Modeling of underground flows. Application to reactive transport

Carole Rosier (Université du Littoral-Côte d'Opale)
joint work with R. Awada, C. Bourel, J. Carrayrou, C. Choquet, S. A. Nazer, M. Tsegmid.

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The aquifer occupy a cylindrical domain $\Omega \subset \mathbb{R}^3$ in the vertical direction e_3. The projection of Ω on an horizontal plane is a domain $\Omega_x \subset \mathbb{R}^2$. The lower base of Ω is the graph of the function $h_{\mathrm{bot}} = h_{\mathrm{bot}}(x)$. The upper base of Ω is the graph of the function $h_{\mathrm{soil}} = h_{\mathrm{soil}}(x)$ defined from Ω_x to $\mathbb{R}$. We assume that

$$h_{\mathrm{soil}}(x) > h_{\mathrm{bot}}(x) \ , \qquad \forall x \in \Omega_x.$$

More precisely the domain is given by:

$$\Omega = \Big\{(x,z) \in \Omega_x \times \mathbb{R} \quad | \quad z \in \Big] h_{\mathrm{bot}}(x), h_{\mathrm{soil}}(x) \Big[\Big\}.$$

We split the boundary $\partial\Omega$ of Ω in three zones (bottom, top and vertical)

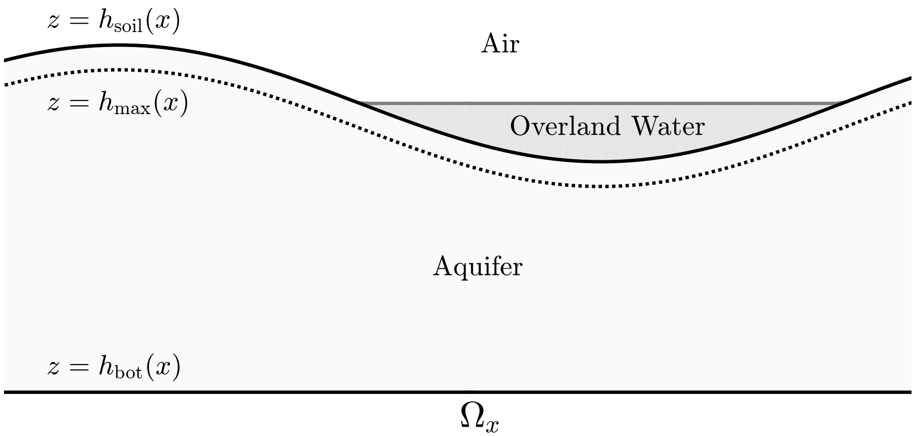
$$\partial\Omega = \Gamma_{\mathrm{bot}} \sqcup \Gamma_{\mathrm{soil}} \sqcup \Gamma_{\mathrm{ver}},$$

$$\Gamma_{bot} := \Big\{(x,z) \in \Omega \mid z = h_{\mathrm{bot}}(x)\Big\} \ , \quad \Gamma_{soil} := \Big\{(x,z) \in \Omega \mid z = h_{\mathrm{soil}}(x)\Big\} \ ,$$

$$\Gamma_{\mathrm{ver}} := \Big\{(x,z) \in \Omega \mid x \in \partial\Omega_x\Big\}.$$

Bidimensional representation of the cylindrical geometry of the problem: $\Omega_x \subset \mathbb{R}$ is an interval

We introduce for $0 < \delta \ll 1$, $h_{\max}(x) := h_{soil}(x) - \delta$.



Permeability tensor K_0.

• The permeability tensor $K_0(x,z)$ is a 3×3 symmetric positive definite tensor which describes the conductivity of the *saturated* soil at the position $(x,z) \in \Omega$. We introduce $K_{xx} \in \mathcal{M}_{22}(\mathbb{R})$, $K_{zz} \in \mathbb{R}^*$ and $\boldsymbol{K}_{xz} \in \mathcal{M}_{21}(\mathbb{R})$ such that

$$\boldsymbol{K}_0 = \begin{pmatrix} \boldsymbol{K}_{xx} & \boldsymbol{K}_{xz} \\ \boldsymbol{K}_{xz}^T & K_{zz} \end{pmatrix}. \tag{1}$$

• The nonlinear hydraulic conductivity is given by $K = \frac{\kappa \rho g}{\mu} K_0$.

Richards hypothesis.

The Richards model is based on the assumption that the air pressure in the underground equals the atmospheric pressure, thus is not an unknown of the problem. One thus assumes that **the moisture content,** $\theta = \theta(P)$, and **the relative conductivity of the soil,** $\kappa = \kappa(P)$, are given as *functions* of the fluid pressure P.

The moisture content :

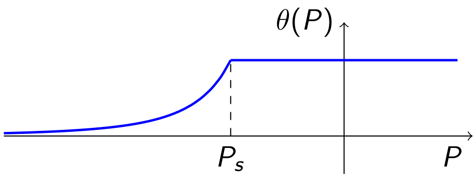
$$\theta = \begin{cases} \phi & \text{(saturated zone)} & \text{if} \quad P(\cdot, x) > P_s, \\ \theta(P) & \text{(with } \theta_- \leq \theta(P) \leq \phi \text{ and } \theta'(P) \geq 0) & \text{if} \quad P(\cdot, x) \leq P_s, \end{cases} \tag{2}$$

where $\theta_- > 0$ corresponds to a residual moisture content which is positive and P_s denotes the saturation pressure (which is a fixed real number).

The associated relative hydraulic mobility :

$$\kappa(P) = \begin{cases} 1 & \text{(saturated zone)} & \text{if} \quad P(\cdot, x) > P_s, \\ \kappa(P) & \text{(with } 0 \leq \kappa(P) \leq 1 \text{ and } \kappa'(P) > 0) & \text{if} \quad P(\cdot, x) \leq P_s. \end{cases} \tag{3}$$

The most classical models are the van Genuchten model and Brooks and Corey model.



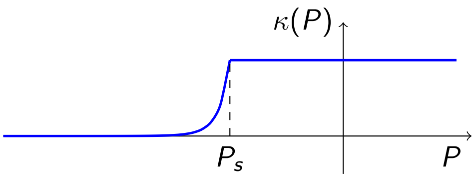


Figure: Saturation and relative permeability in terms of pressure: the Brooks and Corey model.

3D Richards problem

We recall the 3D-Richards equations which are classically used to described the water flow in an aquifer :

$$\begin{cases} \dfrac{\partial \theta(P)}{\partial t} + \nabla \cdot \boldsymbol{v} = 0 & \text{in } \Omega \\ \boldsymbol{v} = -\kappa(P)\, \boldsymbol{K}_0 \left(\frac{1}{\rho g} \nabla P + \boldsymbol{e}_3 \right) & \text{in } \Omega \\ \alpha\, P + \beta\, \boldsymbol{v} \cdot \boldsymbol{n} = F & \text{on } \Gamma_{\mathrm{soil}} \\ \boldsymbol{v} \cdot \boldsymbol{n} = 0 & \text{on } (\Gamma_{\mathrm{bot}} \cup \Gamma_{\mathrm{ver}}) \\ P(0, x, z) = P_{\mathrm{init}}(x, z) & \text{for } \ (x, z) \in \Omega \end{cases} \tag{4}$$

Bear (1972), Pikul (1974), Abbott (1986), Yakirevich (1998), Paulus(2011), Bourel (2020).

