Generalized HMFE Approximation for Compositional Two-Phase Flow

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Outline

1. Continuous formulation
2. HFME discretization
3. Numerical results
   - MOMAS test cases
   - More about heterogeneous soil
   - 2D test case

Outline

Conservation Equations

For $\alpha = (1), (2)$:

$$\phi \frac{\partial (N X^{(\alpha)})}{\partial t} + \mathrm{div}\ \left(N_l x_l^{(\alpha)} \vec{V}_l + N_l S_l \vec{W}_l^{(\alpha)} \right) + \mathrm{div}\ \left(N_g x_g^{(\alpha)} \vec{V}_g + N_g S_g \vec{W}_g^{(\alpha)} \right) =$$

$$\begin{aligned} \vec{V}_i &= -\frac{K k_i(S_i)}{\mu_i} \left(\vec{\nabla} P_i - M_i N_i \vec{g} \right) \quad \text{(generalized Darcy's law)}, \\ \vec{W}_i^{(\alpha)} &= -D_i^{(\alpha)} \phi \vec{\nabla} x_i^{(\alpha)} \quad \text{for } i = l(iquide),\ g(az) \quad \text{(Fick's law)}, \end{aligned}$$

- N (resp. N_l, N_g): total molar concentrations (resp. of l, g)
- $k_{l,g}$: relative permeability
- $\phi, K, \mu_i, D_i^{(\alpha)}$: constants.
- $X^{(\alpha)}$, $x_i^{(\alpha)}$: molar fractions ($X^{(1)} + X^{(2)} = x_i^{(1)} + x_i^{(2)} = 1$)
- $M_i = M^{(1)} x_i^{(1)} + M^{(2)} x_i^{(2)}$: molar mass of phase i

Closure relationships

$S := S_g$

Choice of two main unkonwns

- $P_g - P_l = P_c(S)$
- Compressibility laws:

$$P_{l,g}, x_{l,g}^{(1)} \Rightarrow N_{l,g}$$

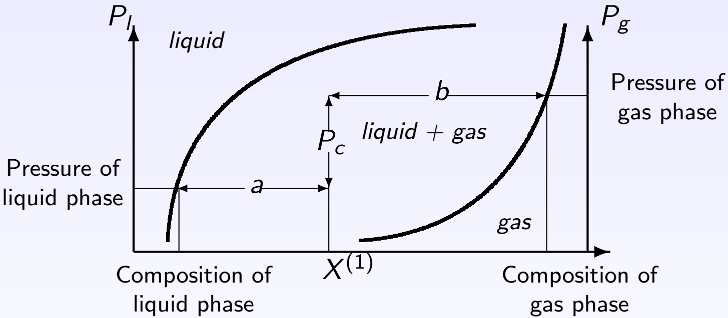
- Equilibrium model: for $0 < S < 1$,

$$x_l^{(1)} = X_m(P, S) \text{ and } x_g^{(1)} = X_M(P, S).$$

- For $S = 0$: $\cancel{x_g^{(1)}}$, for $S = 1$: $\cancel{x_l^{(1)}}$

$$(P, X^{(1)}) \rightarrow \left(S, (x_l^{(1)}), (x_g^{(1)})\right)$$

Equilibrium with $X_m(P,S) = X_m(P_l)$ and $X_M(P,S) = X_M(P_g)$



$$\frac{a}{a+b} = \frac{SN_g}{N}$$

Equilibrium with Henry's law
no water in gas phase, incompressible liquid phase

(1): H_2 (2): H_2O

When there is only a small amount of the light component in the liquid phase, for a saturated fluid:

$$\underbrace{x_g^{(1)} \cdot P_g}_{\substack{\text{partial pressure}\\ \text{of component (1)}\\ \text{in gas phase}}} = H \cdot \underbrace{N_l x_l^{(1)}}_{\substack{\text{molar concentration}\\ \text{of component (1)}\\ \text{in liquid phase}}}$$

