmatrix} \\ \boldsymbol{K} = (K_j)_j = (1, 10^{-14}, 1, 10^{-9}, 1, 10^{-7}, 10^2, 0.4) \end{cases}$

with

- **Linear relations**

$$\boldsymbol{T} = \boldsymbol{a} + \boldsymbol{M}\boldsymbol{b}, \quad \boldsymbol{T} = \boldsymbol{T}^m + \boldsymbol{T}^f, \quad \boldsymbol{T}^m = \begin{pmatrix} \boldsymbol{a}^m + \boldsymbol{M}^m \boldsymbol{b}^m \\ 0 \end{pmatrix}$$

- **Non-linear relations**

$$b_i = K_i \prod_j a_j^{M_{ij}}, \quad \text{for all } i$$

i.e. $\log(K^i) = b_i - \sum_j \boldsymbol{M}_{ij} \log(a_j)$ for all i

i.e.

$$\log(\boldsymbol{K}) = \boldsymbol{b} - \boldsymbol{M} \log(\boldsymbol{a})$$

Chemical Cinetic: example of nitrate creation

New Unkwnowns

- $[NO_3^-]$, $[O_2]$, $[Bac]$

Example of a cinetic reactions

$$NH_4^+ + 2O_2 \longrightarrow NO_3^- + 2H^+ + H_2O,$$

with the reaction rate (non linear)

$$r_1 = r_1([Bac],[O_2],[NH_4^+]) = \mu[Bac]\frac{k_1}{k_1 + [Bac]}\frac{[NH_4^+]}{k_2 + [NH_4^+]}\frac{[O_2]}{k_3 + [O_2]}$$

Cinetic reactions

Acts as **non-linear** source terms in mass conservation equation.

Chemical Cinetic: example of nitrate creation

New Unkwnowns

- $s = ([NO_3^-], [O_2], [Bac])$

Example of a cinetic reactions

$$NH_4^+ + 2O_2 \longrightarrow NO_3^- + 2H^+ + H_2O,$$

with the reaction rate (non linear)

$$r_1 = r_1([Bac], [O_2], [NH_4^+]) = \mu[Bac]\frac{k_1}{k_1 + [Bac]}\frac{[NH_4^+]}{k_2 + [NH_4^+]}\frac{[O_2]}{k_3 + [O_2]}$$

Cinetic reactions

Acts as **non-linear** source terms in mass conservation equation.

Mass-concervation equation

Notations

- $\boldsymbol{c} = (\boldsymbol{T}, \boldsymbol{s})$: quantities transported
- $\boldsymbol{e} = (\boldsymbol{T}^m, \boldsymbol{s})$: quantities transported (mobile contributions)
- $\boldsymbol{d} = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{s})$: concentrations of every chemical species involved
- $\boldsymbol{r} = \boldsymbol{r}(\boldsymbol{d})$ reaction rate (one component for each cinetic reaction)

Equilibrium equations

- Linear relations

$$\boldsymbol{c} = \boldsymbol{A}\boldsymbol{d}, \qquad \boldsymbol{e} = \boldsymbol{E}\boldsymbol{d}$$

- Non-linear relations

$$\log(\boldsymbol{K}) = \Lambda \log(\boldsymbol{d})$$

Mass-concervation equation

For the flow

- θ: Water saturation
- H: Hydraulic head
- v^f: Fluid velocity

$$\begin{cases} \dfrac{\partial \theta}{\partial t} + \operatorname{div} \boldsymbol{v}^f = g^f \\ \boldsymbol{v}^f = -k_r \boldsymbol{K}_0 \nabla H \\ \text{+limit cond.} \end{cases}$$

Transport of multiple reacting species

- c^i: **quantity transported** (in the water)
- e^i: **quantity transported, mobile contrib.**
- $\boldsymbol{v}^{e^i}$: **velocity of the specy** (diffusion + dispersion + transport)
- $\boldsymbol{D} = \boldsymbol{D}(\boldsymbol{v}^f)$: **diffusion + dispersion tensor**

$$\begin{cases} \dfrac{\partial}{\partial t}(\theta c^i) + \operatorname{div}(\boldsymbol{v}^{e^i}) = g_i^c + R^i(\boldsymbol{d}) \\ \boldsymbol{v}^{e^i} := e^i \boldsymbol{v}^f - \theta \boldsymbol{D}(e^i) \nabla e^i \end{cases}$$