GOAL : We look for models exploiting the low thickness of a confined or unconfined aquifer. They consist in capturing very different physical phenomena, the fast and essentially vertical leakage coming from the surface through an unsaturated soil and the slow and essentially horizontal displacement in the saturated part of the aquifer.

STRATEGY : Let $\epsilon > 0$ describe the ratio of the aquifer's depth over its characteristic horizontal length. An asymptotic analysis is used for proving that new models and the 3D-Richards equation are associated with the same effective problem for any time scale.

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1. At short times, the horizontal flow is very small and the vertical one satisfies a 1D-Richards problem.
2. At non-short times, the vertical flow appears instantaneous. The hydraulic head H does not depend on the vertical variable z. This corresponds to the so-called Dupuit hypothesis.
3. At large times, the horizontal flux is non-zero. It is ruled by a 2D-horizontal diffusion equation where the conductivity is the vertical average of the permeability tensor on the *whole* depth of the aquifer.

- In $\Omega_{2d} \times (h, h_{soil})$, the following 1d-Richards equation holds

$$\begin{cases} \partial_t \theta(P) + \partial_z \big(\boldsymbol{q} \cdot e_3 \big) = 0 & \text{in} \quad (0,T) \times \Omega_t, \\ \boldsymbol{q} = -\kappa(P)\, K_{zz} \left(\frac{1}{\rho\, g} \frac{\partial P}{\partial z} + 1 \right) \boldsymbol{e}_3, & \\ a\, P + \boldsymbol{q} \cdot \boldsymbol{e}_3 = F & \text{in} \quad (0,T) \times \Gamma_{\mathrm{soil}}, \\ P\big(t, x, h(t,x)\big) = \rho\, g (\tilde{H} - h) & \text{in} \quad (0,T) \times \Omega_{2d}, \\ P(0, x, z) = P_{\mathrm{init}}(x, z) & \text{in} \quad \Omega_0. \end{cases} \tag{5}$$

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- The level $z = h$ is defined by

$$h(t,x) = \max\Big\{\min\Big\{\tilde{H}(t,x) - \frac{P_s}{\rho\, g}, h_{\max}(x)\Big\}, h_{\mathrm{bot}}(x)\Big\}. \tag{6}$$

- In Ω_t^-, the water pressure P satisfies

$$P(t,x,z) = \rho\, g\big(\tilde{H}(t,x) - z\big) \qquad \text{for} \quad t \in [0,T[\,, \quad (x,z) \in \Omega_t^-. \tag{7}$$

- The hydraulic head $\tilde{H}$ is a solution in Ω_{2d} to the following problem:

$$\begin{cases} -\nabla' \cdot (\tilde{\boldsymbol{K}} \nabla' \tilde{H}) = -(\boldsymbol{q} \cdot \boldsymbol{e}_3)|_{\Gamma_h^+} & \text{for} \quad (t,x) \in]0,T[\times\Omega_{2d}, \\ \tilde{\boldsymbol{K}}(\tilde{H})\, \nabla' \tilde{H} \cdot \vec{\nu} = 0 & \text{for} \quad (t,x) \in]0,T[\times\partial\Omega_{2d} \\ \tilde{H}(0,x) = H_{\mathrm{init}}(x) & \text{for} \quad x \in \Omega_{2d} \end{cases} \tag{8}$$

where the averaged conductivity $\tilde{K}$ is defined by

$$\tilde{\boldsymbol{K}}(H)(t,x) = \int_{h_{\mathrm{bot}}(x)}^{h_{\mathrm{soil}}(x)} \kappa\big(\rho\, g(H(t,x) - z)\big)\, \boldsymbol{S}_0(x,z)\, dz, \tag{9}$$

$$\boldsymbol{S}_0 = \boldsymbol{K}_{xx} - \frac{1}{K_{zz}} \boldsymbol{K}_{xz}(\boldsymbol{K}_{xz}^T), \qquad \boldsymbol{M}_0 = \begin{pmatrix} \boldsymbol{S}_0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Comments on this model

- This model is an alternative to the 3D-Richards problem for describing the flow in a shallow aquifer in a large range of time scales.
- This model is simpler to handle numerically than the $3D$-Richards model : coupling of a $2D$ problem with $1D$ vertical Richards problems.
- This model behaves like the 3D-Richards model for any time scale when the *ratio* ϵ of the thickness over the horizontal length of the aquifer is small.

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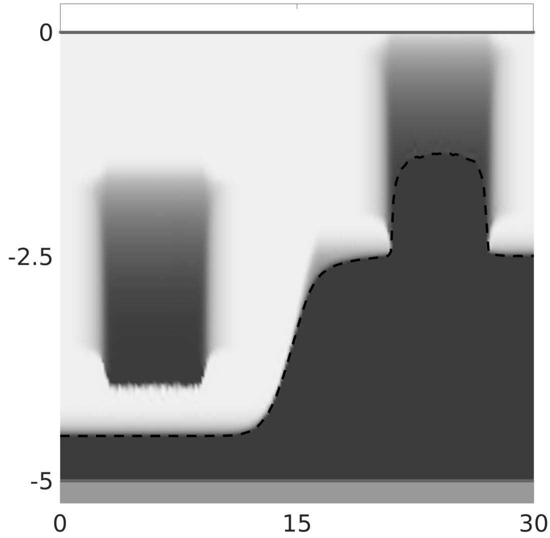
Rmk : This model couples the two kinds of flows appearing in the effective models in the short and long time scale.

▷ The first one is a vertical $1D$ Richards problem in the upper part of the aquifer and is associated with the velocity $\boldsymbol{q}$. It mimics the behavior of the flow in the short time scale case.

▷ The second one is a $2D$ horizontal problem that assume an instantaneous vertical flow in the lower part of the aquifer and is associated with the velocity $\boldsymbol{w}$. It mimics the behavior of the flow in the long time scale case.

Aquifer with impermeable upper layer at time t=1.