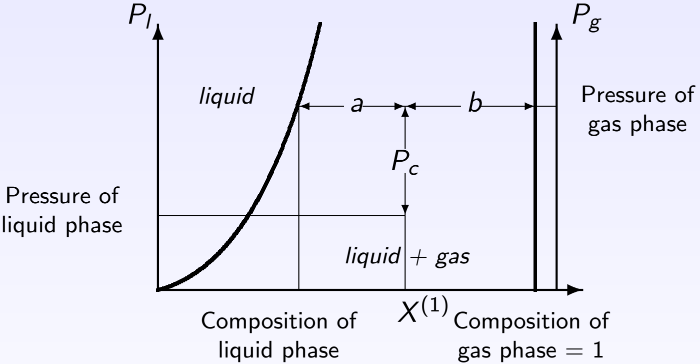
Gas contains only hydrogen:

$$X_M(P,S) \equiv 1$$

Incompressible heavy component in the liquid phase: $N_l x_l^{(2)} =: N_l^{std}$,

$$X_m(P,S) = \frac{P_g}{P_g + H \cdot N_l^{std}}$$

Closure relationships



$$\frac{a}{a+b} = \frac{SN_g}{N}$$

Complementarity Problem

$$\begin{cases} S = 0 \\ x_l^{(1)} = X^{(1)} \leq X_m(P,0) \end{cases}$$
or
$$\begin{cases} S = 1 \\ x_g^{(1)} = X^{(1)} \geq X_M(P,1) \end{cases}$$
or
$$\begin{cases} 0 \leq S \leq 1 \\ x_l^{(1)} = X_m(P,S) \\ x_g^{(1)} = X_M(P,S) \\ X^{(1)} = \dfrac{SN_g x_g^{(1)} + (1-S)N_l x_l^{(1)}}{SN_g + (1-S)N_l} \end{cases}$$

↓ Artificial definitions of the properties of the missing phase

$$\begin{cases} \min\left(S \;,\; X_m(P,S) - x_l^{(1)} \right) = 0 \\ \min\left(1 - S \;,\; x_g^{(1)} - X_M(P,S) \right) = 0 \\ SN_g(X^{(1)} - x_g^{(1)}) + (1-S)N_l(X^{(1)} - x_l^{(1)}) = 0 \end{cases}$$

Outline

System of diffusion-convection equations

For $(\alpha) = (1),\ (2)$

$$\frac{\partial m^{(\alpha)}(x,y)}{\partial t} + \mathrm{div}\ \vec{u}^{(\alpha)}_{diff} + \mathrm{div}\ \vec{u}^{(\alpha)}_{conv} = q^{(\alpha)}$$

$$\vec{u}^{(\alpha)}_{diff} = -\sum_{\tau} b^{(\alpha)}_{\tau}(x,y)\vec{\nabla} f^{(\alpha)}_{\tau}(x,y)$$

$$\vec{u}^{(\alpha)}_{conv} = h^{(\alpha)}(x,y)\vec{g}.$$

$$\begin{array}{lcl} m^{(\alpha)} & = & \phi(SN_g + (1-S)N_l)X^{(\alpha)} \\ b^{(\alpha)}_1 & = & N_g x^{(\alpha)}_g K \frac{k_g}{\mu_g}\ , \\ b^{(\alpha)}_2 & = & N_l x^{(\alpha)}_l K \frac{k_l}{\mu_l}\ , \\ b^{(\alpha)}_3 & = & \mathbf{N_g} D_g S\phi\ , \\ b^{(\alpha)}_4 & = & \mathbf{N_l} D_l (1-S)\phi\ , \\ h^{(\alpha)} & = & \frac{Kk_g}{\mu_g} M_g N_g^2 x^{(\alpha)}_g + \frac{Kk_l}{\mu_l} M_l N_l^2 x^{(\alpha)}_l \end{array}$$

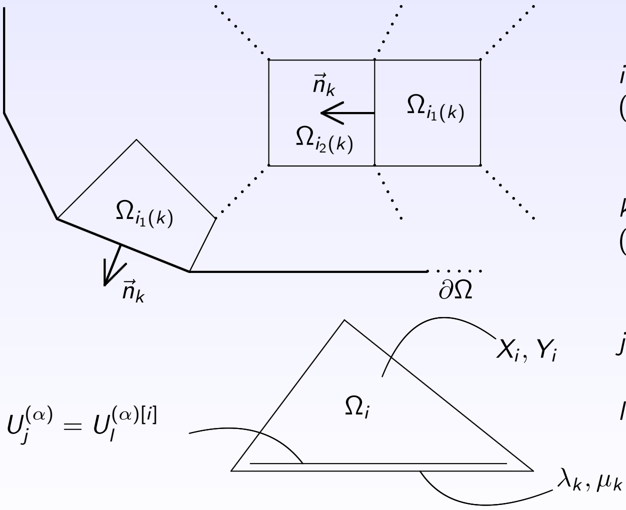
$$\begin{array}{lcl} f^{(\alpha)}_1 & = & P_g \\ f^{(\alpha)}_2 & = & P_l \\ f^{(\alpha)}_3 & = & x^{(\alpha)}_g \\ f^{(\alpha)}_4 & = & x^{(\alpha)}_l \end{array}$$

