Finite Volume Discretization of Multiphase Porous Media Flows for CO2 geological sequestration

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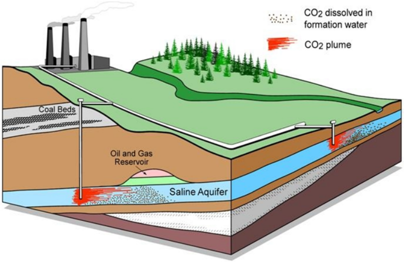
CO2 geological storage in saline aquifer

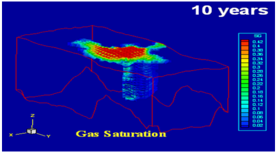
- Objectives
  - Optimization of CO2 injection
  - Optimization of CO2 trapping
  - Risk assessment and management

- Models
  - Compositional MultiPhase flow
  - Geochemistry
  - Geomechanics

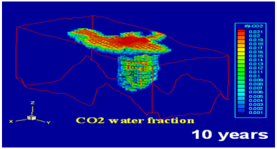


Injection phase: 10 to 50 years

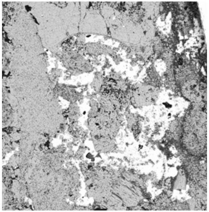
- Two phase Darcy flow
  - Structural trapping
  - Capillary trapping



- CO2 dissolution
  - Solubility trapping



- Near-well alteration
  - Drying and salt precipitation
  - Risk of loss of injectivity



General Notations for compositional multiphase fluid systems

- Phases: $\alpha \in \mathcal{P}$
- Components: $i \in \mathcal{C}$
- Binary matrix of components in phases

$$M = \begin{array}{cc} & (i \in \mathcal{C}) \\ (\alpha \in \mathcal{P}) & \left(\begin{array}{cc|c|cc} 1 & \dots & 0 & \dots & 1 \\ \vdots & \dots & \vdots & \dots & \vdots \\ \hline 0 & \dots & 1 & \dots & 1 \\ \hline \vdots & \dots & \vdots & \dots & \vdots \\ 1 & \dots & 1 & \dots & 0 \end{array}\right) \rightarrow \mathcal{C}_\alpha \\ & \downarrow \\ & \mathcal{P}_i \end{array}$$

Set of present phases

- Due to thermodynamical equilibrium phases $\alpha \in \mathcal{P}$ can appear or disappear
- The unknown $\mathcal{Q}$ denotes the set of present phases on each point of the domain

$$\mathcal{Q}(x) \in \{\mathcal{R} \subset \mathcal{P}\}$$

Formulation using the set of unknowns $\mathcal{Q}$, P, S^α, C^α, $\alpha \in \mathcal{Q}$

$$n_i = \phi \sum_{\alpha \in \mathcal{Q} \cap \mathcal{P}_i} \zeta_\alpha(P, C^\alpha)\; S^\alpha \; C_i^\alpha, \qquad Z = \left(\frac{n_i}{\sum_{j \in \mathcal{C}} n_j} \right)_{i \in \mathcal{C}}$$

$$\left\{ \begin{array}{r} \partial_t n_i + \mathrm{div}\Big(\displaystyle\sum_{\alpha \in \mathcal{Q} \cap \mathcal{P}_i} C_i^\alpha \frac{\zeta_\alpha(P, C^\alpha) k_{r_\alpha}(S)}{\mu_\alpha(P, C^\alpha)} \mathbf{V}^\alpha \Big) = 0,\ i \in \mathcal{C}, \\ \displaystyle\sum_{\alpha \in \mathcal{Q}} S^\alpha = 1, \\ \displaystyle\sum_{i \in \mathcal{C}} C_i^\alpha = 1,\ \alpha \in \mathcal{Q}, \\ f_i^\alpha(P, C^\alpha) = f_i^\beta(P, C^\beta), \alpha \neq \beta \in \mathcal{Q} \cap \mathcal{P}_i,\ i \in \mathcal{C}, \end{array} \right.$$

with

$$\mathbf{V}^\alpha = -\Lambda\Big(\nabla \Big[P + P_{c,\alpha}(S) \Big] - \rho_\alpha(P, C^\alpha)\mathbf{g} \Big), \alpha \in \mathcal{Q}.$$

$\mathcal{Q}$ is typically obtained by the fixed point equation: $\mathcal{Q} = \text{Flash}(P, Z)$.