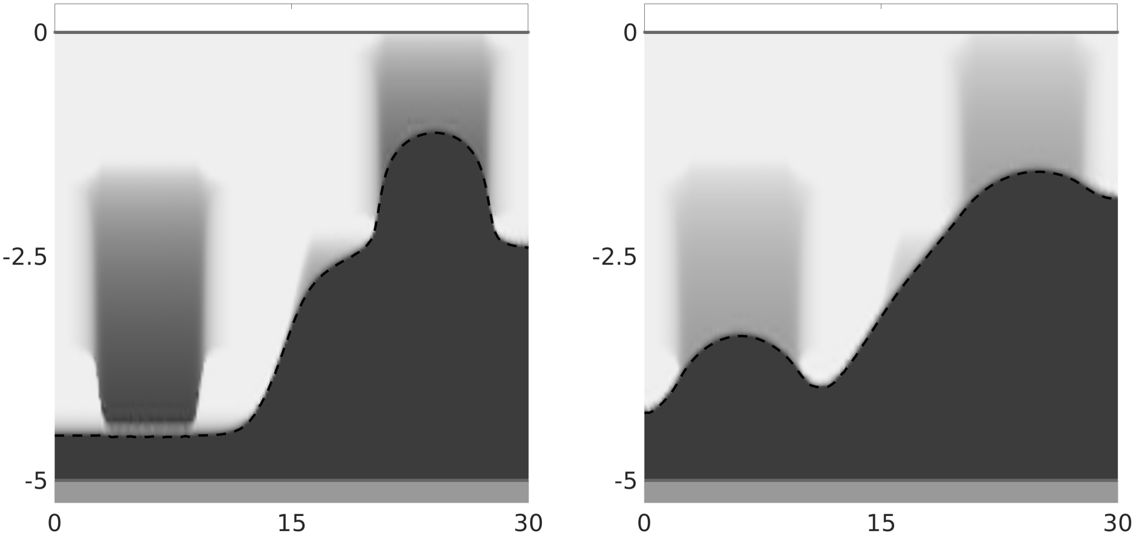
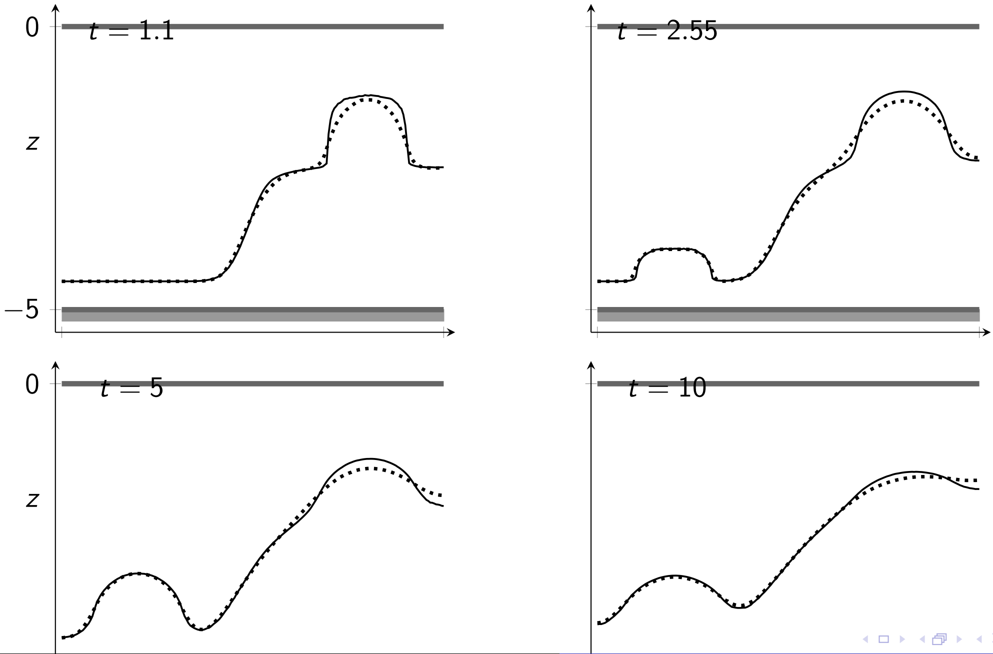


Figure: Qualitative example of the coupled model with interaction with the overland


0
$t = 1.1$
z
-5
$t = 2.55$
0
$t = 5$
z
$t = 10$

Goal : Regardless of the time scale, these two models exhibit the same behavior when the *ratio* of the characteristic thickness to the length of the shallow aquifer tends to zero.

1. We introduce a fixed dimensionless reference domain $\overline{\Omega}$ and a dimensionless real number $\overline{T} > 0$. We fix $\overline{\Omega}_x$, $\overline{h}_{\rm soil}$, and $\overline{h}_{\rm bot}$ such that

$$\overline{\Omega} = \left\{ (\overline{\boldsymbol{x}}, \overline{z}) \in \overline{\Omega}_x \times \mathbb{R} \quad | \quad \overline{z} \in \left] \overline{h}_{\rm bot}(\overline{\boldsymbol{x}}), \overline{h}_{\rm soil}(\overline{\boldsymbol{x}}) \right[\right\}.$$

2. To obtain a rescaled version of original problems in the domain $]0, \overline{T}[\times \overline{\Omega}$, we introduce positive reference numbers L_x, L_z, and T such that the physical variables are given as a function of the dimensionless variables by

$$\boldsymbol{x} = L_x\, \overline{\boldsymbol{x}}, \quad z = L_z\, \overline{z}, \quad t = T\overline{t}/\overline{T}.$$

3. The physical domain Ω may then be viewed as a dilation of the reference domain $\overline{\Omega}$.

$$\Omega_x = L_x\, \overline{\Omega}_x, \quad h_{\rm soil}(\boldsymbol{x}) = L_z\, \overline{h}_{\rm soil}(\overline{\boldsymbol{x}}), \quad h_{\rm bot}(\boldsymbol{x}) = L_z\, \overline{h}_{\rm bot}(\overline{\boldsymbol{x}}).$$

1. Using the rescaled unknowns, we get the 2 dimensionless problems :
   - **Dimensionless Richards problem**
   - **Dimensionless coupled model**
2. We define the following formal asymptotics for the unknowns

$$\begin{array}{ll} \overline{P}_\epsilon^\gamma = \overline{P}_0^\gamma + \epsilon\, \overline{P}_1^\gamma + \epsilon^2\, \overline{P}_2^\gamma + \dots & \overline{\boldsymbol{v}}_\epsilon^\gamma = \overline{\boldsymbol{v}}_0^\gamma + \epsilon\, \overline{\boldsymbol{v}}_1^\gamma + \epsilon^2\, \overline{\boldsymbol{v}}_2^\gamma + \dots, \\ \overline{H}_\epsilon^\gamma = \overline{H}_0 + \epsilon\, \overline{H}_1^\gamma + \epsilon^2\, \overline{H}_2^\gamma + \dots & \overline{h}_\epsilon^\gamma = \overline{h}_0^\gamma + \epsilon\, \overline{h}_1^\gamma + \epsilon^2\, \overline{h}_2^\gamma + \dots,, \quad etc... \end{array}$$

3. Introducing these formal asymptotics in the dimensionless problems, we get effective problems in the main-order at the different time scales.
4. We are interested in the asymptotic behavior of the flow, for small and large values of T. More precisely, we aim to describe the effective flow obtained for short, intermediate, and long time scales, that is, $T = \overline{T}$, $T = \epsilon^{-1}\overline{T}$, and $T = \epsilon^{-2}\overline{T}$, respectively.

Difficulties related to this system:

1. **The time degeneracies** : The analysis of Richards equations is known to be delicate in particular due to the degenerate in time term. Indeed, when considering a free water table, we must face the gradual disappearance of water in the desaturation zone and thus the disappearance of a main unknown of the problem.