Time discretization: 2 possibilities considered

- Euler-scheme, implicit for diffusion terms f_τ but explicit for diffusion coefficients b_τ and explicit for convection terms h,
- or, for the settings for which we can find a suitable nonlinear solver, on an Euler-scheme, implicit for diffusion terms f_τ and for diffusion coefficients b_τ and explicit for convection terms h.

Time step $t_n \to t_{n+1} = t_n + \Delta t$.
Values at time $t = t_n$: exponent ^{0}

Triangulation



$i = 1, \ldots, N_c$
(number of cells)

$k = 1, \ldots, N_E$
(number of edges)

$j = 1, \ldots, 2N_E - N_b$

$l = 1, \ldots, 3$

Conservation Equations

For any cell Ω_i

$$\int_{\Omega_i} \frac{m^{(\alpha)}(x,y) - m^{(\alpha)}(x^0,y^0)}{\Delta t} + \int_{\partial\Omega_i} \vec{u}^{(\alpha)}_{diff} \cdot \vec{n}_{ext_i} + \int_{\partial\Omega_i} h^{(\alpha)}(x,y)\vec{g}\cdot\vec{n}_{ext_i} = \int_{\Omega_i} q^{(}$$

Lowest order:

$$\frac{|\Omega_i|}{\Delta t} m^{(\alpha)}(X_i, Y_i) + B_{loc} U^{(\alpha)[i]} =$$
$$\frac{|\Omega_i|}{\Delta t} m^{(\alpha)}(X_i^0, Y_i^0) - \sum_{k, E_k \subset \partial\Omega_i} h^{(\alpha)*} \epsilon_{ik} g_k + Q_i^{(\alpha)} \quad \forall i \in 1, \dots, N_c.$$

with

$$\epsilon_{ik} g_k = \int_{E_k} \vec{g}\cdot\vec{n}_{ext_i} \quad \text{for } E_k \subset \partial\Omega_i \,, \quad Q_i^{(\alpha)} = \int_{\Omega_i} q^{(\alpha)}.$$

Upwind convection:

$$\text{if } m^{(\alpha)}(x_L, y_L) \le m^{(\alpha)}(x_R, y_R) : \quad h^{(\alpha)*} = \min\left(h^{(\alpha)}(x_L, y_L), h^{(\alpha)}(x_R, y_R)\right)$$
$$\text{if } m^{(\alpha)}(x_L, y_L) > m^{(\alpha)}(x_R, y_R) : \quad h^{(\alpha)*} = \max\left(h^{(\alpha)}(x_L, y_L), h^{(\alpha)}(x_R, y_R)\right).$$

Diffusion equations

For any basis function $\vec{v}_j$ and any cell Ω_i

$$\int_{\Omega_i} \vec{u}_{diff}^{(\alpha)} \cdot \vec{v}_j + \sum_{\tau} \overbrace{\int_{\partial\Omega_i} b_{\tau}^{(\alpha)}(x^0, y^0) f_{\tau}^{(\alpha)}(x, y) \vec{v}_j \cdot \vec{n}_{ext_i}}^{T_{\tau,bd}^{(\alpha)}(i)}$$

$$- \sum_{\tau} \underbrace{\int_{\Omega_i} f_{\tau}^{(\alpha)}(x, y) \mathrm{div} \left(b_{\tau}^{(\alpha)}(x^0, y^0) \vec{v}_j \right)}_{T_{\tau,int}^{(\alpha)}(i)} = 0 .$$

Remind:

$$\sum_{i=1}^{N_c} T_{\tau,bd}^{(\alpha)}(i) = \sum_{k, E_k \subset \partial\Omega} \int_{E_k} b_{\tau}^{(\alpha)}(x^0, y^0) f_{\tau}^{(\alpha)}(x, y) \vec{v}_j \cdot \vec{n}_{ext_\Omega} .$$

