DG approximation of two-component miscible liquid-gas porous media flows

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Introduction

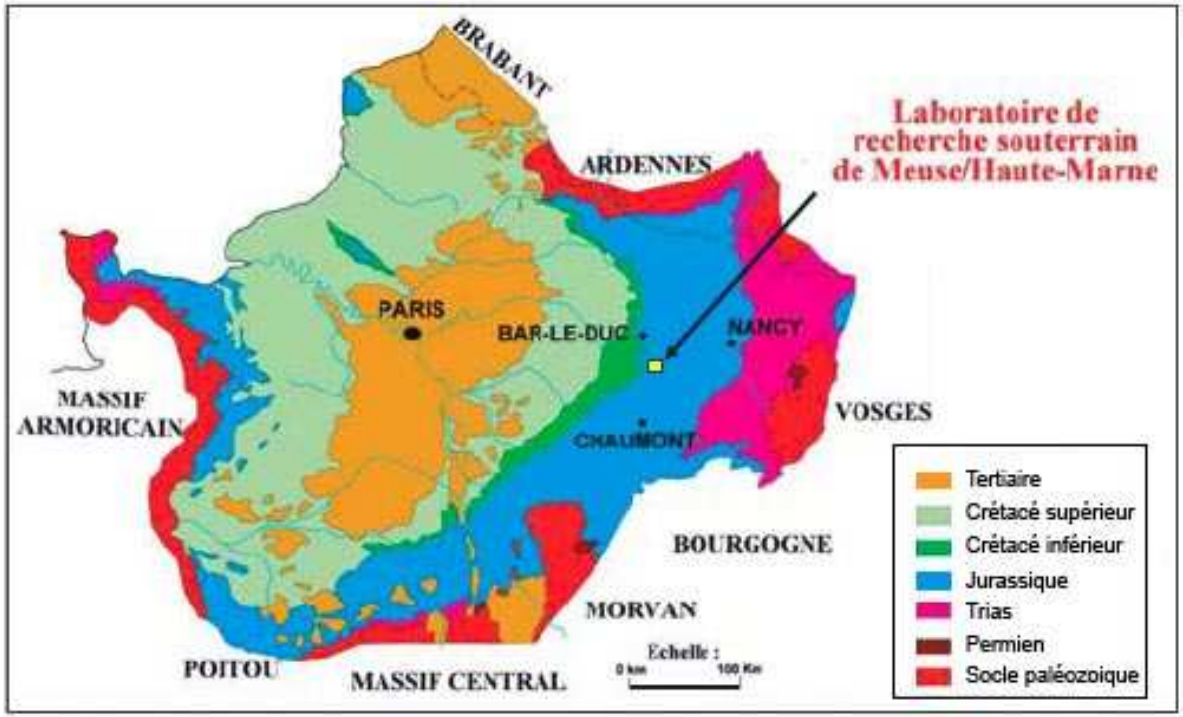
- Multicomponent multiphase porous media flows are encountered in several applications
  - petroleum engineering (oil-water)
  - agricultural engineering, groundwater remediation (air-water)
- Such flows have received enhanced attention recently
  - gas sequestration
  - **underground repositories of radioactive waste**

The issue of radioactive waste I

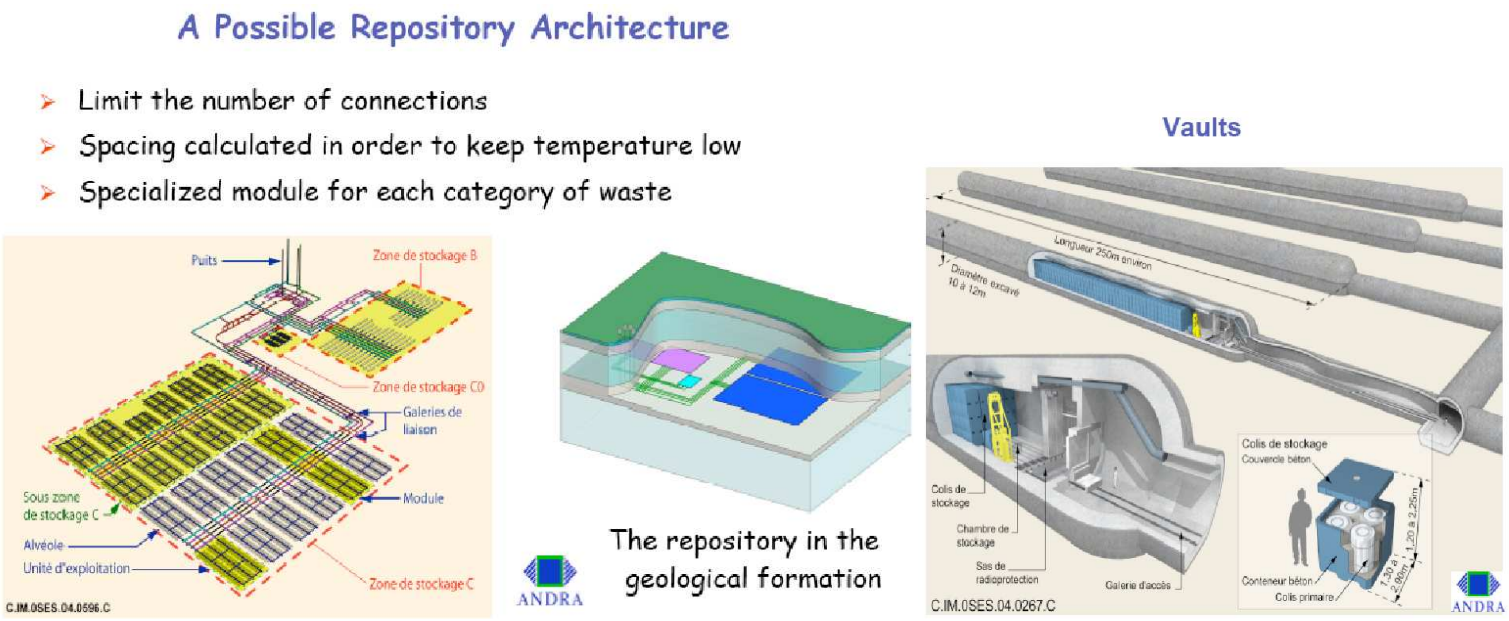
- Production in France estimated at **2 kg/year/citizen**
  - various sources: electro-nuclear plants, health treatments, industrial processes, research, army
- Total conditioned radioactive waste amounts to **1.2 Mm^3**
- **0.2%** of this volume contains **99%** of radioactivity
- HAVL waste High Activity, Long Life **1 Myears**