Components present only in absent phases

For given $\mathcal{Q}$ and i, the set $\mathcal{Q} \cap \mathcal{P}_i$ can be empty.

- Hence, let us define the set

$$\widetilde{\mathcal{C}}_{\mathcal{Q}} = \{ i \,|\, \mathcal{Q} \cap \mathcal{P}_i = \emptyset \}$$

- and the additional independent unknowns n_i for $i \in \widetilde{\mathcal{C}}_{\mathcal{Q}}$.

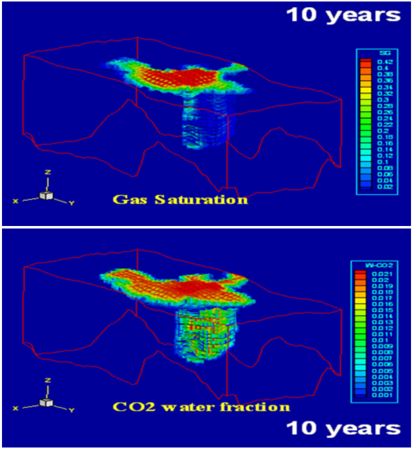
Then, the following total set of unknowns:

$$\boxed{\Big(\mathcal{Q}, P, S^\alpha, C_i^\alpha, n_j\Big)_{i \in \mathcal{C}^\alpha,\, \alpha \in \mathcal{Q},\, j \in \widetilde{\mathcal{C}}_{\mathcal{Q}}}}$$

matches the above total number of equations.

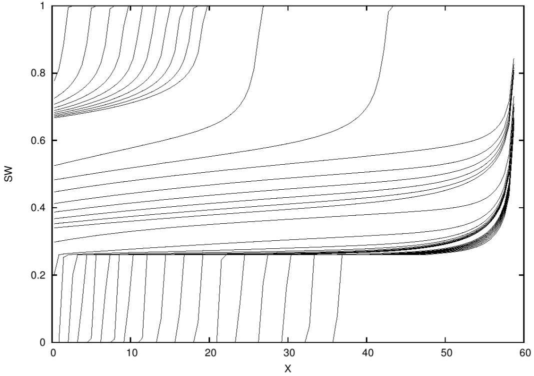
Example: dissolution of CO2 in the water phase

- $\mathcal{P} = \{\text{water}, \text{gas}\}$
- $\mathcal{C} = \{\text{H20}, \text{CO2}\}$
- $M = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$



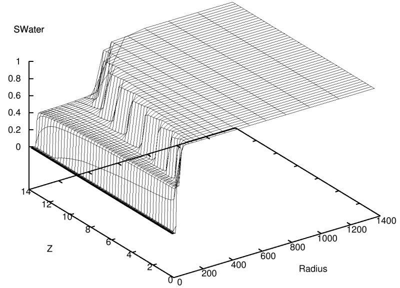
Example: near well drying of water due to CO2 injection

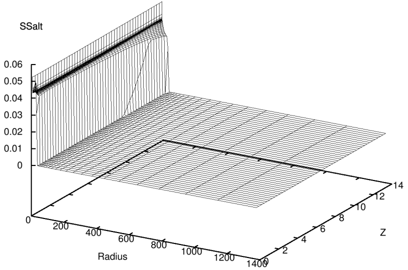
- $\mathcal{P} = \{\text{water}, \text{gas}\}$
- $\mathcal{C} = \{\text{H20}, \text{CO2}, \text{Salt}\}$
- $M = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}$