Basis functions for the scalar fields constant per cell:

$$\begin{aligned} T_{int}^{(\alpha)}(i) &= f_\tau^{(\alpha)}(x_i, y_i) \int_{\partial\Omega_i} b_\tau^{(\alpha)}(x^0, y^0)\vec{v}_j \cdot \vec{n}_{ext_i} \\ &= f_\tau^{(\alpha)}(x_i, y_i) \sum_{k|E_k \subset \partial\Omega_i} \int_{E_k} b_\tau^{(\alpha)}(x^0, y^0)\vec{v}_j \cdot \vec{n}_{ext_i}. \end{aligned}$$

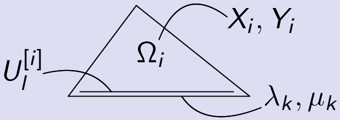
- Values for terms $b_\tau(x^0, y^0)$ over E_k needed: Lagrange multipliers used.
- Case of heterogeneous physics: values of Lagrange multipliers together with the physics corresponding to the current cell $\Rightarrow$ continuity of main unkonwns

For all $i = 1, \cdots, N_c$, $A^{[i]}$ = local mass matrix:

$$A^{[i]}_{l,m} = \int_{\Omega_i} \vec{v}_{j(i,l)} \cdot \vec{v}_{j(i,m)}.$$

We get $\forall i \in 1, \ldots, N_c, \quad E_k \subset \partial\Omega_i$

Diffusion equations



$$\left[A^{[i]} U^{[i](\alpha)}\right]_l + \sum_\tau b_\tau^{(\alpha)}(\lambda_k^0, \mu_k^0) \left(f_\tau^{(\alpha)}(\lambda_k, \mu_k) - f_\tau^{(\alpha)}(X_i, Y_i)\right) = 0.$$

Flux continuity equations

$$\forall k = 1, \ldots, N_E, \text{ with } E_k \subset \Omega, \quad U_k^{[i_1(k)]} + U_k^{[i_2(k)]} = 0.$$

Reduction: static codensation

Iterative scheme used to solve $(\lambda^n, \mu^n) \mapsto (\lambda^{n+1}, \mu^{n+1})$.
Static condensation (used in every step of the iterative scheme):

- for λ, μ given
  1. compute corresponding X, Y in solving local equations in X_i, Y_i associated to each cell Ω_i:
     local implicit functions are considered

     $$\forall i \in I \ (X_i, Y_i) = \psi_i(\lambda, \mu) \Leftrightarrow \tilde{F}_i(\lambda, \mu, X_i, Y_i) = 0$$

     where $\tilde{F}$ is related to the conservation equation.
  2. compute needed residual $G(\lambda, \mu)$ and Jacobian matrices related to the flux continuity equation.

Conservation equations: $\tilde{F}_i^{(\alpha)} : (\mathbb{R}^{N_E} \times \mathbb{R}^{N_E}) \times (\mathbb{R} \times \mathbb{R}) \to \mathbb{R}$

$$\tilde{F}_i^{(\alpha)}(\lambda,\mu,x,y) = \frac{|\Omega_i|}{\Delta t}\left(m^{(\alpha)}(x,y) - m^{(\alpha)}(X_i^0, Y_i^0)\right) + \sum_{E_k \subset \partial\Omega_i} a_{i,k} \sum_{\tau} \left[\, f_\tau^{(\alpha)}(x,y) \; - \; f_\tau^{(\alpha)}(\lambda_k,\mu_k) \,\right] \, b_\tau^{(\alpha)}(\lambda_k^0,\mu_k^0) + \sum_{E_k \subset \partial\Omega_i} h^{(\alpha)^*}(x^{*k}, y^{*k})\epsilon_{ik} g_k - Q_i^{(\alpha)} \quad \forall i \in I.$$

Flux continuity equations: $i := i_d(k)\,,\; x := \psi_i^x(\lambda,\mu)\,,\; y := \psi_i^y(\lambda,\mu)$

$$\tilde{G}_{d,k}^{(\alpha)}(\lambda,\mu) := \sum_{E_{k'} \subset \partial\Omega_i} H^{[i]}{}_{kk'} \sum_{\tau} \left[\, f_\tau^{(\alpha)}(x,y) \; - \; f_\tau^{(\alpha)}(\lambda_{k'},\mu_{k'}) \,\right] \, b_\tau^{(\alpha)}(\lambda_{k'}^0, \mu_{k'}^0$$

$$G_k^{(\alpha)}(\lambda,\mu) = \tilde{G}_{1,k}^{(\alpha)}(\lambda,\mu) + \tilde{G}_{2,k}^{(\alpha)}(\lambda,\mu)$$

Implementation Aspects

M++

C++ finite elements library ("Mesh, multigrid and more")
Provides the possibility to define automatically global iterative methods (here damped Newton's method with Armijo-rule) from local Jacobian matrices and residuals:
assembling of the method is automatic.