The issue of radioactive waste II

- HAVL waste could be stored in underground repository
  - **ANDRA** (French Agency for Radioactive Waste Management)
  - preliminary study established feasibility in **2005**
  - **clay host rock** located at $\approx$ 500 m depth
  - decision to be taken in **2014**, operating could start in **2025**



The issue of radioactive waste III



- Underground research facility currently operating
- Various academic research programs have been launched
- **GNR MOMAS Mathematical modeling and numerical simulation**

www.gdrmomas.org

The issue of radioactive waste IV

- Multiple barriers to contain radionuclides (RN)
  - conditioning of waste, steel containers
  - manufactured barriers (bentonite, steel)
  - host rock (quite favorable properties)
- Main time scales
  - 10^2 **years** operating and observing the facility, reversibility
  - 10^4 **years** degradation of manufactured barriers
  - 10^6 **years** migration of RN through geosphere up to biosphere

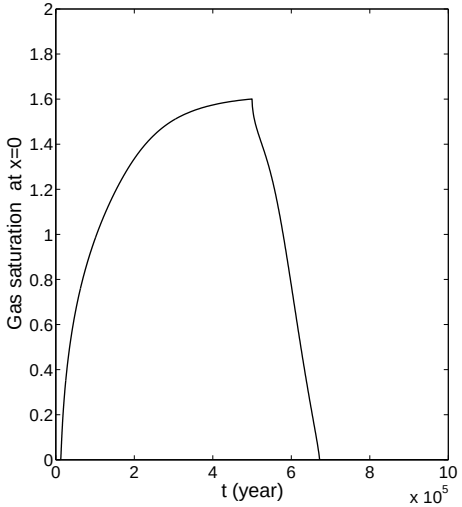
Hydrogen production and migration

- Corrosion of metallic components (and marginally water radiolysis)

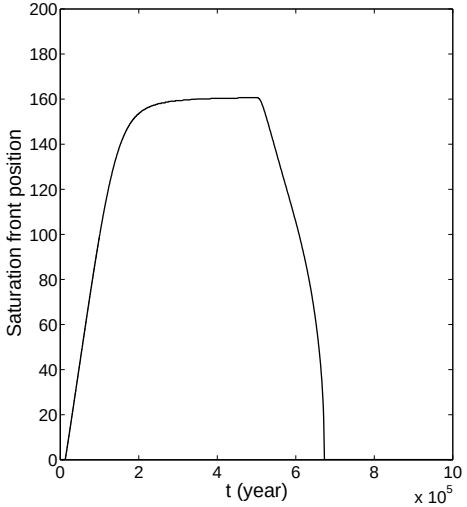
$$Fe + 2H_20 \rightarrow Fe(OH)_2 + H_2$$

- Understand hydrogen migration through host rock
- Two-phase (liquid, gas), two-component (water, hydrogen) flow, gas phase is compressible
- **Gas phase (dis)appearance**

gas saturation at inflow



position of gas phase front



Outline

- Setting
- Numerical method
- Results

Setting

- Governing equations
- Choice of main unknowns
- Mathematical model

Governing equations I

- **Basic notation**
  - subscript $\alpha \in \{l, g\}$ for phase
  - superscript $\beta \in \{w, h\}$ for component
  - ϱ_α^β density of component β in phase α
  - s_α saturation of phase α, $s_l + s_g = 1$
  - p_α pressure of phase α

- Mass conservation equation for each component

$$\Phi \sum_{\alpha \in \{l,g\}} \partial_t (s_\alpha \varrho_\alpha^\beta) + \sum_{\alpha \in \{l,g\}} \nabla \cdot (\varrho_\alpha^\beta \mathbf{q}_\alpha + \mathbf{j}_\alpha^\beta) = F^\beta$$

  with Φ porosity, $\mathbf{q}_\alpha$ volumetric flow rate of phase α, $\mathbf{j}_\alpha^\beta$ mass diffusion flux of component β in phase α

- [Bear '78, Chavent & Jaffré '78, Helmig '97]

Governing equations II

- Darcy–Muskat law for volumetric flow rates (neglecting gravity)

$$\mathbf{q}_\alpha = -K\lambda_\alpha(s_\alpha)\nabla p_\alpha \qquad \forall \alpha \in \{l, g\}$$

  with K absolute permeability, λ_α mobility of phase α ($\lambda_\alpha = 0$ if phase α is absent)

- Capillary pressure $\pi : [0, 1) \to [0, +\infty)$

$$p_g = p_l + \pi(s_g)$$

- Assume incompressibility in liquid phase and neglect water vaporization

$$\varrho_l^w = \varrho_l^{\mathrm{std}} \qquad \varrho_g^w = 0$$

Governing equations III

- Ideal gas law in gas phase and hydrogen phase changes in thermodynamic equilibrium (Henry's law)

$$\varrho_g^h = C_g p_g \qquad \varrho_l^h = C_h p_g$$

- Fick's law for dissolved hydrogen diffusion flux (dilute approximation)

$$\mathbf{j}_l^h = -\Phi s_l D_l^h \nabla \varrho_l^h \qquad \mathbf{j}_l^w = -\mathbf{j}_l^h$$