Plan

1. Geometry and 3d-Richards equations
2. Dominant componants of the flow: effective problems
3. A coupled model coupling dominant componants
4. Numerical scheme
5. Considering reactive transport
6. Reactive transport: Dominant componant and coupled model
7. Numerical scheme

Dominant componant for the transport problem

Reactive transport

$$\begin{cases} \dfrac{\partial}{\partial t}(\theta c^i) + \mathrm{div}(\boldsymbol{v}^{e^i}) = g^{c^i} + R^i(\boldsymbol{d}) \\ \boldsymbol{v}^{e^i} := e^i\, \boldsymbol{v}^f - \theta D \nabla e^i \end{cases}$$

Chemical equilibrium

$$\begin{cases} \boldsymbol{c} = \boldsymbol{A}\boldsymbol{d}, \\ \boldsymbol{e} = \boldsymbol{A}^m \boldsymbol{d}, \\ \log \boldsymbol{K} = \boldsymbol{B} \log(\boldsymbol{d}) \end{cases}$$

Transport in short time scale: 1d-vertical

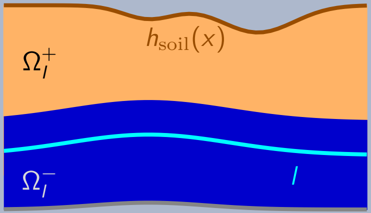
$$\begin{cases} \dfrac{\partial}{\partial t}(\theta c^i) + \dfrac{\partial v_3^{e^i}}{\partial z} = g^{c^i} + R^i(\boldsymbol{d}) \\ v_3^{e^i} := e^i\, v_3^f - \theta D \dfrac{\partial e^i}{\partial z} \end{cases}$$

Long time problem: 2d-horizontal

$$\begin{cases} d^i(t,x,z) = \tilde{d}^i(t,x) \\ \dfrac{\partial}{\partial t} \displaystyle\int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}} \theta c^i\, dz - \mathrm{div}_x\, \tilde{\boldsymbol{w}}^i = 0 \\ \tilde{\boldsymbol{w}}^i = \tilde{e}^i \tilde{\boldsymbol{w}}^f - \tilde{\theta} D^i \nabla_{\overline{x}} \tilde{e}^i \end{cases}$$

1d-vertical transport in Ω_l^+

$$\begin{cases} c^i = \tilde{c}^i & \text{for } z = l \end{cases}$$



Constant concentrations in Ω_l^-:

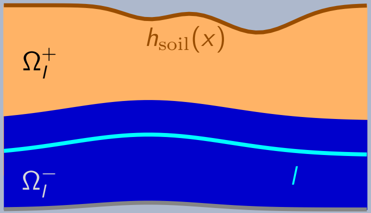
$$\boldsymbol{d}(t,x,z) = \tilde{\boldsymbol{d}}(t,x), \quad \boldsymbol{c}(t,x,z) = \tilde{\boldsymbol{c}}(t,x), \quad \boldsymbol{e}(t,x,z) = \tilde{\boldsymbol{e}}(t,x)$$

2d problem

Coupled model in physical variables

1d-vertical transport in Ω_l^+

$$\begin{cases} \dfrac{\partial(\theta c^i)}{\partial t} + \dfrac{\partial v_3^{e^i}}{\partial z} = g^{c^i} + R^i(\boldsymbol{d}) \\ v_3^{e^i} := e^i\, v_3^f - \theta D \dfrac{\partial e^i}{\partial z} \\ c^i = \tilde{c}^i \qquad \text{for } z = l \end{cases}$$



Constant concentrations in Ω_l^-:

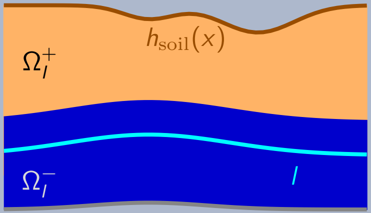
$$\boldsymbol{d}(t,x,z) = \tilde{\boldsymbol{d}}(t,x), \quad \boldsymbol{c}(t,x,z) = \tilde{\boldsymbol{c}}(t,x), \quad \boldsymbol{e}(t,x,z) = \tilde{\boldsymbol{e}}(t,x)$$