Modular code

makes it possible to separate difficulties linked to the static model
(i.e. "How to define f_τ, $b_\tau, \dots$")
and PDE-aspects
(i.e. "Assembling", or "How to use f_τ, $b_\tau, \dots$").

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    - MOMAS test cases
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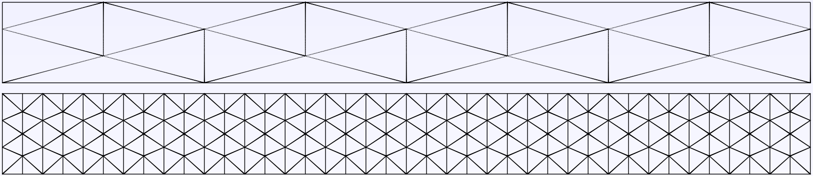
Problem 1

- Main unknowns: $P_l, X^{(1)}$
- $t = 0 : X^{(1)} = 10^{-5}$
- $\Delta t = 0.2$ and $\Delta t = 4$ centuries
- Meshes:

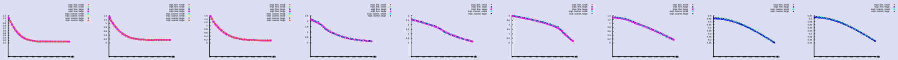


- Compare implicit and explicit treatment of diffusion coefficients

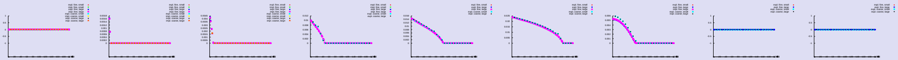
Problem 1

- $t = 100, 140, 200, 500, 1000, 5000, 6700, 8400, 10000$ centuries

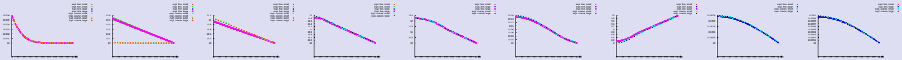
Total hydrogen concentration (i.e. $N \cdot X^{(1)}$)



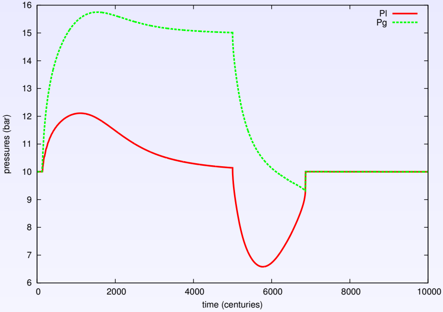
Gas saturation

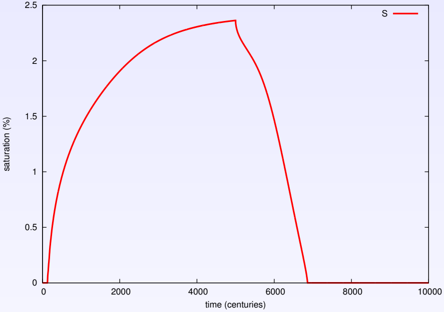


Liquid pressure



Problem 1: input values



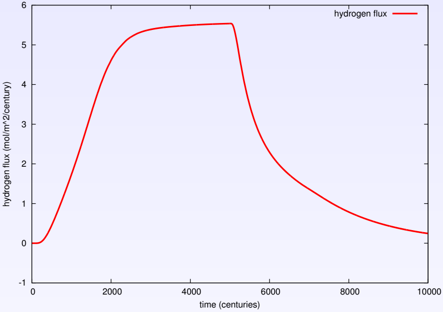


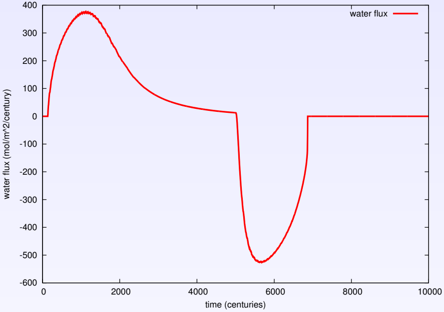
Left: liquid pressure (red) and gas pressure (green) (axis: 6 bar - 16 bar)

Right: gas saturation in $x = 0$ (axis: 0,0% - 2.5%)

in $x = 0$ function of time (axis: 0 - 10000 centuries).