Example: near well drying of water due to CO2 injection and salt precipitation

- $\mathcal{P} = \{\text{water}, \text{gas}, \text{mineral}\}$
- $\mathcal{C} = \{\text{H20}, \text{CO2}, \text{Salt}\}$
- $M = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$





Cell Centered Finite Volume Discretization of Compositional MultiPhase Flows

Discretization: set of cells $\mathcal{K} \in \mathcal{M}$, neighbouring cells $\mathcal{L} \in \mathcal{T}_{\mathcal{K}}$ sharing the face $\mathcal{K}\mathcal{L}$.

Let $X_{\mathcal{K}} = \Big(P_{\mathcal{K}}, S^{\alpha}_{\mathcal{K}}, C^{\alpha}_{i,\mathcal{K}}, n_{j,\mathcal{K}}\Big)_{i \in \mathcal{C}^{\alpha},\, \alpha \in \mathcal{Q}_{\mathcal{K}},\, j \in \widetilde{\mathcal{C}}_{\mathcal{Q}_{\mathcal{K}}}}$ the set of unknowns in the cell $\mathcal{K}$.

$$\frac{n_i(X_{\mathcal{K}}) - n_i(X^n_{\mathcal{K}})}{\Delta t}\,|\mathcal{K}| + \sum_{\mathcal{L} \in \mathcal{T}_{\mathcal{K}}} \sum_{\alpha \in \mathcal{Q}_{\mathcal{K}_{up}} \cap \mathcal{P}_i} \left(C^{\alpha}_i \,\frac{\zeta_{\alpha}\, k_{r_{\alpha}}}{\mu_{\alpha}}\right)(X_{\mathcal{K}_{up}})\; F^{\alpha}_{\mathcal{K}\mathcal{L}} = 0$$

for all $\mathcal{K} \in \mathcal{M}$, $i \in \mathcal{C}$, with

- $F^{\alpha}_{\mathcal{K}\mathcal{L}} = -F^{\alpha}_{\mathcal{L}\mathcal{K}}$ a cell centered conservative discretization of the Darcy Flux $\displaystyle\int_{\mathcal{K}\mathcal{L}} \mathbf{V}^{\alpha} \cdot \mathbf{n}_{\mathcal{K}\mathcal{L}} d\sigma$
- the upwinding $\quad \mathcal{K}_{up} = \begin{cases} \mathcal{K} \ \text{ if } \ F^{\alpha}_{\mathcal{K}\mathcal{L}} \geq 0, \\ \mathcal{L} \ \text{ if } \ F^{\alpha}_{\mathcal{L}\mathcal{K}} < 0. \end{cases}$

Cell Centered Finite Volume Discretization of Compositional MultiPhase Flows

The local closure equations are fully coupled to the conservation equations

$$\mathcal{C}_{\mathcal{K}}\Big(X_{\mathcal{K}}\Big) = 0$$

Solution algorithm: Newton type algorithm

- Residual computation
- Linear system reduction and solution
- Update of the unknowns $X_{\mathcal{K}}$ on the mesh $\mathcal{M}$
- Update of the set of phases on the mesh $\mathcal{M}$

$$\mathcal{Q}_{\mathcal{K}} = \mathrm{Flash}(P_{\mathcal{K}}, Z_{\mathcal{K}})$$

Cell Centered, Consistent and Conservative discretization of the Darcy fluxes

$$F_{\mathcal{K}\mathcal{L}} = -F_{\mathcal{L}\mathcal{K}} \sim \int_{\mathcal{K}\mathcal{L}} -\Lambda\,\nabla P \cdot \mathbf{n}_{\mathcal{K}\mathcal{L}} d\sigma$$

