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 Mm³**

- **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**

[Image of a map showing the location of a repository for radioactive waste]
The issue of radioactive waste III

A Possible Repository Architecture

- Limit the number of connections
- Spacing calculated in order to keep temperature low
- Specialized module for each category of waste

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)
  \[ \text{Fe} + 2\text{H}_2\text{O} \rightarrow \text{Fe(OH)}_2 + \text{H}_2 \]

- Understand hydrogen migration through host rock

- Two-phase (liquid, gas), two-component (water, hydrogen) flow, gas phase is compressible

- **Gas phase (dis)appearance**

![Graph](image)
Outline

- Setting
- Numerical method
- Results
Setting

- Governing equations
- Choice of main unknowns
- Mathematical model
Governning equations I

- **Basic notation**
  - subscript $\alpha \in \{l, g\}$ for phase
  - superscript $\beta \in \{w, h\}$ for component
  - $\rho_\alpha^\beta$ density of component $\beta$ in phase $\alpha$
  - $s_\alpha$ saturation of phase $\alpha$, $s_l + s_g = 1$
  - $p_\alpha$ pressure of phase $\alpha$

- **Mass conservation equation for each component**

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

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

- [Bear ’78, Chavent & Jaffré ’78, Helmig ’97]
Governing equations II

- Darcy–Muskat law for volumetric flow rates (neglecting gravity)
  \[ q_\alpha = -K \lambda_\alpha (s_\alpha) \nabla p_\alpha \quad \forall \alpha \in \{l, g\} \]
  with \( K \) absolute permeability, \( \lambda_\alpha \) mobility of phase \( \alpha \) (\( \lambda_\alpha = 0 \) if phase \( \alpha \) is absent)

- Capillary pressure \( \pi : [0, 1) \rightarrow [0, +\infty) \)
  \[ p_g = p_l + \pi(s_g) \]

- Assume incompressibility in liquid phase and neglect water vaporization
  \[ \varrho_l^w = \varrho_l^{\text{std}} \quad \varrho_g^w = 0 \]
Governing equations III

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

\[ \varrho_g^h = C_g p_g, \quad \varrho_l^h = C_h p_g \]

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

\[ j_l^h = -\Phi s_l D_l^h \nabla \varrho_l^h, \quad j_l^w = -j_l^h \]

- Governing equations

\[
\begin{align*}
\Phi \varrho_{l}^{\text{std}} \partial_t s_l + \nabla \cdot (\varrho_{l}^{\text{std}} q_l - j_l^h) &= F_w \\
\Phi \partial_t (\varrho_{l}^h s_l + C_g p_g s_g) + \nabla \cdot (\varrho_{l}^h q_l + C_g p_g q_g + j_l^h) &= F^h
\end{align*}
\]
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

\[ y = (y_1, y_2), \quad y_1 := p_l, \quad y_2 := \rho^h_l \]

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

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

\( \pi^{-1} : \mathbb{R} \rightarrow [0, 1) \) 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 $C_h p_0$ (15 g/m$^3$)
  - mass conservation equations scaled by $\rho_{\text{std}}$ 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

$$
\sigma_i(y) = \sum_{j \in \{1,2\}} A_{ij}(y) \nabla y_j
$$
Mathematical model II

- **System coefficients**

\[
\begin{align*}
  b_1(y) &= -\Phi s_g(y) \\
  b_2(y) &= \Phi a(s_g(y)) y_2 \\
  A_{11}(y) &= p_0 K \lambda_l(1 - s_g(y)) \\
  A_{12}(y) &= -(C_{h}p_0/\varrho_{l}^{\text{std}})\Phi(1 - s_g(y))D_{l}^{h} \\
  A_{21}(y) &= y_2 p_0 K \lambda_l(1 - s_g(y)) \\
  A_{22}(y) &= y_2 p_0 K \lambda_g(s_g(y))\omega + \Phi(1 - s_g(y))D_{l}^{h}
\end{align*}
\]

with \(a(s) = 1 + (\omega - 1)s\) and \(\omega = C_{g}/C_{h} (\approx 50)\)

- 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 \(\mu m^2/s\))**

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

- **Under assumption** \(A_{12} \approx 0\), ellipticity iff \(p_0K\lambda_l(1) < 4\Phi D_l^h\)

- **Alternative assumption for ellipticity is smallness condition on hydrogen** [Mikelić ’09]
Mathematical model IV

- Under assumption $A_{12} \approx 0$, change of variables
  
  $$y_1 = u_1 + \omega^{-1} e^{\omega u_2} \quad y_2 = e^{\omega u_2}$$

  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** \((i \in \{1, 2\})\)

\[
\frac{1}{\tau^m} (b_i(y^m) - b_i(y^{m-1})) - \sum_{j \in \{1, 2\}} \nabla \cdot (A_{ij}(y^m) \nabla y_j^m) = F_i^m
\]
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 $y_{m,l+1}^i$ s.t. ($i \in \{1, 2\}$)

\[
\sum_{j \in \{1, 2\}} \frac{1}{\tau_m} \partial_j b_i(y_i^m) y_{j,l+1}^m - \sum_{j \in \{1, 2\}} \nabla \cdot (A_{ij}(y_i^m) \nabla y_{j,l+1}^m) = G_{i,l}^m
\]