Problem 1: output fluxes



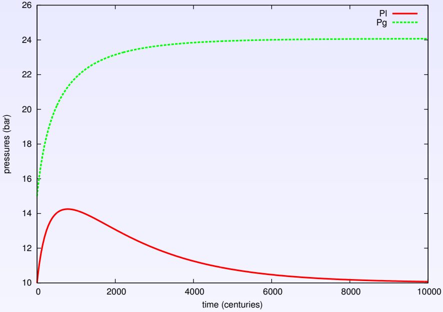


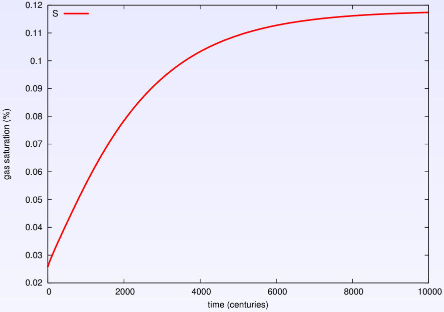
Left: output gas flux
(axis: -1 - 6 mol/m^2/century
i.e. -2 - $12 \cdot 10^{-5}$ kg/m^2/year)

Right: output water flux
(axis: 0 - 400 mol/m^2/century
i.e. 0 - 400 kg/m^2/year)

function of time (axis: 0 - 10000 centuries).

Problem 2 a: input values



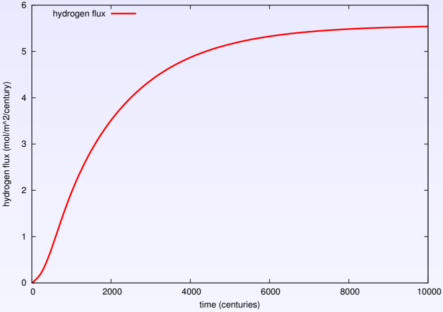


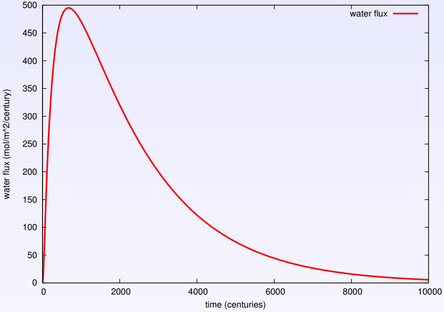
Left: liquid pressure (red) and gas pressure (green) (axis: 10 bar - 26 bar)

Right: gas saturation in $x = 0$ (axis: 0,02% - 0.12%)

in $x = 0$ function of time (axis: 0 - 10000 centuries).

Problem 2 a: output fluxes



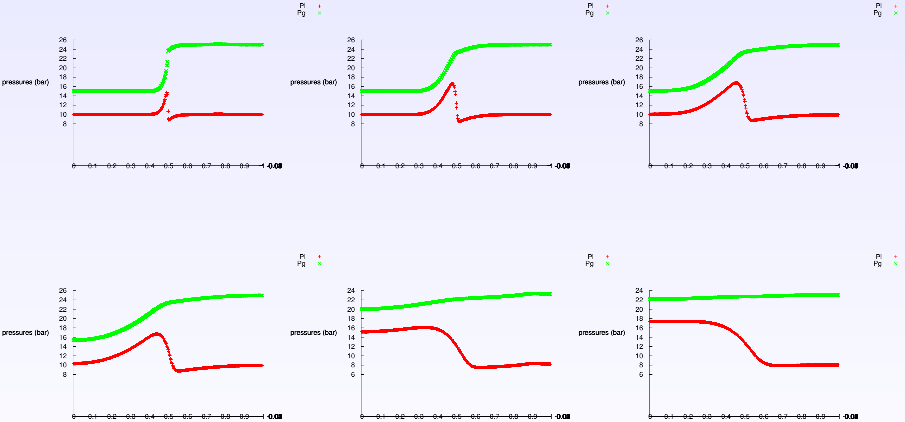


Left: output hydrogen flux
(axis: 0 - 6 mol/m^2/century
i.e. 0 - $12 \cdot 10^{-5}$ kg/m^2/year)