- Two Point Flux Approximation (TPFA):

  $$F_{\mathcal{K}\mathcal{L}} = \frac{\Lambda_{\mathcal{K}\mathcal{L}}|\mathcal{K}\mathcal{L}|}{d_{\mathcal{K}\mathcal{L}}} \Big(P_{\mathcal{K}} - P_{\mathcal{L}}\Big),$$

  conservative, monotone, cheap but not consistent and convergent on realistic meshes
- MultiPoint Flux Approximation schemes (MPFA):

  $$F_{\mathcal{K}\mathcal{L}} = \sum_{\mathcal{N} \in \mathcal{S}_{\mathcal{K}\mathcal{L}}} T_{\mathcal{K}\mathcal{L}}^{\mathcal{N}} P_{\mathcal{N}},$$

  conservative, consistent, but not always coercive and convergent

Vertex Approximate Gradient (VAG) scheme

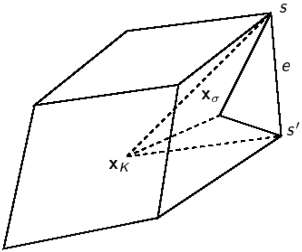
Discrete function space: vertex and cell unknowns

$$V_{\mathcal{D}} = \{u_s \in \mathbb{R}, s \in \mathcal{V}, u_K \in \mathbb{R}, K \in \mathcal{T} \mid u_s = 0 \text{ on } \partial\Omega\}$$

Gradient reconstruction on $V_{\mathcal{D}}$ (conforming example):

$$\mathbf{x}_\sigma = \sum_{s \in \mathcal{V}_\sigma} \frac{1}{\mathrm{Card}\mathcal{V}_\sigma} \mathbf{x}_s, \quad u_\sigma = \sum_{s \in \mathcal{V}_\sigma} \frac{1}{\mathrm{Card}\mathcal{V}_\sigma} u_s$$

$$\nabla_{K,\sigma,e} u = \sum_{s \in \mathcal{V}_\sigma} (u_s - u_K) g^s_{K,\sigma,e}$$



Piecewise constant gradient in $L^2(\Omega)^d$:

$$\nabla_{\mathcal{D}} u = \nabla_{K,\sigma,e} u \ \text{ on each tetrahedra } , \mathbf{x}_K, \mathbf{x}_\sigma, \mathbf{x}_s, \mathbf{x}_{s'}, \ \text{ with } e = ss'$$

Discrete variational formulation and fluxes

Bilinear form on $V_{\mathcal{D}} \times V_{\mathcal{D}}$

$$\left\{ \begin{aligned} a_{\mathcal{D}}(u, v) &= \int_{\Omega} \Lambda \, \nabla_{\mathcal{D}} u \cdot \nabla_{\mathcal{D}} v \, dx \\ &= \sum_{K \in \mathcal{T}} \sum_{s, s' \in \mathcal{V}_K} A_K^{s,s'} \left(u_{s'} - u_K \right) \left(v_s - v_K \right) \\ &= \sum_{K \in \mathcal{T}} \sum_{s \in \mathcal{V}_K} F_{K,s}(u) \left(v_K - v_s \right) \end{aligned} \right.$$

with the flux between the cell K and the vertex s defined by

$$F_{K,s}(u) = \sum_{s' \in \mathcal{V}_K} A_K^{s,s'} \left(u_K - u_{s'} \right)$$

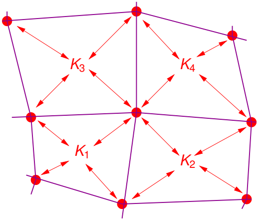
Vertex Gradient Finite Volume Scheme

The variational formulation: find $u \in V_{\mathcal{D}}$ such that

$$a_{\mathcal{D}}(u, v) = \sum_{K \in \mathcal{T}} v_K \int_K f \, dx \quad \text{for all } v \in V_{\mathcal{D}}$$

is equivalent to

$$\begin{cases} \displaystyle\sum_{s \in \mathcal{V}_K} F_{K,s}(u) = \int_K f \, dx \text{ for all } K \in \mathcal{T}, \\ \displaystyle\sum_{K \in \mathcal{T}_s} -F_{K,s}(u) = 0 \text{ for all } s \in \mathcal{V} \setminus \partial\Omega \end{cases}$$