- **Governing equations**

$$\Phi \varrho_l^{\mathrm{std}} \partial_t s_l + \nabla \cdot (\varrho_l^{\mathrm{std}} \mathbf{q}_l - \mathbf{j}_l^h) = F^w$$
$$\Phi \partial_t (\varrho_l^h s_l + C_g p_g s_g) + \nabla \cdot (\varrho_l^h \mathbf{q}_l + C_g p_g \mathbf{q}_g + \mathbf{j}_l^h) = F^h$$

Choice of main unknowns I

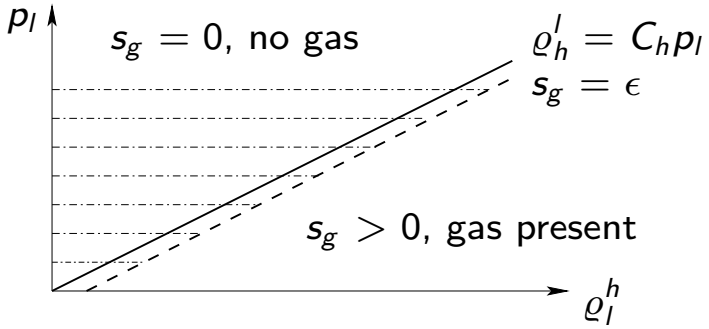
- Possible absence of gas phase in a priori unknown parts of domain
- Choosing one of the saturations as one of the main unknowns is **inappropriate if gas phase disappears**
  - s_g is identically 0
  - s_l is identically 1
- Unified formulation of governing equations highly desirable to avoid intricate numerical solvers
- Artificially enforcing $s_g \geq \epsilon > 0$ is **inappropriate** (can lead to both dissolved hydrogen and gas pressure overestimation)

Choice of main unknowns II

- Following [Bourgeat, Jurak & Smaï '09], we choose as main unknowns

$$y = (y_1, y_2), \qquad y_1 := p_l, \qquad y_2 := \varrho_l^h$$

allowing for a **unified formulation** including gas phase disappearance



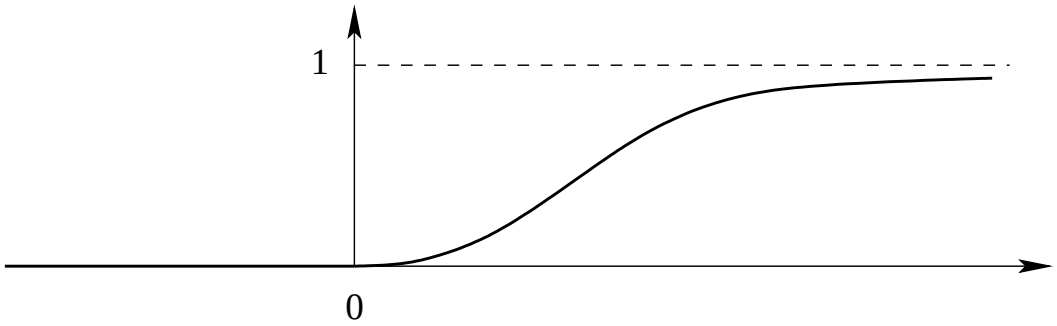
- See also
  - [Jaffré & Sboui '10] for a reformulation based on complementary constraints
  - [Abadpour & Panfilov '09] for method with negative saturations

Choice of main unknowns III

- Gas saturation recovered from capillarity and thermodynamic equilibrium

$$s_g(p_l, \varrho_l^h) = s_g(y) = \pi^{-1}\left(\frac{y_2}{C_h} - y_1\right)$$

$\pi^{-1} : \mathbb{R} \to [0, 1)$ inverse capillary pressure function extended by zero



- s_g is a continuous function of y
  - **continuously differentiable** for van Genuchten capillary pressure model
  - **not differentiable** at entry pressure for Brooks–Corey model

Mathematical model I

- Nondimensional form
  - reference pressure p_0 (1 MPa), reference density $C_h p_0$ (15g/m^3)
  - mass conservation equations scaled by ϱ_l^{std} and $C_h p_0$
- Governing equations

$$\partial_t b_1(y) - \nabla \cdot (A_{11}(y)\nabla y_1 + A_{12}(y)\nabla y_2) = F_1$$
$$\partial_t b_2(y) - \nabla \cdot (A_{21}(y)\nabla y_1 + A_{22}(y)\nabla y_2) = F_2$$

with $b_i(y)$ nondimensional and $A_{ij}(y)$ in m^2/s

- **IC** on y, **BC** either Dirichlet on y or Neumann on total fluxes

$$\boldsymbol{\sigma}_i(y) = \sum_{j\in\{1,2\}} A_{ij}(y)\nabla y_j$$

Mathematical model II

- **System coefficients**

$$
\begin{aligned}
b_1(y) &= -\Phi s_g(y) \\
b_2(y) &= \Phi a(s_g(y)) y_2 \\
A_{11}(y) &= p_0 K \lambda_l (1 - s_g(y)) \\
A_{12}(y) &= -(C_h p_0 / \varrho_l^{\mathrm{std}}) \Phi (1 - s_g(y)) D_l^h \\
A_{21}(y) &= y_2 p_0 K \lambda_l (1 - s_g(y)) \\
A_{22}(y) &= y_2 p_0 K \lambda_g (s_g(y)) \omega + \Phi (1 - s_g(y)) D_l^h
\end{aligned}
$$

with $a(s) = 1 + (\omega - 1)s$ and $\omega = C_g / C_h$ (≈ 50)