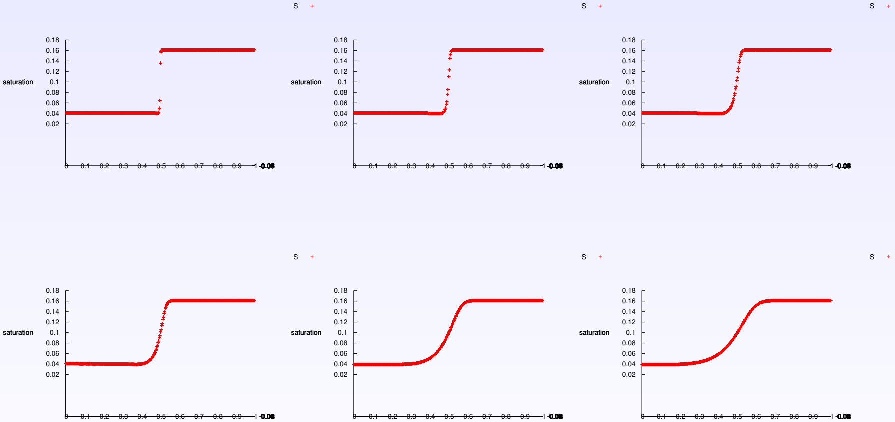
Right: output water flux
(axis: 0 - 500 mol/m^2/century
i.e. 0 - 500 kg/m^2/year)

function of time (axis: 0 - 10000 centuries).

Problem 3: pressures

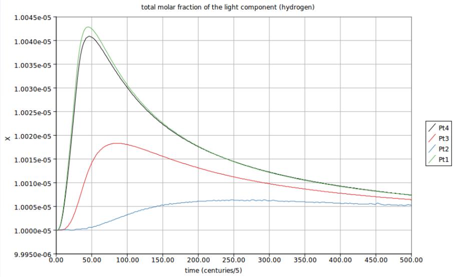


Problem 3: saturations

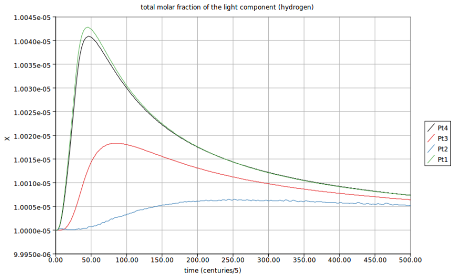


Problem 4

Problem 5



total molar fraction of the light component (hydrogen)
x
time (centuries/5)
Pt4
Pt3
Pt2
Pt1

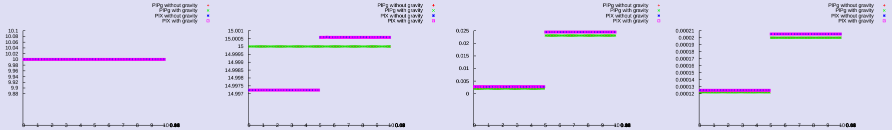


total molar fraction of the light component (hydrogen)
x
time (centuries/5)
Pt4
Pt3
Pt2
Pt1

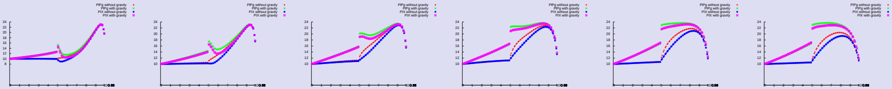
Heterogeneous example

Main Unknowns: P_l, $X^{(1)}$ or P_l, P_g.