   Alt H.W., Luckhaus S., Quasilinear Elliptic-Parabolic Differential Equations, Math. Z. 183, 311-341 (1983).

2. **The free boundary problem between the saturated and unsaturated zones**

3. **The lack of control of the gradient of the pressure in the horizontal direction** : Since the horizontal hydraulic conductivity is null, we have an 1D-equation but defined in a 3D domain. Hence there is a lack of control of the pressure's gradient in the horizontal space variables.

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- $h(t,x) = \max\Big\{\min\Big\{\tilde{H}(t,x) - \frac{P_s}{\rho\, g}, h_{\mathrm{max}}(x) = h_{\mathrm{soil}}(x) - \delta\Big\}, h_{\mathrm{bot}}(x) - \delta\Big\}.$

S. Al Nazer, M. Tsegmid, C. R. (2022)

- We consider that the fluid is compressible by assuming that **the pressure P is related to the density ρ** as follows :

$$\frac{d\rho}{\rho} = \alpha_P dP \Leftrightarrow \rho = \rho_0 e^{\alpha_P (P-P_0)}.$$

The real number $\alpha_P \geq 0$ is the fluid compressibility coefficient and P_0 is the pressure of reference. We assume that the fluid is weakly compressible: $\alpha_P \ll 1$.

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- In natural conditions and especially in an aquifer, one observes small fluid mobility. A consequence is $\nabla\rho \cdot q \ll 1$ which leads to the following simplification in the mass conservation equation :

$$\partial_t \theta(P) + \theta\alpha_P \, \partial_t P + \nabla \cdot q = 0. \tag{10}$$

- In Ω_t the following 3d-Richards equation holds

$$\begin{cases} \partial_t \theta(P) + \theta \alpha_P \, \partial_t P + \nabla \cdot q = 0 & \text{for} \quad t \in]0, T[, \quad (x,z) \in \Omega_t, \\ \alpha \, P + \beta \, q \cdot \vec{\nu} = F & \text{on} \quad (0,T) \times \Gamma_{\text{soil}}, \\ q \cdot \vec{\nu} = 0 & \text{on} \quad (0,T) \times \Gamma_{\text{ver}}, \\ P\big(t, x, h(t,x)\big) = P_s & \text{in} \quad \Omega_{2d}, \\ P(0,x,z) = P_0(x,z) & \text{in} \quad \Omega_0. \end{cases}$$

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- In Ω_t^- $\quad P(t,x,z) = \rho g(H-h) \quad$ for $\; t\in[0,T[\,, \quad (x,z)\in\Omega_t^-$.
- The averaged hydraulic head satisfies

$$\begin{cases} S_0(h-h_{\rm bot})\partial_t H - \nabla'\cdot(\tilde{J}(H)\nabla' H) = -q_{|z=h_{\rm soil}}\cdot\vec{\nu} - \nabla'\cdot\left(\int_h^{h_{\rm soil}} q\,dz\right) \\ \qquad\qquad - \int_h^{h_{\rm soil}} \left(\frac{\partial\theta(P)}{\partial t} + \theta(P)\alpha_P\frac{\partial P}{\partial t}\right) dz, \\ \tilde{J}\nabla' H\cdot\vec{\nu} = 0 \quad \text{on} \quad (0,T)\times\partial\Omega_{2d}, \quad h(0,x) = h_0(x) \quad \text{in} \quad \Omega_{2d}. \end{cases}$$

- The models $\mathcal{M}_\delta$ are a good approximation of the compressible 3d-Richards in shallow aquifers.
- The effective problems associated with the compressible 3d-Richards problem and with the problems $\mathcal{M}_\delta$ (when ϵ is very small) coincide
    - in the long and intermediate time scale for all $\alpha_p \geq 0$,
    - in the short time scale for $\alpha_p = 0$.
- They can be seen as the coupling of the two flows characterized by the effective models at the short and long time scales : the first one is a quasi-vertical 1d-Richards problem in the upper part of the aquifer, the second one is a 2d horizontal problem assuming an instantaneous vertical flow in the lower part of the aquifer.
- The models $\mathcal{M}_\delta$ can be seen as perturbations of the Dupuit- 1D Richards problem when we consider small quantities $\boldsymbol{N}_0$, α_P, δ.

Mathematical assumptions

- **Functions θ and κ** are pressure-dependent and we assume

$$\theta \in \mathcal{C}^1(\mathbb{R}), \quad 0 < \theta_- := \phi s_0 \leq \theta(x) \leq \theta_+, \quad \theta'(x) \geq 0 \ \forall x \in \mathbb{R},$$

$$\kappa \in \mathcal{C}(\mathbb{R}), \quad 0 < \kappa_- \leq \kappa(x) \leq \kappa_+ \ \forall x \in \mathbb{R}.$$

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These assumptions are sufficient to define the primitive function $\mathcal{P}_1$ such that

$$\mathcal{P}_1(P) = \theta(P) + \alpha_P \int^P \theta(s)\, ds.$$

A direct computation gives $\mathcal{P}_1'(P) = \theta'(P) + \alpha_P \theta(P) > \alpha_P \theta_- > 0$. Since $\mathcal{P}_1$ is a bijective application, the existence of p such that

$$p = \mathcal{P}_1(P)$$

is equivalent to the existence of P solution of the original problem.

Transformation by $\mathcal{P}_1$ of the "Richards equation"

The transform $\mathcal{P}_1$ of "Richards Equation" is given by

$$\partial_t p - \nabla \cdot \Big(\tau(p)\, B \nabla p\Big) - \nabla \cdot \Big(\kappa(\mathcal{P}_1^{-1}(p)) B \vec{e_3}\Big) = 0.$$

with

$$\tau(p) = \frac{1}{\rho g} \frac{\kappa(\mathcal{P}_1^{-1}(p))}{(\theta' + \alpha_P \theta)(\mathcal{P}_1^{-1}(p))}.$$

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Note that, due to hypotheses on θ and κ, there exist two positive reals τ_- and τ_+ such that

$$0 < \tau_- := \frac{\kappa_-}{\rho g\, \alpha_P \theta_+} \leq \tau(p) \leq \tau_+ := \frac{\kappa_+}{\rho g\, \alpha_P \theta_-}. \tag{11}$$

Transformation of the equation in H

Let $\delta > 0$ and $d = (h_{\text{soil}} - h_{\text{bot}})$, we introduce the function $T_l : \mathbb{R} \mapsto \mathbb{R}$ defined by

$$T_l(H) = h - h_{\text{bot}} = \max\left\{\min\left\{H - \frac{P_s}{\rho\, g}, h_{\max}\right\}, h_{\text{bot}} + \delta\right\} - h_{\text{bot}}.$$

Transformation of the equation in H

Let $\delta > 0$ and $d = (h_{\rm soil} - h_{\rm bot})$, we introduce the function $T_l : \mathbb{R} \mapsto \mathbb{R}$ defined by

$$T_l(H) = h - h_{\rm bot} = \max\Big\{\min\Big\{H - \frac{P_s}{\rho\, g}, h_{\rm max}\Big\}, h_{\rm bot} + \delta\Big\} - h_{\rm bot}.$$