- First equation is parabolic in y_1, degenerating into elliptic if gas phase disappears
- Second equation is parabolic in y_2, degenerating into elliptic if dissolved hydrogen disappears

Mathematical model III

- **Structure of space differential operator**
- Ellipticity iff

$$(A_{12} + A_{21})^2 < 4A_{11}A_{22}$$

- Typical orders of magnitude (in $\mu\text{m}^2/\text{s}$)

$$A_{11} \approx 50, \quad A_{12} \approx 0.7, \quad A_{21} \approx 50, \quad A_{22} \approx 450$$

- Under assumption $A_{12} \approx 0$, ellipticity iff $p_0 K \lambda_l(1) < 4\Phi D_l^h$
- Alternative assumption for ellipticity is smallness condition on hydrogen [Mikelić '09]

Mathematical model IV

- Under assumption $A_{12} \approx 0$, change of variables

$$y_1 = u_1 + \omega^{-1} e^{\omega u_2} \qquad y_2 = e^{\omega u_2}$$

yields coupled elliptic-parabolic system [Smaï '09]

$$\partial_t b^*(u) - \nabla \cdot (A^*(u) \nabla u) = F$$

- b^* is the gradient of a **convex potential**
- $A^*(u)$ is **symmetric positive definite**
- Fits Alt–Luckhaus theory for existence of weak solutions
- See also [Amaziane, Jurak & Žgalić-Keko '11; Khalil & Saad '11] for mathematical analysis of compressible immiscible case

Numerical method

- Time discretization: backward Euler
- Linearization: inexact Newton
- Space discretization: discontinuous Galerkin (dG)

Time discretization

- Recall governing equations ($i \in \{1,2\}$)

$$\partial_t b_i(y) - \sum_{j\in\{1,2\}} \nabla \cdot (A_{ij}(y)\nabla y_j) = F_i$$

- Time discretization by backward Euler scheme ($i \in \{1,2\}$)

$$\frac{1}{\tau^m}(b_i(y^m) - b_i(y^{m-1})) - \sum_{j\in\{1,2\}} \nabla \cdot \left(A_{ij}(y^m)\nabla y_j^m\right) = F_i^m$$

Linearization

- Incomplete Newton method with fully coupled approach
  - fixed-point for nonlinearities in diffusion operator
  - linearization in time derivative
- For all $m = 1, \ldots, M$ **(time loop)** and for all $l \geq 0$ **(linearization loop)**, find y_{l+1}^m s.t. $(i \in \{1, 2\})$

$$\sum_{j \in \{1,2\}} \frac{1}{\tau^m} \partial_j b_i(y_l^m) y_{j,l+1}^m - \sum_{j \in \{1,2\}} \nabla \cdot \left(A_{ij}(y_l^m) \nabla y_{j,l+1}^m \right) = G_{i,l}^m$$

yielding a system of linear coupled PDEs in space

Space discretization I

- dG methods can be viewed as
  - FE-based methods using discrete functions with jumps
  - FV-based high-order methods using numerical fluxes
- Vigorous development since the late 90s
  - [Cockburn, Karniadakis & Shu '00; Hesthaven & Warburton '08]
  - unified analysis Poisson problem [Arnold, Brezzi, Cockburn & Marini '02], Friedrichs systems [AE & Guermond '06]
- DG methods for two-phase immiscible porous media flows
  - [Bastian '99; Bastian & Rivière '03; Eslinger '05; Klieber & Rivière '06; Epshteyn & Rivière '07; AE, Mozolevski & Schuh '09]
- Upcoming book **Mathematical aspects of discontinuous Galerkin methods**, D. Di Pietro & AE, Springer, 2011

Space discretization II

- $\{\mathcal{T}_\delta\}_{\delta>0}$ family of shape-regular meshes (possibly with hanging nodes)
- $\mathcal{F}_\delta^{\mathrm{i}}$ collects interfaces, $\mathcal{F}_\delta^{\mathrm{b}}$ boundary faces, $\mathcal{F}_\delta := \mathcal{F}_\delta^{\mathrm{b}} \cup \mathcal{F}_\delta^{\mathrm{i}}$
- Average operator $\{\cdot\}$, jump operator $[\![\cdot]\!]$, face normal $\mathbf{n}_F$
- For polynomial degree $k \geq 1$,

$$V_\delta^k := \{v_\delta \in L^2(\Omega);\ \forall T \in \mathcal{T}_\delta,\ v_\delta|_T \in \mathbb{P}_k(T)\}$$

- Discrete pressure and hydrogen density both sought in V_δ^k

Space discretization III

- Interior penalty dG bilinear form $(i, j \in \{1, 2\})$

$$
\begin{aligned}
a_\delta^{ij}(y_\delta; u_\delta, v_\delta) = & \sum_{T \in \mathcal{T}_\delta} \int_T A_{ij}(y_\delta) \nabla u_\delta \cdot \nabla v_\delta \\
& - \sum_{F \in \mathcal{F}_\delta^{\mathrm{i}} \cup \mathcal{F}_\delta^{\mathrm{D}}} \int_F \mathbf{n}_F \cdot \{A_{ij}(y_\delta) \nabla u_\delta\} [\![v_\delta]\!] \\
& - \theta^{ij} \sum_{F \in \mathcal{F}_\delta^{\mathrm{i}} \cup \mathcal{F}_\delta^{\mathrm{D}}} \int_F \mathbf{n}_F \cdot \{A_{ij}(y_\delta) \nabla v_\delta\} [\![u_\delta]\!] \\
& + \sum_{F \in \mathcal{F}_\delta^{\mathrm{i}} \cup \mathcal{F}_\delta^{\mathrm{D}}} \eta_F^{ij} \frac{\sigma k^2}{\delta_F} \int_F [\![u_\delta]\!] [\![v_\delta]\!]
\end{aligned}
$$

