# 3D numerical simulation of coupled processes between two-phase flows and geochemical reactions in porous media

E. Ahusborde, B. Amaziane, **M. Id Moulay***

CNRS / Univ Pau & Pays Adour/ E2S UPPA,Laboratoire de Mathématiques et de leurs Applications de Pau - Fédération IPRA, UMR5142 64000, Pau, France.

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*mohamed.id-moulay@univ-pau.fr*

# Outline


1. Motivation and Goals
2. Reactive transport model
3. Numerical scheme
4. Validation & numerical results
5. Conclusion & Perspectives

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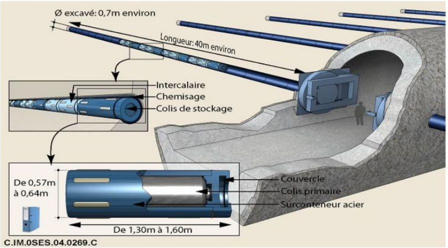
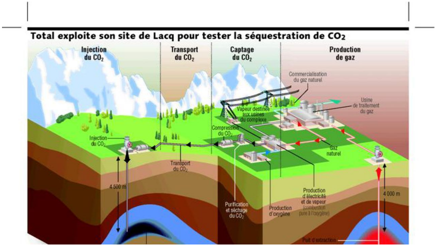
# Motivation




Geological storage of nuclear waste
*Figure: www.andra.fr*

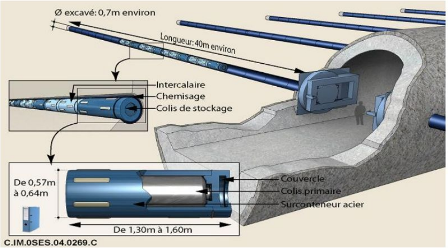



$CO_2$ sequestration

(Lacq-$CO_2$ - pilot general scheme) [1]

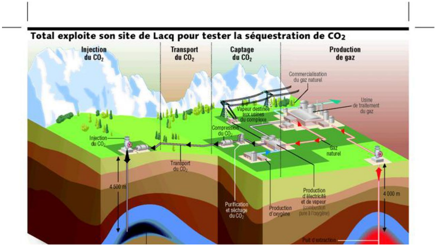
➢ The aim of **reactive transport modelling** in these applications is to make **forecasts** on large time-scales using numerical simulation on **storage reliability**.


[1] C. Prinet, S. Thibeau, M. Lescanne, J. Monne, Lacq-Rousse CO2 Capture and Storage Demonstration Pilot: Lessons Learnt From Two and a Half Years Monitoring, Energy Procedia, 37: 3610-3620,2013.




Geological storage of nuclear waste

*Figure: www.andra.fr*




$CO_2$ sequestration

(Lacq-$CO_2$ - pilot general scheme) [1]

➢ Necessity to take into account **interactions** between **chemical** species, the rock matrix and the flow

[1] C. Prinet, S. Thibeau, M. Lescanne, J. Monne, Lacq-Rousse CO2 Capture and Storage Demonstration Pilot: Lessons Learnt From Two and a Half Years Monitoring, Energy Procedia, 37: 3610-3620,2013.

# Goals

- Development of a **fully coupled**, **fully implicit, finite volume** scheme for **two-phase** multicomponent flows with reactive transport in porous media.
- Implementation of a two-phase multicomponent **reactive transport module** ***2pNc − react*** in the DuMu$^X$ framework
- Validation of the module on **3D test cases in literature including $CO_2$ sequestration**
- **Comparison** of the **fully coupled fully implicit** and **operator splitting** approaches on particular test cases in a unified environnement.
- **Improvement** of the fully coupled module:
  - improving the **nonlinear** solver (Newton method)
  - including **High performance computing**

→ Very competitive parallel reactive transport simulator

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# Geochemical model

- Example of chemical system for $CO_2$ sequestration:

$OH^- + H^+ \rightleftharpoons H2O_{(l)}$

$HCO_3^- + H^+ \rightleftharpoons H2O_{(l)} + CO2_{(l)}$

$CO2_{(l)} \rightleftharpoons CO2_{(g)}$

$H2O_{(l)} \rightleftharpoons H2O_{(g)}$

$CaCO_3 + H^+ \rightleftharpoons HCO_3^- + Ca^{2+}$

Mass action law and reactions rate

**Mass conservation equations: (1)**

❖ **Two-phase** compositionnel flow :