Moreover, the hypothesis $\delta > 0$ is sufficient to define the primitive function $\mathcal{T}_1$ such that

$$u = \mathcal{T}_1(H) = \begin{cases} \delta\Big(H - \frac{P_s}{\rho\, g} - h_{\rm bot}\Big) - \dfrac{\delta^2}{2} & \text{if} \quad H \leq h_{\rm bot} + \delta + \frac{P_s}{\rho\, g}, \\ \dfrac{1}{2}\Big(H - \frac{P_s}{\rho\, g} - h_{\rm bot}\Big)^2 & \text{if} \quad h_{\rm bot} + \delta + \frac{P_s}{\rho\, g} \leq H \leq h_{\rm max} + \frac{P_s}{\rho\, g}, \\ d\Big(H - \frac{P_s}{\rho\, g} - h_{\rm bot}\Big) - \dfrac{d^2}{2} & \text{if} \quad H \geq h_{\rm max} + \frac{P_s}{\rho\, g}. \end{cases} \tag{12}$$

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Hence, we have

$$\frac{1}{d} \leq \|(\mathcal{T}_1^{-1})'\|_\infty \leq \frac{1}{\delta}. \tag{13}$$

$$S_0\partial_t u - \nabla' \cdot \left(\tilde{L}(u)\nabla' u\right) = -\int_{h_{\mathrm{bot}}+T_l(\mathcal{T}_1^{-1}(u(t,x)))}^{h_{\mathrm{soil}}} \frac{\partial p}{\partial t}\, dz - \nabla_x \cdot \left(\int_{h_{\mathrm{bot}}+T_l(\mathcal{T}_1^{-1}(u(t,x)))}^{h_{\mathrm{soil}}} q\, dz\right)$$

$$-q_{|z=h_{\mathrm{soil}}} \cdot \vec{\nu} \quad in \qquad (0,T)\times\Omega_{2d},$$

$$\tilde{L}(u)\nabla' u \cdot \vec{\nu} = 0 \quad \text{on} \quad (0,T)\times\partial\Omega_{2d}, \quad u(0,x) = \mathcal{T}_1\left(\tilde{H}_0(x)\right) \quad \text{in} \quad \Omega_{2d},$$

$$S_0\partial_t u - \nabla' \cdot \left(\tilde{L}(u)\nabla' u\right) = -\int_{h_{\mathrm{bot}}+T_l(\mathcal{T}_1^{-1}(u(t,x)))}^{h_{\mathrm{soil}}} \frac{\partial p}{\partial t}\, dz - \nabla_x \cdot \left(\int_{h_{\mathrm{bot}}+T_l(\mathcal{T}_1^{-1}(u(t,x)))}^{h_{\mathrm{soil}}} q\, dz\right)$$

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$$\partial_t p - \nabla \cdot \left(\tau(p)\, B\, \nabla p\right) - \nabla \cdot \left(\kappa(\mathcal{P}_1^{-1}(p)) B \vec{e_3}\right) = 0 \quad \text{in} \quad \mathcal{O}_T,$$

$$\mathrm{p}\big|_{\Gamma_t} = \mathcal{P}_1(P_s) \quad \text{in} \quad (0,T), \qquad \left(\tau(p)\, B\, \nabla p + \kappa(\mathcal{P}_1^{-1}(p)) B \vec{e_3}\right) \cdot \vec{\nu} = 0 \quad \text{on} \quad (0,T) \times \Gamma_{ver},$$

$$\mathrm{p}(0,x,z) = \mathrm{P}_1(P_0)(x,z) \text{ in } \Omega_0.$$

Let $p \in W(0,T;\Omega)$ such that $p = 0$ in $\mathcal{O}_T^c$.

$$\int_{h(t,x)}^{h_{soil}(x)} \frac{\partial p}{\partial t}\, dz = \int_{h_{\mathrm{bot}}(x)}^{h_{soil}(x)} \chi_{z \geq h(t,x)} \frac{\partial p}{\partial t}\, dz$$

is the function of $(H^1(\Omega_{2d}))'$ such that $\forall v \in H^1(\Omega_{2d}) \subset H^1(\Omega)$, for $\eta_0 > 0$ small enough

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$$\begin{aligned}
\langle \int_{h(t,x)}^{h_{soil}} \frac{\partial p}{\partial t} dz,\ v\rangle_{H^1(\Omega_{2d})',H^1(\Omega_{2d})} \\
= \langle \int_{h_{\rm bot}}^{h_{soil}} \rho_{\eta_0} * \chi_{\{z \geq (h_{\rm bot}+\delta/2)\}} \frac{\partial p}{\partial t} dz,\ v\rangle_{H^1(\Omega_{2d})',H^1(\Omega_{2d})} \\
= \langle \frac{\partial p}{\partial t}, \underbrace{\rho_{\eta_0} * \chi_{\{z \geq (h_{\rm bot}+\delta/2)\}}\, v}_{\in V(\Omega)} \rangle_{V'(\Omega),V(\Omega)},
\end{aligned}$$

where $\rho \in C^\infty(\mathbb{R})$, $\rho \geq 0$, is supported in the unit ball and satisfies $\int_{\mathbb{R}} \rho(\mathbf{x}) d\mathbf{x} = 1$. We set $\rho_{\eta_0}(x) = \rho(x/\eta_0)/\eta_0$, η_0 is chosen such that $\mathrm{Supp}(\rho_{\eta_0} * \chi_{\{z \geq (h_{\rm bot}+\delta/2)\}}) \subset \{z,\ z \geq (h_{\rm bot} + \delta/4)\}$ and $\rho_{\eta_0} * \chi_{\{z \geq (h_{\rm bot}+\delta/2)\}} = 1$ if $z \geq (h_{\rm bot} + 3\delta/4)$.

▷ For any $T > 0$, let $\mathcal{O}_T$ be the open domain of $\mathbb{R}^+ \times \Omega$ defined by
$\mathcal{O}_T = \{(t,x,z) \in (0,T) \times \Omega,\ h(t,x) < z\}$, where h is the position of the interface Γ_t.

$$\Omega_t = \{(x,z) \in \Omega,\ z \in]h(t,x), h_{\rm soil}[\}, \quad \mathcal{O}_T^c = ((0,T) \times \Omega) \setminus \mathcal{O}_T,$$
$$\Gamma = \partial\mathcal{O}_T \text{ (boundary of } \mathcal{O}_T), \quad \Gamma' = \Gamma \setminus \Omega_0 \text{ (lateral boundary of } \mathcal{O}_T).$$

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▷ $H^{0,1}(\mathcal{O}_T) = \{u \in L^2(\mathcal{O}_T),\ \nabla u \in L^2(\mathcal{O}_T) \times L^2(\mathcal{O}_T)\}$, endowed with the Hilbertian norm $\|u\|^2_{H^{0,1}(\mathcal{O}_T)} = \int_{\mathcal{O}_T} |u|^2 dxdt + \int_{\mathcal{O}_T} |\nabla u|^2 dxdt$.