Space discretization IV

- Discrete problem: For all $v_{i,\delta} \in V_\delta^k$, $i \in \{1,2\}$,

$$\sum_{j\in\{1,2\}} \frac{1}{\tau^m} \int_\Omega \partial_j b_i(y_{\delta,l}^m) y_{j,\delta,l+1}^m v_{i,\delta} + \sum_{j\in\{1,2\}} a_\delta^{ij}(y_{\delta,l}^m; y_{j,\delta,l+1}^m, v_{i,\delta})$$
$$= \int_\Omega G_{i,l}^m v_{i,\delta} + \text{bc's}$$

- Penalty and symmetry terms only on diagonal blocks ($i = j$)
- Penalty strategy reasonable if ellipticity can be asserted

Space discretization V

- DG method **weakly enforces**
  - zero PDE residual on each element $T \in \mathcal{T}_\delta$
  - Dirichlet/Neumann BC's on all boundary faces
  - on all mesh interfaces $F \in \mathcal{F}_\delta^{\mathrm{i}}$, the transmission conditions

$$[\![y_i]\!] = 0, \qquad \mathbf{n}_F \cdot [\![\boldsymbol{\sigma}_i(y)]\!] = 0, \qquad \forall i \in \{1, 2\}$$

- For heterogeneous media with different rock types
  - **weighted-averages** can be considered ([AE, Stephansen & Zunino '09] for linear convection-diffusion)
  - for immiscible flows where gas saturation is one of the main unknowns, **nonlinear interface conditions** must be enforced [AE, Mozolevski & Schuh '09]

Results

- Three test cases (1D)
  - **Gas-phase (dis)appearance** [MOMAS benchmark]
  - **Ill-prepared initial condition** [MOMAS benchmark]
  - **Heterogeneous medium** [Bourgeat, Jurak & Smaï '11]
- In all cases, we use
  - van Genuchten model for capillary pressure and Mualem model for relative permeability
  - piecewise linear polynomials in dG method ($k = 1$)
  - 10^{-8} convergence criterion in L^2-norm for inexact Newton

Gas-phase (dis)appearance I

- Domain $\Omega = (0, 200)$ (m) initially saturated by water
- Hydrogen injection at $x = 0$ during 10^5 years
- Injection rate $q_{\mathrm{inj}} = 5.57{\cdot}10^{-6}$ kg /m^2/year
- Simulation time 10^6 years
- Initial and BC's

$$
\begin{aligned}
-\mathbf{n}\cdot\boldsymbol{\sigma}_1|_{x=0} &= 0 & -\mathbf{n}\cdot\boldsymbol{\sigma}_2|_{x=0} &= q_{\mathrm{inj}}\chi_{[0,T_{\mathrm{inj}}]}(t)\\
p_l|_{x=200} &= 10^6 \text{ (Pa)} & \varrho_l^h|_{x=200} &= 0\\
p_l|_{t=0} &= 10^6 \text{ (Pa)} & \varrho_l^h|_{t=0} &= 0
\end{aligned}
$$

- Uniform mesh with 200 elements, time steps within [125;5000] years

Gas-phase (dis)appearance II

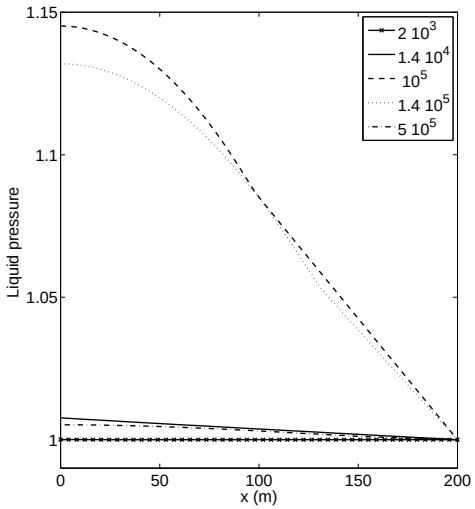
Problem data

Porous medium		Fluid characteristics	
Param.	Value	Param.	Value
Φ	0.15 (-)	D_l^h	$3\ 10^{-9}$ m^2/s
K	$5\ 10^{-20}$ m^2	μ_l	$1\ 10^{-3}$ Pa·s
P_r	$2\ 10^6$ Pa	μ_g	$9\ 10^{-6}$ Pa·s
n	1.49 (-)	$H(303K)$	$7.65\ 10^{-6}$ $mol/Pa/m^3$
s_{lr}	0.4 (-)	M^h	$2\ 10^{-3}$ kg/mol
s_{gr}	0 (-)	ϱ_l^{std}	10^3 kg/m^3