2d problem

Coupled model in physical variables

1d-vertical transport in Ω_l^+

$$\begin{cases} \dfrac{\partial(\theta c^i)}{\partial t} + \dfrac{\partial v_3^{e^i}}{\partial z} = g^{c^i} + R^i(\boldsymbol{d}) \\ v_3^{e^i} := e^i\, v_3^f - \theta D \dfrac{\partial e^i}{\partial z} \\ c^i = \tilde{c}^i \qquad\qquad \text{for } z = l \end{cases}$$



Constant concentrations in Ω_l^-:

$$\boldsymbol{d}(t,x,z) = \tilde{\boldsymbol{d}}(t,x), \quad \boldsymbol{c}(t,x,z) = \tilde{\boldsymbol{c}}(t,x), \quad \boldsymbol{e}(t,x,z) = \tilde{\boldsymbol{e}}(t,x)$$

2d problem

$$\frac{\partial}{\partial t}\int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}} \theta c^i\, dz - \mathrm{div}_x\, \tilde{\boldsymbol{w}}^i = \int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}} R^i(\boldsymbol{d})\, dz, \quad \tilde{\boldsymbol{w}}^i = \tilde{e}^i \tilde{\boldsymbol{w}}^f - \tilde{\theta} D^i \nabla_{\overline{x}} \tilde{e}^i$$

Full Coupled reactive-transport problem

Coupled Reactive transport

$$\frac{\partial}{\partial t}(\theta c^i) + \frac{\partial v_3^{e^i}}{\partial z} = R^i(\boldsymbol{d}) \qquad \text{in } \Omega_l^+$$

$$\frac{\partial}{\partial t}\Big(\int_{h_{\rm bot}}^{h_{\rm soil}} \theta c^i \, dz\Big) - \mathrm{div}_x \, \tilde{\boldsymbol{w}}^i = \int_{h_{\rm bot}}^{h_{\rm soil}} R^i(\boldsymbol{d}) \, dz,$$

$$v_3^{e^i} = e^i \, v_3^f - \theta D \frac{\partial e^i}{\partial z} \qquad \text{in } \Omega_l^+$$

$$\tilde{\boldsymbol{w}}^i = \tilde{e}^i \tilde{\boldsymbol{w}}^f - \tilde{\theta} D^i \nabla_{\overline{x}} \tilde{e} i$$

In Ω_l^-

$$\boldsymbol{d}(t,x,z) = \tilde{\boldsymbol{d}}(t,x), \quad \boldsymbol{c}(t,x,z) = \tilde{\boldsymbol{c}}(t,x), \quad \boldsymbol{e}(t,x,z) = \tilde{\boldsymbol{e}}(t,x)$$

Chemical equilibrium:

$$\boldsymbol{c} = \boldsymbol{A}\boldsymbol{d}, \qquad \boldsymbol{e} = \boldsymbol{A}^m \boldsymbol{d}, \qquad \log \boldsymbol{K} = \boldsymbol{B} \log(\boldsymbol{d})$$

Full Coupled reactive-transport problem

Coupled Reactive transport

$$\frac{\partial}{\partial t}(\theta c^i) + \frac{\partial v_3^{e^i}}{\partial z} = R^i(\boldsymbol{d}) \qquad \text{in } \Omega_l^+$$

$$v_3^{e^i} = e^i\, v_3^f - \theta D \frac{\partial e^i}{\partial z} \qquad \text{in } \Omega_l^+$$

In Ω_l^-

$\boldsymbol{d}(t,x,z) = \tilde{\boldsymbol{d}}(t,x), \quad \boldsymbol{c}(t,x,z) = \tilde{\boldsymbol{c}}(t,x), \quad \boldsymbol{e}(t,x,z) = \tilde{\boldsymbol{e}}(t,x)$

+2d problem

Chemical equilibrium:

$$\boldsymbol{c} = \boldsymbol{A}\boldsymbol{d}, \qquad \boldsymbol{e} = \boldsymbol{A}^m\boldsymbol{d}, \qquad \log \boldsymbol{K} = \boldsymbol{B}\log(\boldsymbol{d})$$

Plan

Implicit time scheme

$(t_n)_n$: **discretization of** $[0, T]$, δ_t: **time step.**

$$\boldsymbol{c}^n(x,z) \simeq \boldsymbol{c}(t_n,x,z)\ , \quad c^{i,n}(x,z) \simeq c^i(t_n,x,z)...$$