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▷ $F(\mathcal{O}_T)$ denotes the closure in $H^{0,1}(\mathcal{O}_T)$ of functions of $\mathcal{D}(\bar{\mathcal{O}}_T)$ null in a neighborhood of Γ_t and $F'(\mathcal{O}_T)$ its topological dual.

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▷ $\mathcal{B}(\mathcal{O}_T) = \left\{u \in F(\mathcal{O}_T) \middle|\ \frac{du}{dt} \in F'(\mathcal{O}_T)\right\}$, endowed with the Hilbertian norm
$\|\cdot\|_{\mathcal{B}(\mathcal{O}_T)} = \left(\|\cdot\|^2_{F(\mathcal{O}_T)} + \|\partial_t \cdot\|^2_{F'(\mathcal{O}_T)}\right)^{1/2}$.

Definition

We call weak solution, any solution (u, p) with $u \in W(0, T, \Omega_{2d})$ and $p \in W_0(0, T, \Omega)$ such that for all $(\phi_1, \phi_2) \in L^2(0, T; H^1(\Omega_{2d})) \times L^2(0, T; V(\Omega))$

$$S_0 \int_0^T \langle \frac{\partial u}{\partial t}, \phi_1 \rangle_{H^1(\Omega_{2d})', H^1(\Omega_{2d})} \, dt + \int_0^T \int_{\Omega_{2d}} \big(\tilde{L}(u) \nabla' u \cdot \nabla' \phi_1 \big) dx \, dt =$$

$$\int_0^T \langle \partial_t p, \rho_{\eta_0} * \chi_{\{z \geq (h_{\rm bot} + \delta/2)\}} \phi_1 \rangle_{H^1(\Omega_{2d})', H^1(\Omega_{2d})} \, dt + \int_0^T \int_{\Omega_{2d}} \left(\left(F \, \phi_1 + \int_{h(t,x)}^{h_{\rm soil}} q \, dz \cdot \nabla' \phi_1 \right) \right.$$

$$\langle \partial_t p, \phi_2 \rangle_{F'(\mathcal{O}_T), F(\mathcal{O}_T)} + \int_0^T \Big(\int_{\Omega_t} \big(\tau(p) \, \tilde{B} \nabla p + \kappa(\mathcal{P}_1^{-1}(p)) \tilde{B} \, \vec{e_3} \big) \cdot \nabla \phi_2 \big) \, dx \Big) \, dt$$

$$= \int_0^T \int_{\Omega_{2d}} F \; \phi_{2|_{\Gamma_{\rm soil}}} dx \, dt \quad (14)$$

$$p = 0 \text{ in } \mathcal{O}_T^c, \quad p(0, x, z) = \mathcal{P}_1(P_0)(x, z) \text{ in } \Omega_0,$$

Global existence for (p, u)

Theorem

Assuming hypotheses previously stated, then system in (u, p) admits a weak solution satisfying

- $u \in L^2(0, T; H^1(\Omega_{2d}))$ and $\partial_t u \in L^2(0, T; (H^1(\Omega_{2d}))')$,
- $p \in L^2(0, T; V(\Omega))$ and $\partial_t p \in L^2(0, T; V'(\Omega))$.

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As a consequence, we claim the following result

Theorem

Let us assume theprevious hypotheses. Let $\delta \in]0, d[$. Then, the model $\mathcal{M}_\delta$ admits a weak solution (H, P) with $H \in L^2(0, T, H^1(\Omega_{2d}))$ and $P \in L^2(0, T, H^1(\Omega))$.

Sketch of the proof

▷ J. L. Lions, *Sur les problèmes mixtes pour certains systèmes paraboliques dans des ouverts non cylindriques; Annales de l'Institut Fourier 7, 1957, p. 143-182*.

▷ A. L. Mignot, *Méthodes d'approximation des solutions de certains problèmes aux limites linéaires, Rendiconti del Seminario Matematico della Università di Padova, tome 40 (1968), p. 1-138.*

- The problem consists of a strongly nonlinear coupled system, so we apply a fixed point approach.
- We prove a result of existence and uniqueness for each decoupled equation.
  One of the main difficulties of the study is that we are working on time-dependent domains. This difficulty is solved by using the work of Lions and Mignot for parabolic equations on non-cylindrical domains. This consists in suitably extending the solution outside the variable domain, thus bringing us back to a fixed domain.
- We establish compactness results which allow us to prove the global existence in time of the initial problem.

- N_X number of components, N_X^m and N_X^f numbers of mobile and fixed components,
- N_E the number of species, N_E^m and N_E^f numbers of mobile and fixed species,
- $(X, E) \in (\mathbb{R}^+)^{N_X^m + N_E^m}$ and $(S, E_S) \in (\mathbb{R}^+)^{N_X^f + N_E^f}$ vector of mobile and fixed species concentrations,
- $T = (T_i) \in \mathbb{R}^{N_X}$ with T_i be the total quantity of the component $i \in \{1, \dots, N_X\}$,

i: Reactions among mobile species:

$$\sum_{j=1}^{N_X^m} A_{ij}^m X_j \rightleftarrows E_i \quad i = 1, ..., N_E^m;$$

ii: Reactions between mobile and fixed species:

$$\sum_{j=1}^{N_X^m} A_{ij}^f X_j + \sum_{j=1}^{N_X^s} A_{ij}^{ff} S_j \rightleftarrows E_{S\,i} \quad i = 1, ..., N_E^f.$$

Mass conservation equations

$$\begin{cases} E_i = K_i^m \prod_{j=1}^{N_X^m} X_j^{A_{ij}^m} & i \in \{1, \ldots, N_E^m - N_X^m\}, \\ E_{S\,i} = K_i^f \prod_{j=1}^{N_X^m} X_j^{A_{ji}^f} \prod_{j=1}^{N_X^f} S_j^{A_{ji}^{ff}} & i \in \{1, \ldots, N_E^f - N_X^f\}. \end{cases} \tag{15}$$

By substituting the mass action laws into the mass conservation equations, we get

$$\begin{aligned} T_j^m &= \sum_{i=1}^{N_E^m} A_{ij}^m \Big(K_i^m \prod_{k=1}^{N_X^m} X_k^{A_{ik}^m} \Big) + \sum_{i=1}^{N_E^f} A_{ij}^f \Big(K_i^s \prod_{k=1}^{N_X^m} X_k^{A_{ik}^f} \prod_{k=1}^{N_X^f} S_k^{A_{ik}^f} \Big) \quad j = 1, \ldots, N_X^m \\ T_j^s &= \sum_{i=1}^{N_E^m} A_{ij}^{ff} \Big(K_i^s \prod_{k=1}^{N_X^m} X_k^{A_{ij}^f} \prod_{k=1}^{N_X^f} S_k^{A_{ij}^{ff}} \Big) \quad j = 1, \ldots, N_X^f. \end{aligned} \tag{16}$$

where $K = (K^m, K^f) \in \mathbb{R}^{N_E - N_X}$ is the equilibrium constant vector.