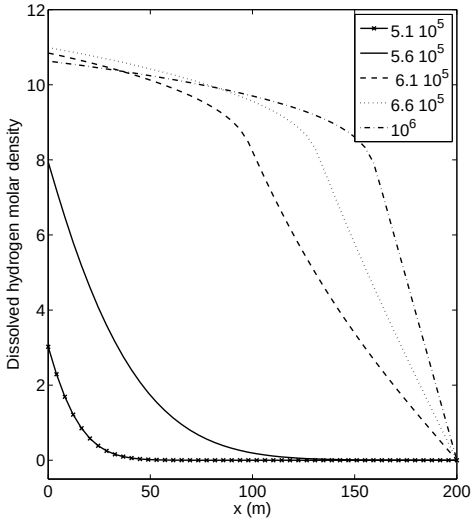
Gas-phase (dis)appearance III

- **Snapshots for times in $[0, 10^5]$ years**

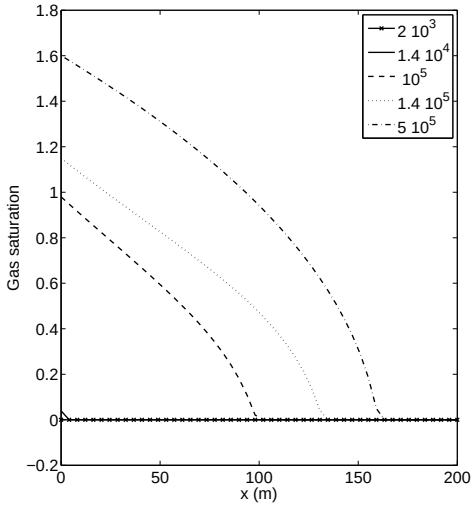
liquid pressure (MPa)



diss. hyd. molar density (mol/m^3)



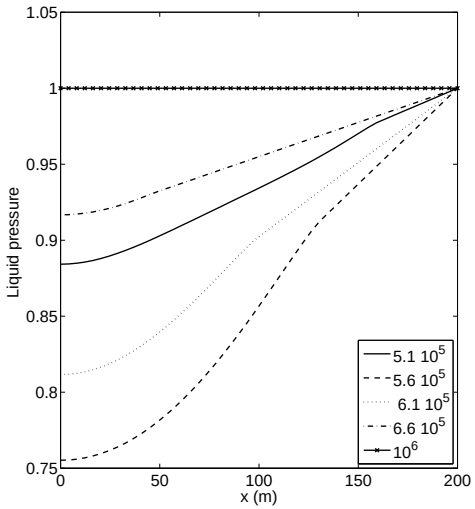
gas saturation (%)



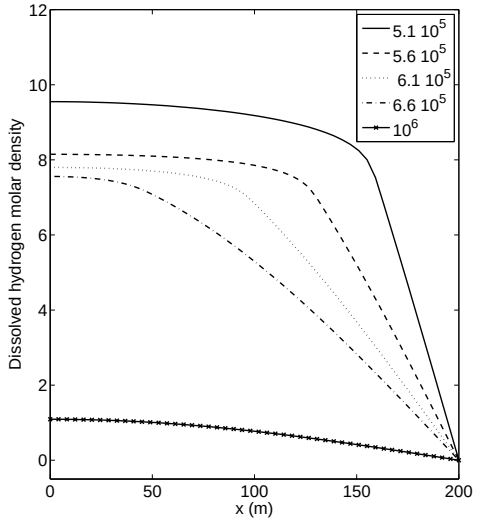
Gas-phase (dis)appearance IV

- **Snapshots for times in $[10^5, 10^6]$ years**

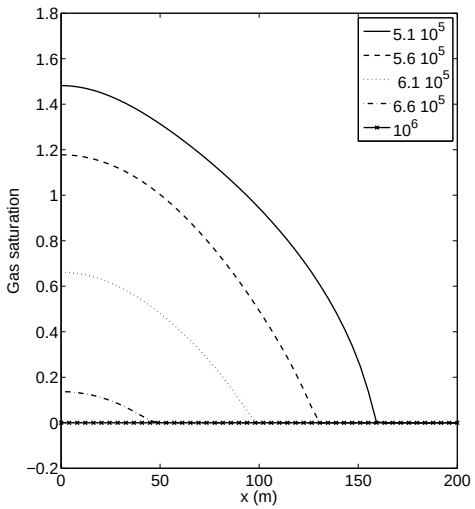
liquid pressure (MPa)



diss. hyd. molar density (mol/m^3)



gas saturation (%)



Ill-prepared initial condition I

- Domain $\Omega = (0,1)$ (m) with zero flux BC's and no external sources
- Initial conditions

$$p_l(x,0) = 10^6 \text{ (Pa)} \quad x \in (0,1)$$

$$p_g(x,0) = \begin{cases} 1.5{\cdot}10^6 \text{ (Pa)} & \text{if } x \in (0,0.5) \\ 2.5{\cdot}10^6 \text{ (Pa)} & \text{if } x \in (0.5,1) \end{cases}$$

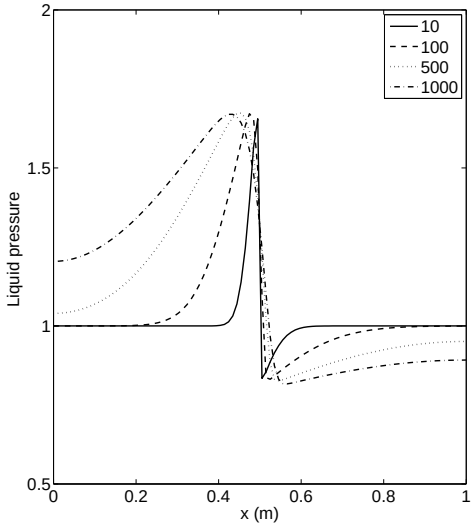
  so that system is initially out of mechanical equilibrium

- Similar medium and fluid parameters (except $K = 10^{-16}$ m^2) as previous case
- Simulation time 10^6 s
- Uniform mesh with 512 elements, time steps within $[1;10^4]$ s