➢ $S_l$ liquid saturation
➢ $P_n$ gas pressure
➢ $x^i_\alpha$ molar fractions of components

**Closure relations:**

- Darcy's law,
- capillary pressure law,
- state equations,
- solubility laws

**Difficulties:** degeneracy, non linearities, phase exchange

$$\frac{\partial}{\partial t}(\phi \rho_\alpha S_\alpha x^i_\alpha) + \nabla.(\rho_\alpha x^i_\alpha \overrightarrow{q_\alpha} - \rho_\alpha \phi S_\alpha D_\alpha \nabla x^i_\alpha) = r^i, \quad i \in I \quad \alpha \in \{l, g\} \qquad (1)$$

# Geochemical model

- Example of chemical system for $CO_2$ sequestration:

$OH^- \rightleftharpoons H2O_{(l)} - H^+$
$HCO_3^- \rightleftharpoons H2O_{(l)} + CO2_{(l)} - H^+$

$CO2_{(g)} \rightleftharpoons CO2_{(l)}$

$H2O_{(g)} \rightleftharpoons H2O_{(l)}$

$CaCO_3 \rightleftharpoons HCO_3^- + Ca^{2+} - H^+$

Some notations :

- $I$ = set of all the chemical components involved in the chemical reactions
  - $I_p$ = primary components
  - $I_s$ = secondary components

- Main unknowns are the primary components
- **Secondary** species can be seen as product or intermediary variables

They are **eliminated** through their reaction rate by linear combination of the **mass conservation equations**, ex:

$$r_{H2O(l)} = - r_{H2O(g)} - r_{HCO3-} - r_{OH-}$$

$$\frac{\partial}{\partial t}(\phi \rho_\alpha S_\alpha x^i_\alpha) + \nabla.(\rho_\alpha x^i_\alpha \vec{q_\alpha} - \rho_\alpha \phi S_\alpha D_\alpha \nabla x^i_\alpha) = r^i, \quad i \in I \quad \alpha \in \{l, g\} \qquad (2)$$

[1] M. W. Saaltink, C. Ayora, and J. Ramírez. A mathematical formulation for reactive transport that eliminates mineral concentrations. Water Resources Research, 34:1649–1656, 1998.

# Geochemical model

- Example of chemical system for $CO_2$ sequestration:

$OH^- \rightleftharpoons H2O_{(l)}$

$HCO_3^- \rightleftharpoons H2O_{(l)} + CO2_{(l)}$

$CO2_{(g)} \rightleftharpoons CO2_{(l)}$

$H2O_{(g)} \rightleftharpoons H2O_{(l)}$

$CaCO_3 \rightleftharpoons HCO_3^- + Ca^{2+} - H^+$

Some notations :

❖ $I$ = set of all the chemical components involved in the chemical reactions

- ➢ $I_p$ = primary components
  - $I_{pm}$ = primary mobile components
  - $I_{pi}$ = primary immobile components
- ➢ $I_s$ = secondary components
  - ■ $I_{se}$ = components in equilibrium reactions
    - $I_{spm}$ = mobile species
    - $I_{spe}$ = precipitated species
    - $I_{si}$ = sorbed species
  - ■ $I_{sk}$ = components in kinetic reactions

Equilbrium mass action law:

$$a^j = K_j \prod_{i \in I_p} \left(a^i\right)^{\nu_{ji}}, j \in I_{se}$$

Kinetic mass action law: ex $CaCO_3$

$$\frac{dc_s^i}{dt} = -K_i^s A_i^s \left(1 - K_i \prod_{j \in I_p} \left(a_l^j\right)^{\nu_{ji}}\right), \quad i \in I_{sk}$$

# Geochemical model

- Example of chemical system for $CO_2$ sequestration:

$OH^- \rightleftharpoons H2O_{(l)}$

$HCO_3^- \rightleftharpoons H2O_{(l)} + CO2_{(l)}$

$CO2_{(g)} \rightleftharpoons CO2_{(l)}$

$H2O_{(g)} \rightleftharpoons H2O_{(l)}$

$CaCO_3 \rightleftharpoons HCO^-_3 + Ca^{2+} - H^+$

➢ The $I_{2p}$ components presents in both phases sometimes play part in phase displacement and thermodynamic state of the phase

Some notations :