Coupled Reactive transport

$$\frac{1}{\partial t}(\theta^n c^{i,n} - \theta^{n-1}c^{i,n-1}) + \frac{\partial v_3^{e^{i,n}}}{\partial z} = R^i(\boldsymbol{d}^n) \qquad \text{in } \Omega_l^+$$

$$v_3^{e^{i,n}} = e^{i,n}\, v_3^{f,n} - \theta D \frac{\partial e^{i,n}}{\partial z} \qquad \text{in } \Omega_l^+$$

In Ω_l^-

$$\boldsymbol{d}^n(t,x,z) = \tilde{\boldsymbol{d}}^n(t,x), \quad \boldsymbol{c}^n(t,x,z) = \tilde{\boldsymbol{c}}^n(t,x), \quad \boldsymbol{e}^n(t,x,z) = \tilde{\boldsymbol{e}}^n(t,x)$$

+2d problem

Chemical equilibrium:

$$\boldsymbol{c}^n = \boldsymbol{A}\boldsymbol{d}^n, \qquad \boldsymbol{e}^n = \boldsymbol{A}^m\boldsymbol{d}^n, \qquad \log \boldsymbol{K} = \boldsymbol{B}\log(\boldsymbol{d}^n)$$

Picard fixed-point

Strategy

- At each time scale n, we know: $\boldsymbol{d}^{n-1}$
- We build a sequence $(\boldsymbol{d}^{n_k})_k$ such that

$$\boldsymbol{d}^{n_0} = \boldsymbol{d}^{n-1}, \qquad \boldsymbol{d}^{n_k} \to \boldsymbol{d}^n \text{: solution of the implicit problem}$$

Coupled Reactive transport: give the solution c^{i,n_k}

We know $\boldsymbol{c}^{n_{k-1}}$, $\boldsymbol{e}^{n_{k-1}}$, $\boldsymbol{d}^{n_{k-1}}$, $\tilde{\boldsymbol{c}}^{n_{k-1}}$...

$$\frac{1}{\partial t}(\theta^n c^{i,n_k} - \theta^{n-1} c^{i,n-1}) + \frac{\partial \hat{v}_3^{c^{i,n_k}}}{\partial z} = R^i(\boldsymbol{d}^{n_{k-1}}) \qquad \text{in } \Omega_l^+$$

$$\hat{v}_3^{c^{i,n_k}} = v_3^{c^{i,n_k}} + \left(v_3^{e^{i,n_{k-1}}} - v_3^{c^{i,n_{k-1}}}\right) \qquad \text{in } \Omega_l^+$$

In Ω_l^-

$$\boldsymbol{d}^n(t,x,z) = \tilde{\boldsymbol{d}}^n(t,x), \quad \boldsymbol{c}^n(t,x,z) = \tilde{\boldsymbol{c}}^n(t,x), \quad \boldsymbol{e}^n(t,x,z) = \tilde{\boldsymbol{e}}^n(t,x)$$

+2d problem

Chemical equilibrium: give $\boldsymbol{d}^{n_k}$ and $\boldsymbol{e}^{n_k}$

$$\boldsymbol{c}^{n_k} = \boldsymbol{A}\boldsymbol{d}^{n_k}, \qquad \boldsymbol{e}^{n_k} = \boldsymbol{A}^m \boldsymbol{d}^{n_k}, \qquad \log \boldsymbol{K} = \boldsymbol{B} \log(\boldsymbol{d}^{n_k})$$

Convergence of Picard algorithm

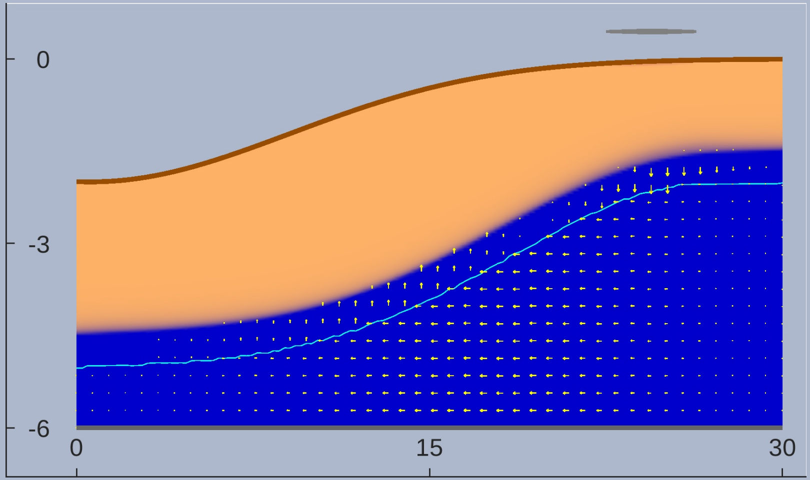
Difficulty: During resolution c^{n_k} must be positive !