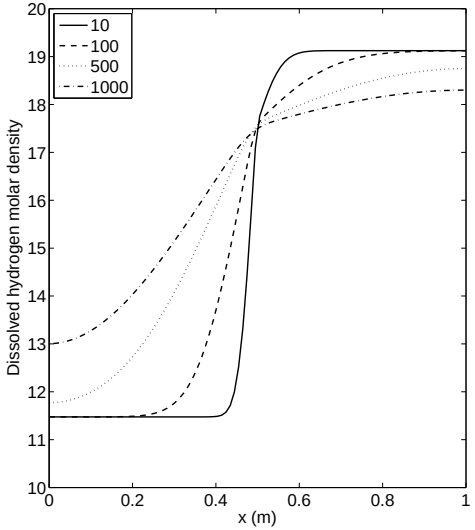
Ill-prepared initial condition II

- **Snapshots for times [0,10^3] s**

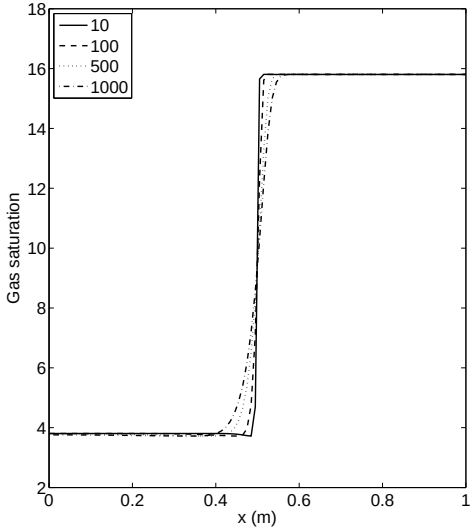
liquid pressure (MPa)



diss. hyd. molar density (mol/m^3)



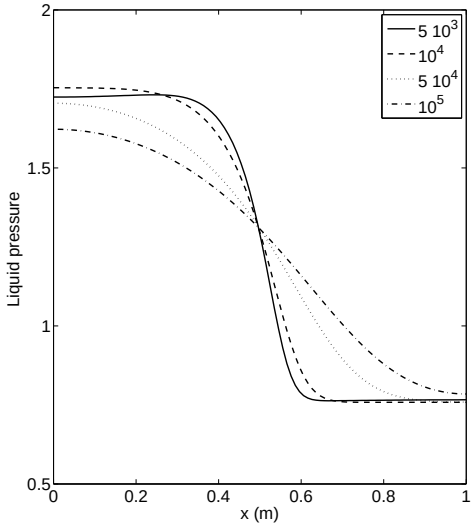
gas saturation (%)



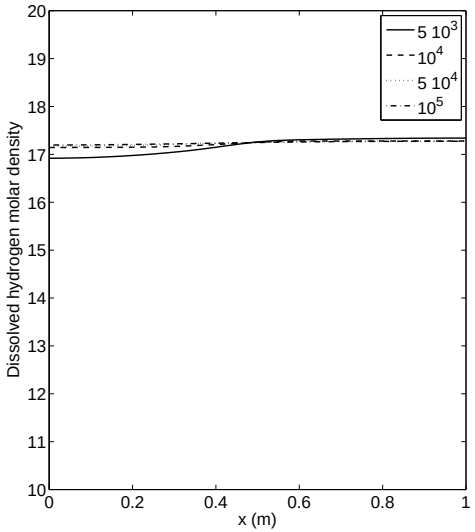
Ill-prepared initial condition III

- **Snapshots for times [$5{\cdot}10^3$,10^5] s**

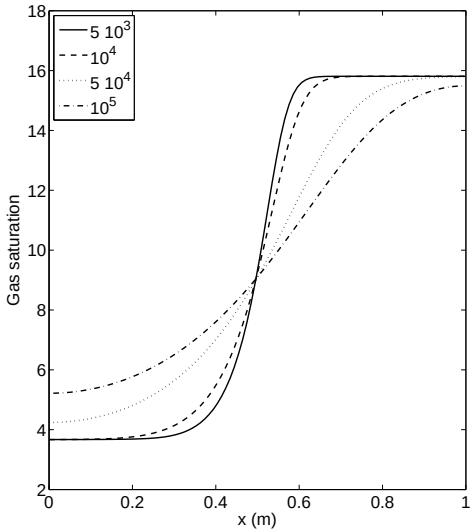
liquid pressure (MPa)



diss. hyd. molar density (mol/m^3)



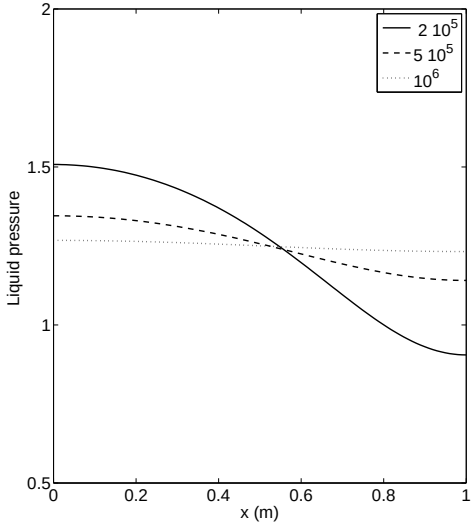
gas saturation (%)