❖ $I$ = set of all the chemical components involved in the chemical reactions

➢ $I_p$ = primary components

- $I_{pm}$ = primary mobile components
- $I_{pi}$ = primary immobile components

➢ $I_s$ = secondary components

- $I_{se}$ = components in equilibrium reactions
  - $I_{spe}$ = precipitated species
  - $I_{si}$ = sobred species
- $I_{sk}$ = components in kinetic reactions

➢ $I_{2p}$ = components present in both phases ($H_2O$, $CO_2$)

➢ $I_{rt}$ = remaining components

# Mathematical model

Two-phase compositional flow: $I_{2p}$ components mass conservation

$$\frac{\partial}{\partial t}\left(\theta_l c_l^i + \theta_g c_g^{\bar{i}}\right) + L_l(c_l^i) + L_g(c_g^{\bar{i}}) + \sum_{j\in I_s\setminus I_{2p}} \nu_{ji}\left[\frac{\partial}{\partial t}(\theta_{\alpha_j} c_{\alpha_j}^j) + L_{\alpha_j}(c_{\alpha_j}^j)\right] = 0, \qquad i\in I_p\cap I_{2p}, \quad (3)$$

$$a_g^{\bar{i}} = K^i a_l^i, \qquad \bar{i}\in I_s\cap I_{2p}. \quad (4)$$

---

Reactive transport problem: $I_p \setminus I_{2p}$

$$\frac{\partial}{\partial t}\left(\theta_\alpha c_{\alpha_i}^i + \sum_{j\in I_s\setminus I_{sk}} \nu_{ji}\theta_{\alpha_j} c_{\alpha_j}^j\right) + L_{\alpha_i}(c_{\alpha_i}^i) + \sum_{j\in I_s} L_{\alpha_j}(\nu_{ji} c_{\alpha_j}^j) = 0, \qquad i\in I_{pm}\cap I_{rt} \quad \alpha_i = \{l,\ g\}, \quad (5)$$

$$\frac{\partial}{dt}\left(c_s^i + \sum_{j\in I_{si}\cup I_{spe}} \nu_{ji} c_s^j\right) = 0, \qquad i\in I_{pi} \quad (6)$$

$$a_{\alpha_j}^j = K^j \prod_{i\in I_p} (a_{\alpha_i}^i)^{\nu_{ji}}, \qquad j\in (I_{rt}\cap I_s)\setminus I_{sk}, \alpha_i = \{l,\ g\} \quad (7)$$

$$\frac{dc_s^i}{dt} = -K_i^s A_i^s\left(1 - K_i \prod_{j\in I_p}\left(a_l^j\right)^{\nu_{ji}}\right), \qquad i\in I_{rt}\cap I_{sk}. \quad (8)$$

where: $L_\alpha(c_\alpha^i) = \nabla.(c_\alpha^i \overrightarrow{q_\alpha} - \phi S_\alpha D_\alpha^i \nabla c_\alpha^i)$, $\quad \theta_\alpha = \phi S_\alpha \ \alpha = \{l,\ g\} \quad \theta_s = 1$.

**Solving approaches:**

- Operator splitting methods: Splitting into two sub-problems.
- Fully implicit methods: Coupling the two sub-problems.

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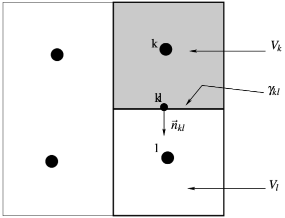
- Fully coupled, fully implicit scheme based on **Direct Substitutional Approach**
- **Implicit Euler scheme** for time discretization
- **Vertex or Cell-centered finite volume** approach for spatial discretization




- **Fully upwinding** scheme for convective terms

$$\{\cdot\}_{kl}^{n+1} = \begin{cases} \{\cdot\}_k^{n+1} & \text{if } \vec{q}_\alpha \cdot \vec{n}_{kl} > 0 \\ \{\cdot\}_1^{n+1} & \text{else.} \end{cases} \tag{9}$$

- $\nabla P_\alpha, \nabla c_\alpha^i$ are calculated on the interface between the cells using $\mathbb{P}_1/\mathbb{Q}_1$ **conforming Finite Element** scheme with piecewise linear elements for the diffusive terms.