Conservative fluxes:

$$F_{s,K}(u) = -F_{K,s}(u) = \sum_{s \in \mathcal{V}_K} A_K^{s,s'} \left(u_K - u_{s'} \right)$$

VAG scheme for MultiPhase Darcy flow discretization

The VAG scheme is unconditionaly coercive on general meshes (including non conforming, with non planar faces, ...) and leads to a compact vertex scheme after elimination of the cell unknowns.

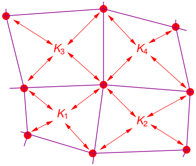
The conservative linear fluxes

$$F_{s,K}(u) = -F_{K,s}(u) = \sum_{s\in\mathcal{V}_K} A_K^{s,s'}\left(u_{s'} - u_K\right)$$

can be used for the discretization of MultiPhase Darcy flow.

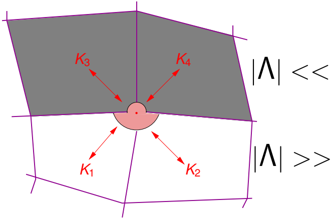
Set $\mathcal{M}$ of cells $\mathcal{K}$:

$$\mathcal{M} = \mathcal{T} \cup \mathcal{V}$$



Which pore volume at the vertices?

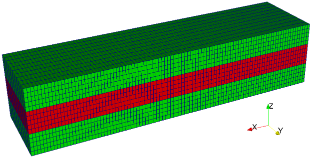
- Conservative redistribution of pore volume from the cells to the vertices
- Pore volume taken from the highest permeability cells around the vertex
  - Total pore volume: $\widetilde{\phi}_K = \displaystyle\int_K \phi \, dx$
  - Indicator of the transmissivity :
    - $B_{K,s} = \displaystyle\sum_{s' \in \mathcal{V}_K} A_K^{s,s'}$
    - $\widetilde{B}_{K,s} = \mu \dfrac{B_{K,s}}{\displaystyle\sum_{L \in \mathcal{T}_s} B_{L,s}}$



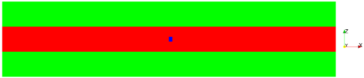
  - $\phi_{\mathcal{K}} = \begin{cases} \widetilde{\phi}_K \displaystyle\sum_{K \in \mathcal{T}_s} \widetilde{B}_{K,s} & \text{if } \mathcal{K} = s \in \mathcal{V}, \\ \widetilde{\phi}_K (1 - \displaystyle\sum_{s \in \mathcal{V}_K} \widetilde{B}_{K,s}) & \text{if } \mathcal{K} = K \in \mathcal{T}. \end{cases}$

Heterogeneous case
Data of the test case

- Injection of immiscible CO_2 in a liquid phase
- Reservoir size : $[-100, 100] \times [0, 50] \times [0, 45]\ m^3$
- Heterogeneity ratio of 10^4
- Coarse grid : $100 \times 10 \times 15$ control volumes

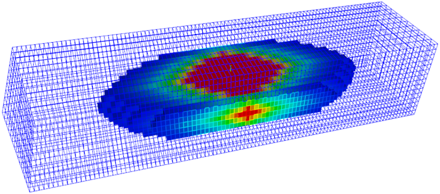


mesh and layers :
permeable medium
barrier



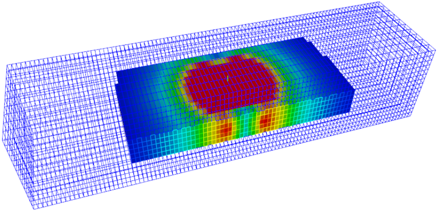
injector well at the center of the section $y = 25\ m$