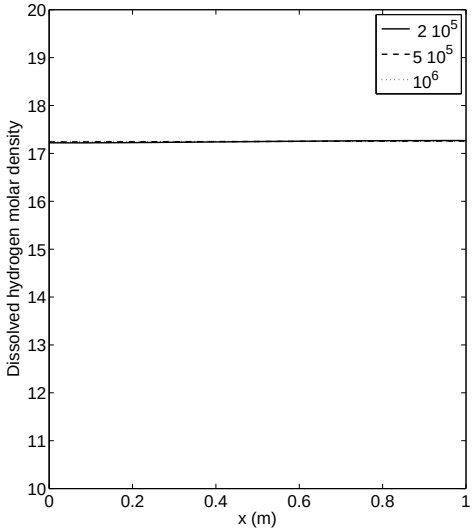
Ill-prepared initial condition IV

- **Snapshots for times [$2{\cdot}10^5$,10^6] s**

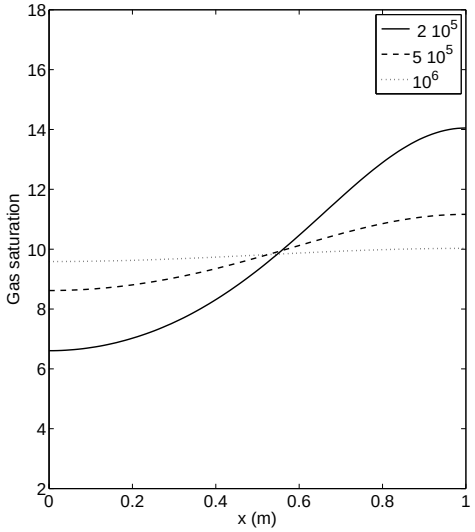
liquid pressure (MPa)



diss. hyd. molar density (mol/m^3)



gas saturation (%)

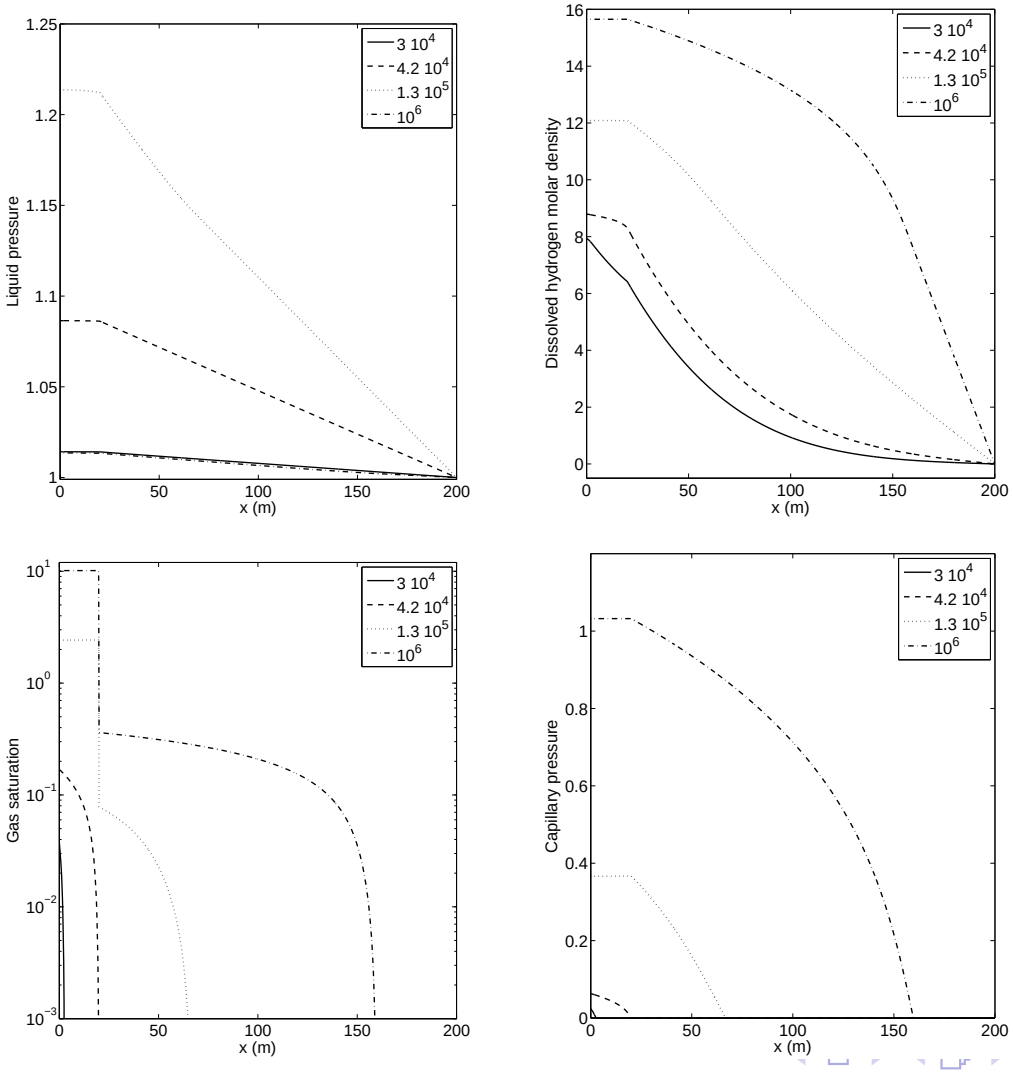


Heterogeneous medium I

- Similar to test case 1 except that medium consists of two rock types occupying $\Omega_1 = (0, 20)$ and $\Omega_2 = (20, 200)$ (m) and that hydrogen injection is not stopped
- Rock occupying Ω_2 has a finer texture $\Rightarrow$ **capillary barrier at interface** $x = 20$
- Uniform mesh with 160 elements (fitted to rock interface), time steps within [200;20000] years

Heterogeneous medium II

Snapshots at times $\{3{\cdot}10^4, 4.2{\cdot}10^4, 1.3{\cdot}10^5, 10^6\}$ years



Conclusions

- Two-component miscible liquid-gas porous media flow model motivated by hydrogen migration in underground radioactive waste repositories
- Choice of main unknowns to handle absence of gas phase
- DG space discretization combined with backward Euler scheme and incomplete Newton linearization
- Further work
  - **deeper analysis** of mathematical model
  - **multidimensional** test cases with heterogeneities