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 & Riviè re ’03; Eslinger ’05; Klieber & Riviè re ’06; Epshteyn & Riviè re ’07; AE, Mozolevski & Schuh ’09]

Space discretization II

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

\[ V^k_\delta := \{v_\delta \in L^2(\Omega); \forall T \in \mathcal{T}_\delta, v_\delta|_T \in \mathbb{P}_k(T)\} \]

- Discrete pressure and hydrogen density both sought in \(V^k_\delta\)
Space discretization III

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

\[
a_\delta^{ij}(y_\delta; u_\delta, v_\delta) = \sum_{T \in T_\delta} \int_T A_{ij}(y_\delta) \nabla u_\delta \cdot \nabla v_\delta
- \sum_{F \in F^i_\delta \cup F^D_\delta} \int_F \mathbf{n}_F \cdot \{A_{ij}(y_\delta) \nabla u_\delta\}[[v_\delta]]
- \theta^{ij} \sum_{F \in F^i_\delta \cup F^D_\delta} \int_F \mathbf{n}_F \cdot \{A_{ij}(y_\delta) \nabla v_\delta\}[[u_\delta]]
+ \sum_{F \in F^i_\delta \cup F^D_\delta} \eta^{ij} \frac{\sigma k^2}{\delta_F} \int_F [[[u_\delta]][[v_\delta]]]
\]
Space discretization IV

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

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

- 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 \( F \in \mathcal{F}_\delta \), the transmission conditions
    \[
    [[\gamma_i]] = 0, \quad n_F \cdot [[[\sigma_i(y)]]] = 0, \quad \forall i \in \{1, 2\}
    \]

- 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 \( q_{\text{inj}} = 5.57 \cdot 10^{-6} \) kg /m\(^2\)/year
- Simulation time \( 10^6 \) years
- Initial and BC’s

\[-n \cdot \sigma_1|_{x=0} = 0 \quad -n \cdot \sigma_2|_{x=0} = q_{\text{inj}} \chi[0, T_{\text{inj}}](t)\]

\[p_l|_{x=200} = 10^6 \text{ (Pa)} \quad \rho_l^h|_{x=200} = 0\]

\[p_l|_{t=0} = 10^6 \text{ (Pa)} \quad \rho_l^h|_{t=0} = 0\]

- Uniform mesh with 200 elements, time steps within \([125;5000]\) years
## Gas-phase (dis)appearance II

### Problem data

<table>
<thead>
<tr>
<th>Porous medium</th>
<th>Fluid characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Param.</td>
<td>Value</td>
</tr>
<tr>
<td>Φ</td>
<td>0.15 (-)</td>
</tr>
<tr>
<td>$K$</td>
<td>$5 \times 10^{-20}$ m$^2$</td>
</tr>
<tr>
<td>$P_r$</td>
<td>$2 \times 10^6$ Pa</td>
</tr>
<tr>
<td>$n$</td>
<td>1.49 (-)</td>
</tr>
<tr>
<td>$s_{lr}$</td>
<td>0.4 (-)</td>
</tr>
<tr>
<td>$s_{gr}$</td>
<td>0 (-)</td>
</tr>
</tbody>
</table>
Gas-phase (dis)appearance III

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

- Liquid pressure (MPa)
- Dissolved hydrogen molar density (mol/m$^3$)
- Gas saturation (%)
Gas-phase (dis)appearance IV

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

![Graphs showing liquid pressure, dissolved hydrogen molar density, and gas saturation over time.](image)
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 $K = 10^{-16} \text{ m}^2$) as previous case
- Simulation time $10^6 \text{ s}$
- Uniform mesh with 512 elements, time steps within $[1;10^4] \text{ s}$
Ill-prepared initial condition II

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

<table>
<thead>
<tr>
<th>Graph</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Left</td>
<td>Liquid pressure (MPa)</td>
</tr>
<tr>
<td>Middle</td>
<td>Dissolved hydrogen molar density (mol/m$^3$)</td>
</tr>
<tr>
<td>Right</td>
<td>Gas saturation (%)</td>
</tr>
</tbody>
</table>

![Graphs showing liquid pressure, dissolved hydrogen molar density, and gas saturation over time for different initial conditions.](image)
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)
- Dissolved hydrogen molar density (mol/m$^3$)
- Gas saturation (%)

![Graphs of liquid pressure, dissolved hydrogen molar density, and gas saturation over time](image-url)
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 $\Omega_2$ 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