Heterogeneous case
Front of the gas saturation

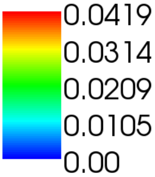


TPFA scheme

Two-Point Flux Approximation



VAG scheme

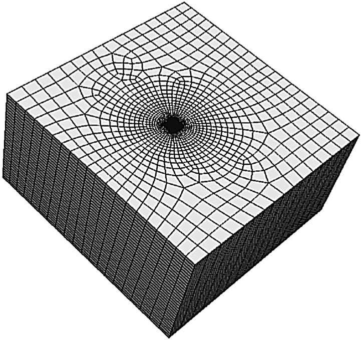


Gas saturation

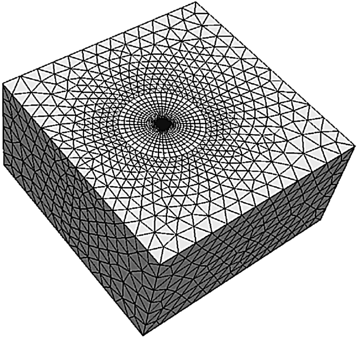
VAG is less sensitive to Grid Orientation Effect.

Near-Well case
Data of the test case

- Injection of miscible CO_2 in a liquid phase
- Deviated well
- Medium homogeneous but anisotropic

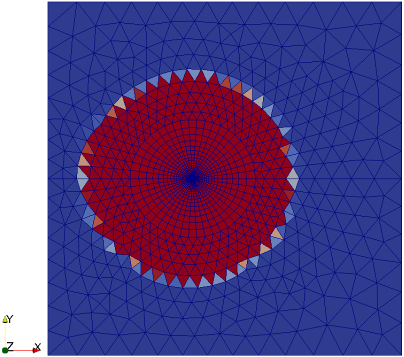


Hexehedral mesh

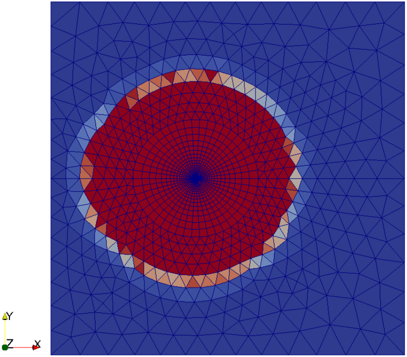


Hybrid mesh

Hybrid Near-Well mesh
Concentration of CO_2 in water phase

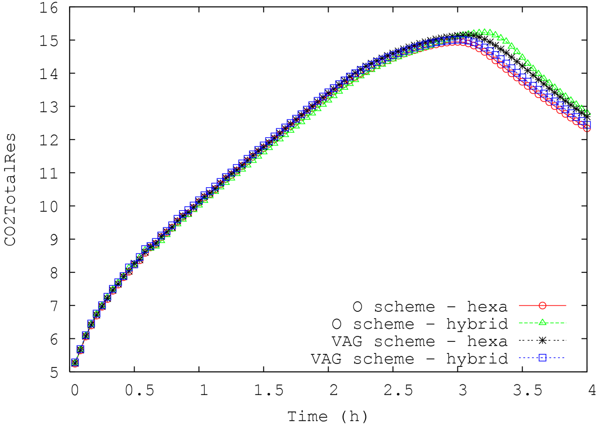


MPFA O-scheme



VAG scheme

Heterogeneous case
Mass of CO_2 in the reservoir



Rate of variation of the mass of CO_2 inside the reservoir

Conclusions

- General formulation of MultiPhase flow for a large class of models in CO2 geological storage
- Vertex based discretization of Darcy fluxes
  - Unconditionaly coercive on general meshes
  - Easy to implement on general meshes (including non conforming, non planar faces, degenerate hexahedra, ...)
  - Easy to implement in usual cell centered MPFA reservoir simulator (based on the graph of transmissivities)
  - Compact scheme
  - Much more efficient than MPFA on tetrahedral meshes
- Need to be further tested on industrial test cases