Initial conditions: P_l, P_g, S, X

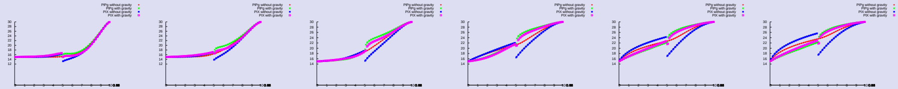


Liquid pressure

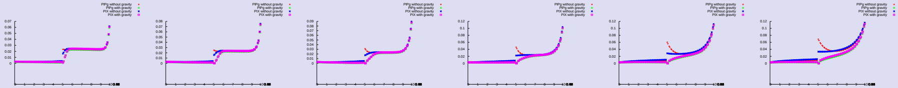


Heterogeneous example

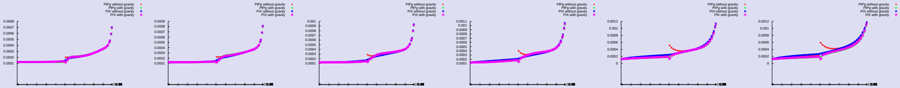
Gas pressure



Gas saturation

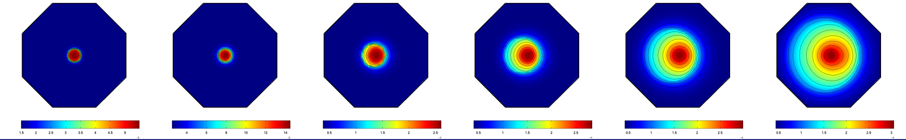


Light component molar fraction

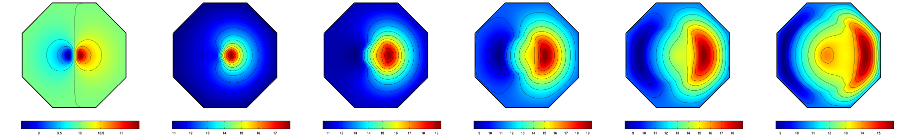


Two-dimensional test case

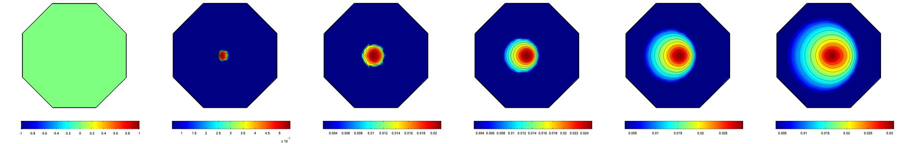
Light component molar fraction



Liquid pressure



Gas saturation



Alternative model

For $\alpha = (1),\ (2)$

$$\frac{\partial m^\alpha(x,y)}{\partial t} + \mathrm{div}\ \vec{u}^\alpha_{diff} + \mathrm{div}\ \vec{u}^\alpha_{conv} = q^\alpha$$

$$\vec{u}^\alpha_{diff} = -\sum_\tau b^\alpha_\tau(x,y)\vec{\nabla} f^\alpha_\tau(x,y)$$

$$\vec{u}^\alpha_{conv} = h^\alpha(x,y)\vec{g}.$$

$$\begin{aligned}
m^\alpha &= \phi(SN_g + (1-S)N_l)X \\
b_1^\alpha &= N_g x_g^\alpha K \tfrac{k_g}{\mu_g}\ , & f_1^\alpha &= P_g \\
b_2^\alpha &= N_l x_l^\alpha K \tfrac{k_l}{\mu_l}\ , & f_2^\alpha &= P_l \\
b_3^\alpha &= \cancel{\mathbf{N_g}} D_g S\phi\ , & f_3^\alpha &= \mathbf{N_g} x_g^\alpha \\
b_4^\alpha &= \cancel{\mathbf{N_l}} D_l(1-S)\phi\ , & f_4^\alpha &= \mathbf{N_l} x_l^\alpha \\
h^\alpha &= \tfrac{Kk_g}{\mu_g} M_g N_g^2 x_g^\alpha + \tfrac{Kk_l}{\mu_l} M_l N_l^2 x_l^\alpha
\end{aligned}$$

lemma

We assume that physical laws and parameters are chosen so that

(H2) $S_g = 0 \Rightarrow P_g = P_l$;

(H3) $N_l x_l^{(2)}$ is independent of X;

(H4) $q^{(2)} = 0$;

(H5) $D_i^{(1)} = D_i^{(2)} =: D_i$ for $i = l, g$.

We consider a regular computation domain Ω.

(i) (Alternative model) Any possible solution of the alternative model with Dirichlet boundary conditions and initial conditions such that

$$\begin{cases} S_g(t=0,.) \equiv 0 \\ P_l(t=0,.) \equiv const \\ P_l(t=0,.) \text{ satisfies the Dirichlet boundary conditions} \end{cases}$$

fulfill

$$P_l(t,.) \equiv P_l(t=0,.) \text{ as long as } S_g \equiv 0.$$

(ii) (Standard model) This is not valid with the standard model.

THANK YOU FOR YOUR ATTENTION