$$T^m = T^{mm} + T^{mf}, \quad T^{mm} = X + \mathbf{A}^m E, \quad T^{mf} = \mathbf{A}^f E_S, \quad T^f = S + \mathbf{A}^f E_S. \tag{17}$$

- N_{Sk} number of species produced by the kinetic reactions, N_{Sk}^m number of these species that are mobile,
- $Sk^m \in (\mathbb{R}^+)^{N_{Sk}^m}$ and $Sk^f \in (\mathbb{R}^+)^{N_{Sk}^f}$ the concentration of these mobile and fixed species,
- N_r^k number of kinetic reactions.

$$\mathbf{B}^{fa} \in \mathbb{R}^{N_C^f \times N_r^k}, \quad \mathbf{B}^{fc} \in \mathbb{R}^{N_{Sk}^f \times N_r^k}. \tag{18}$$

We introduce the unknowns vector $Y := (X, E, Sk^m, S, E_S, Sk^f)$. The reaction velocity (flux) is given by the function $r = f(Y) \in \mathbb{R}^{N_r^k}$

$$\partial_t Y^f = \mathbf{B}^{fc} r(Y) =: R^{fc}(Y). \tag{19}$$

Reactive-transport equations for mobile species

We introduce the matrices $\mathbf{B}^{ma} \in \mathbb{R}^{N_C^m \times N_r^k}$, $\mathbf{B}^{mc} \in \mathbb{R}^{N_E^m \times N_r^k}$. We have

$$\partial_t T^m + \mathbf{L}(T^{mm}) = \mathbf{B}^{ma} r(Y) =: R^{ma}(Y), \quad \partial_t Y^m + \mathbf{L}(Y^m) = \mathbf{B}^{mc} r(Y) =: R^{mc}(Y) \quad (20)$$

where $\mathbf{L}$ is the differential operator defined for all i by

$$\mathbf{L}_i(c) = L(c_i) = div(\boldsymbol{v}^{c_i}), \quad \boldsymbol{v}^{c_i} = c_i \boldsymbol{v} - \alpha_i |\boldsymbol{v}| D^i \nabla c_i .$$

Full problem

Finally, the full problem consists in finding $(T^m, T^f, T^{mm}, X, E, Sk^m, S, E_S, Sk^f)$,

$N_X + N_X^m + N_E + N_{Sk}$ unknowns such that

$$\begin{cases} T^m = T^{mm} + \boldsymbol{A}^{mf}\ E_S, & (N_X^m \text{ equations})\\ T^{mm} = X + \boldsymbol{A}^{mm} E, & (N_X^m \text{ equations})\\ T^f = S + \boldsymbol{A}^{ff} E_S, & (N_X^f \text{ equations})\\ E_i = K_i^m \prod_{j=1}^{N_X^m} X_j^{A_{ji}^m}, & ((N_E^m - N_X^m) \text{ equations})\\ E_{S\,i} = K_i^f \prod_{j=1}^{N_C^m} X_j^{A_{ji}^f} \prod_{j=1}^{N_C^f} S_j^{A_{ji}^{ff}}, & ((N_E^f - N_X^f) \text{ equations})\\ \partial_t T^f = R^{fa}(Y), & (N_X^f \text{ equations})\\ \partial_t Y^f = R^{fc}(Y), & (N_{Sk}^f \text{ equations})\\ \partial_t T^m + \mathbf{L}(T^{mm}) = R^{ma}(Y), & (N_X^m \text{ equations})\\ \partial_t Y^m + \mathbf{L}(Y^m) = R^{mc}(Y). & (N_{Sk}^m \text{ equations}) \end{cases} \tag{21}$$

for a total of $N_X + N_X^m + N_E + N_{Sk}$ equations.

Application to the transport of nitrates

- Components and Species
  - $E_1 = [H^+], E_2 = [NH_4^+], E_3 = [NH_3], E_4 = [OH^-]$ then $N_E^m = 4$,
  - $E_{S1} = [SoilH], E_{S2} = [Soil^-], E_{S3} = [SoilH_2^+], E_{S4} = [SoilNH_4^+]$ then $N_E^f = 4$,
  - $X_1 = [H^+], X_2 = [NH_4^+], S_1 = [SoilH]$ then $N_X^m = 2$ and $N_X^f = 1$.
- Species produced by the kinetic reactions
  - $Sk_1^m = [NO_3^-], Sk_2^m = [O_2], Sk_1^f = [Bac]$.
- Mass action laws of chemical equilibrium reactions
  - $[OH^-] = 10^{-14}[H^+]^{-1}$,
  - $[NH_3] = 10^{-9,3}[NH_4^+][H^+]^{-1}$,
  - $[SoilNH_4^+] = 0.39[NH_4^+][H^+]^{-1}[SoilH]$,
  - $[Soil^-] = 10^{-7}[H^+]^{-1}[SoilH]$,
  - $[SoilH_2^+] = 10^2[H^+][SoilH]$.

Full problem

- Mass conservation equations
  - $T_{[H^+]} = [H^+] - [OH^-] - [NH_3] - [SoilH] + [SoilH_2^+] - [SoilNH_4^+]$,
  - $T_{[NH_4^+]} = [NH_4^+] + [NH_3] + [SoilNH_4^+]$,
  - $T_{[SoilH]} = [SoilH] + [Soil^-] + [SoilH_2^+] + [SoilNH_4^+]$.
- Reaction velocities
  - $r_1 = 10 \times \dfrac{[Bac]}{1 + [Bac]} \times \dfrac{[NH_4^+]}{1 + [NH_4^+]} \times \dfrac{[O_2]}{0,77 + [O_2]}$
  - $r_2 = 8 \times 10^{-8} P_{[O_2]} - 6 \times [O_2]$
- Reactive transport equations

$$\begin{cases} \partial_t T_{[H^+]} + \mathbf{L}(T^m_{[H^+]}) = 2 \times r_2, \\ \partial_t T_{[NH_4^+]} + \mathbf{L}(T^m_{[NH_4^+]}) = -r_2, \\ \partial_t T_{[NO_3^-]} + \mathbf{L}(T^m_{[NO_3^-]}) = r_2, \\ \partial_t [O_2] + \mathbf{L}([O_2]) = -2 \times r_2 + r_1(1 - s(P)), \\ \partial_t [Bac] = 10^{-3} r_2 - 10^{-5}[Bac] + 10^{-7}. \end{cases} \tag{22}$$

- We presented a class of new models for water flows in shallow aquifers, giving an alternative to the classical 3D-Richards model.
- Using asymptotic expansions, we showed that the 3D-Richards model and Dupuit-Richards models behave identically, on every considered time scale.
- The numerical results correspond well to those obtained by the original 3D-Richards model.
- This class of models is useful, in particular, for studying the transport of chemical components in aquifers. Indeed, it turns out that many chemical reactions occur in the first meters of the subsoil, where oxygen is still present.

Thank you for your attention !