- Need a transport scheme **preserving positivity**
- Can be false **before** the convergence being reached...

  $\hookrightarrow$ we use a truncature procedure to obtain convergence

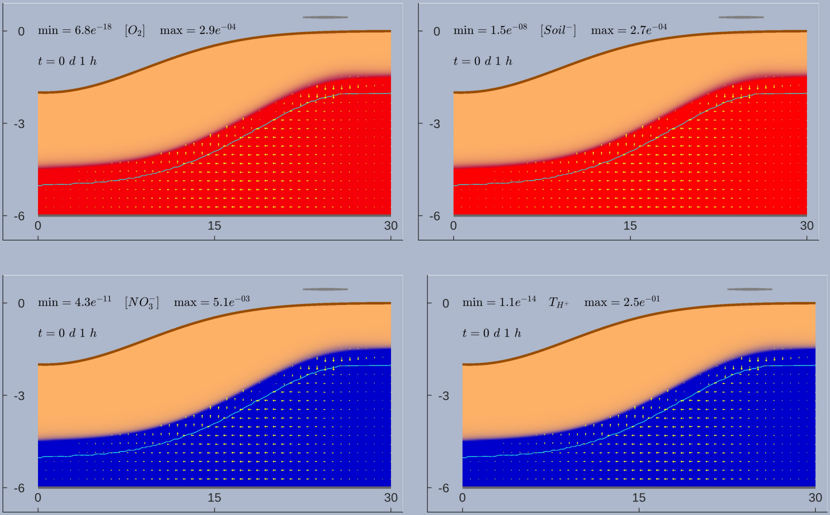
First transport experiment

One specy, **only transport** (no cinetic, no equilibrium)



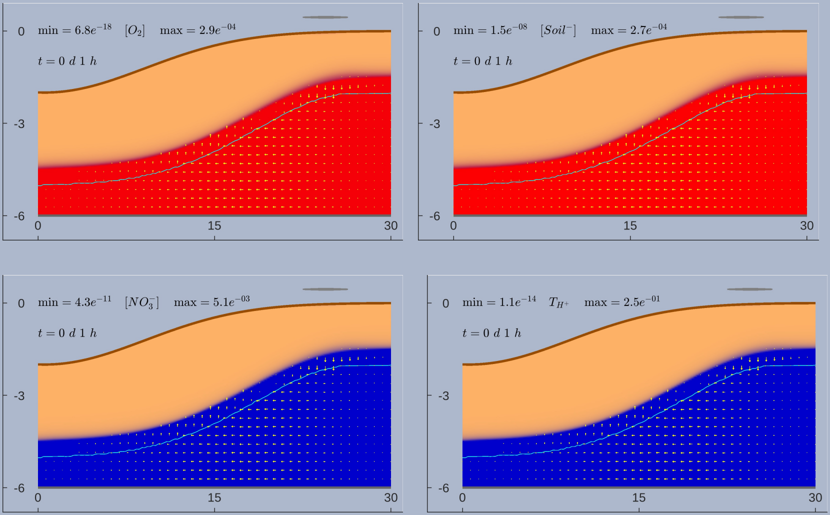
Complete experiment

11 species, 6 transported quantities, equilibrium and cinetic



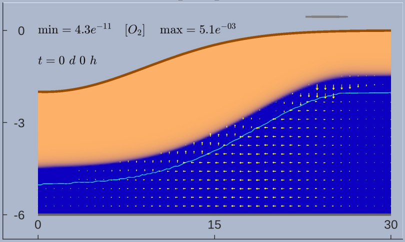
Complete experiment

11 species, 6 transported quantities, equilibrium and cinetic

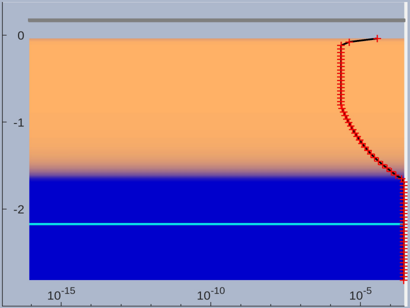


Complete experiment: cross-section view

$[O_2]$



$[0_2]$ vertical cross-section



Complete experiment: cross-section view