Reduction to Homogeneous Dirichlet Boundary Condition

We first reduce the boundary condition on interface Γ_t to homogeneous Dirichlet boundary condition by setting $\bar{p} = p - \mathcal{P}_1(P_s)$. So we consider the original system with $\mathcal{P}_1(P_s) = 0$.

$$\partial_t p - \nabla \cdot \left(\tau(p)\,\nabla p\right) - \frac{\rho_0\, g}{\mu} \nabla \cdot \left(\kappa(\mathcal{P}_1^{-1}(p))K_0 \vec{e_3}\right) = Q \quad \text{in} \quad \mathcal{O}_T, \tag{23}$$

$$p\big|_{\Gamma_t} = 0 \quad \text{in} \quad (0,T), \qquad \nabla\left(\mathcal{P}_1^{-1}(p) + \rho_0 g z\right) \cdot \vec{\nu} = 0 \quad \text{on} \quad (0,T) \times (\Gamma_{soil} \cup \Gamma_{ver}),$$

$$p(0,x,z) = \mathcal{P}_1(P_0)(x,z) \quad \text{in} \quad \Omega_0. \tag{24}$$

Fixed point step

We now construct the framework to apply the Schauder fixed point theorem. For the fixed point strategy, we introduce two convex subsets $(W_1,\ W_2)$ of $W(0,T,\Omega_{2d}) \times W(0,T,\Omega)$, namely

$$W_1 \quad := \quad \{u \in W(0,T,\Omega_{2d});\ u(0)=u_0, \|u\|_{L^2(0,T;H^1(\Omega_{2d}))} \leq C_u \text{ and } \|u\|_{L^2(0,T;(H^1(\Omega_{2d}))')} \leq C'_u\}.$$

and

$$W_2 \quad := \quad \{p \in W(0,T,\Omega);\ p(0)=p_0, \|p\|_{L^2(0,T;H^1(\Omega))} \leq C_p \text{ and } \|p\|_{L^2(0,T;(H^1(\Omega))')} \leq C'_p\},$$

constants $(C_p,\ C'_p)$ and $(C_u,\ C'_u)$ being defined thereafter.

Existence and Uniqueness for decoupled problem in u

Let $(\bar{u}, \bar{p}) \in W_1 \times W_2$, we begin by considering the unique weak solution u of the following linearized problem

$$S_0 \partial_t u - \nabla' \cdot \left(\tilde{L}(\bar{u}) \nabla' u\right) = -\int_{h_{\mathrm{bot}}}^{h_{\mathrm{soil}}} \frac{\partial \bar{p}}{\partial t}\, dz - \nabla' \cdot \left(\int_{\bar{h}}^{h_{\mathrm{soil}}} \bar{q}\, dz \right) - F \quad \text{in} \quad (0,T) \times \Omega_{2d}, \quad (25)$$

$$\tilde{L}(\bar{u}) \nabla' u \cdot \vec{\nu} = 0 \quad \text{on} \quad (0,T) \times \partial\Omega_{2d}, \qquad u(0,x) = \mathcal{T}_1(\tilde{H}_0)(x) \quad \text{in} \quad \Omega_{2d}, \quad (26)$$

where $\bar{q} = -\kappa\left(\mathcal{P}_1^{-1}(\bar{p})\right) B \nabla \left(\frac{\mathcal{P}^{-1}(\bar{p})}{\rho g} + z \right)$ and $\bar{h}(t,x) := h_{\mathrm{bot}} + T_l\left(\mathcal{T}_1^{-1}\left(\bar{u}(t,x)\right)\right)$.

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Lemma

Let $\tilde{H}_0 \in L^2(\Omega_{2d})$, there exists a unique weak solution $u \in W(0,T,\Omega_{2d})$ of (25)-(26) such that

$$\|u\|_{L^2(0,T;H^1(\Omega_{2d}))} \leq C_u \quad \text{and} \quad \|u\|_{L^2(0,T;(H^1(\Omega_{2d}))')} \leq C'_u,$$

where C_u and C'_u only depend on the data of the problem.

Regularization of equation in p

- Let $\psi \in C^\infty(\mathbb{R}^2)$, $\psi \geq 0$, with support in the unit ball such that $\int_{\mathbb{R}^2} \psi(x)dx = 1$. For $\eta > 0$ small enough, we set $\psi_\eta(x) = \psi(x/\eta)/\eta^2$. We extend h by zero outside Ω_{2d} and we define $\tilde{h}$ by the convolution product with respect to the space variable

$$\tilde{h} = \psi_\eta * h.$$

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• Let $\bar{p} \in W_1$ and $\tilde{h} \in L^2(0, T; C^{\infty}(\bar{\Omega}_{2d}))$ where h is given by the previous Lemma. We thus consider the following linearized and regularized problem in Ω_T : Find $p_\eta \in W(0, T, \Omega)$ s.t. $\forall \phi \in L^2(0, T; V)$ s.t. $\phi = 0$ in $\mathcal{O}_T^c$(null on the interface Γ_t)

$$\langle \partial_t p_\eta, \phi \rangle_{F',F} + \int_0^T \Big(\int_\Omega \big(\tau(\bar{p}) B \nabla p_\eta + \kappa(\mathcal{P}_1^{-1}(\bar{p})) B \vec{e_3}\big) \cdot \nabla \phi \Big) dx\, dt = \int_0^T \int_{\Omega_{2d}} F\ \phi dx\, dt,$$

$$p_\eta = 0 \text{ in } \mathcal{O}_T^c, \quad \text{and } p_\eta(0, x, z) = \mathcal{P}_1(P_0)(x, z) \quad \text{in} \quad \Omega_0.$$

Existence and Uniqueness for decoupled problem in p

Lemma

For any $\eta > 0$, there exists a unique function p_η in $W(0, T, \Omega)$ solution of regularized problem. It fulfills the uniform estimates

$$\|p_\eta\|_{L^2(0,T;H^1(\Omega))} \leq C_p \quad \text{and} \quad \|p_\eta\|_{L^2(0,T;(H^1(\Omega))')} \leq C'_p, \tag{27}$$

where C_p and C'_p only depend on the data of the original problem.

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where C_p and C'_p only depend on the data of the original problem.

The proof of this Proposition is done in two steps. We first use the method of auxiliary domains presented by Mignot to solve difficulties related to the free boundary. That is, we extend the functions out of the domain of study by zero, then we introduce a penalized problem and go to the limit to return to the linearized problem

Existence of a solution for the regularized problem

Lemma

- *Let* $(\bar{u}, \bar{p}) \in W(0, T, \Omega) \times W(0, T, \Omega_{2d})$ *the unique solution of* (25)-(26) *and* (27), *thus*
  - *There exists* $\mathcal{C}$ *a nonempty, closed, convex, bounded set in* $W(0, T, \Omega_{2d}) \times W(0, T, \Omega)$ *satisfying* $\mathcal{F}(\mathcal{C}) \subset \mathcal{C}$,
  - *The application* $\mathcal{F}$ *defined by the fixed point procedure is weakly sequentially continuous in* $W(0, T, \Omega_{2d}) \times W(0, T, \Omega)$.

• Letting $\eta \to 0$ in weak formulations resulting from system in (p, u), we prove the existence of a weak solution. This ends the proof of Theorem 1.

Thank you for your attention !