# Numerical scheme

❖ **Newton-Raphson method** to solve the nonlinear system

→ The jacobian is calculated by numerical differentiation

→ **New Jacobian reassembling strategy** → Jacobian is partially reassembled only when more accuracy over the jacobian terms is needed to achieve convergence

→ **Heuristic suggest of time step strategy** → Adaptive Newton time step strategy based **maximum relative shift** at the first iteration and the number of Newton iterations

# Numerical scheme

- ❖ **Linear solver :** Krylov space methods
  - ➢ Bi-conjugate Gradient Stabilized
  - ➢ Restarted GMRES

❖ **AMG** preconditioner with **ILU0** smoother

- ❖ **The Framework**

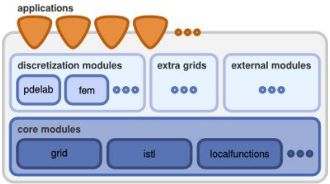
Open-source **Parallel** platform

DuMu$^X$

**DuMux, DUNE for Multi-{Phase, Component, Scale, Physics, ...}**

Dune

http://dune-project.org/




Development and Implementation of ***2pNc-react*** a reactive transport module in DuMu$^X$

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- Test case presented in [1].

[1] Y. Fan, L. J. Durlofsky, and H. A. Tchelepi. A fully-coupled flow-reactive-transport formulation based on element conservation, with application to $CO_2$ storage simulations. Advances in Water Resources, 42:47–61, 2012.

- 3D domain, 100$m$ of thickness, 15$km$ of length and 15$km$ of width.
- Injection well at 25$m$ of the top of the aquifer.
- Injection during 20 years ($18.6 \times 10^9$ metric tons).
- Time of simulation = 2000 years.

| | | | |
|---|---|---|---|
| Porosity | $\phi = 0.18$ | Absolute permeability | $K = 10^{-13} m^2$ |
| Capillary pressure law | $P_c = 0$ | Relative permeability | $k_{rl} = (S_l^*)^4$<br>$k_{rl} = (S_l^*)^4$<br>$S_l^* = \dfrac{S_l - S_{lr}}{1 - S_{lr}}$<br>$S_{lr} = 0.2$ |
| Temperature | $T = 323$ K | | |
| Liquid diffusion | $D_m = 1.\,10^{-9} m^2.s^{-1}$ | Gas diffusion | Model based on [1] |
| Liquid density | Model based on [2] | Liquid viscosity | Model based on [2] |
| Gas density | Model based on [1] | Gas viscosity | Model based on [2] |

[1] B. Xu, K. Nagashima, J. M. DeSimone, and C. S. Johnson. Diffusion of water in liquid and supercritical carbon dioxide: an NMR study. The Journal of Physical Chemistry A, 107, 2003.

[2] J. J. Adams, S. Bachu, Equations of state for basin geofluids: algorithm review and intercomparison for brines, Geofluids 2, 257–271, 2002.

[3] R. Span, W. Wagner, A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100 K at pressures up to 800 MPa, Journal of Physical and Chemical Reference Data 25, 1509–1596, 1996.

[4] A. Fenghour, W. A. Wakeham, V. Vesovic, The Viscosity of Carbon Dioxide, Journal of Physical and Chemical Reference Data 27, 31–44, 1998.

- Chemical system composed of 12 elements (3 minerals) and 6 reactions (3 kinetic reactions and 3 equilibrium).

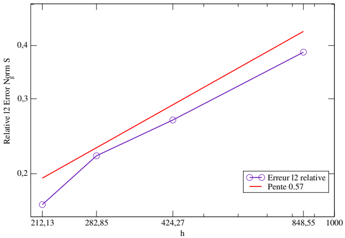
| No. | Reactions | $\log_{10}(K_k^{eq})$ |
|---|---|---|
| (1) | $CO_{2(l)} + H_2O = H^+ + HCO_3^-$ | -13.2631 |
| (2) | $CO_3^{2-} + H^+ = HCO_3^-$ | -6.3221 |
| (3) | $OH^- + H^+ = H_2O$ | -10.2342 |
| (4) | $\text{Anorthite} + 8H^+ = 4H_2O + Ca^{2+} + 2Al^{3+} + 2SiO_{2(l)}$ | 25.82 |
| (5) | $\text{Calcite} + H^+ = Ca^{2+} + HCO_3^-$ | 1.6 |
| (6) | $\text{Kaolinite} + 6H^+ = 5H_2O + 2Al^{3+} + 2SiO_{2(l)}$ | 6.82 |

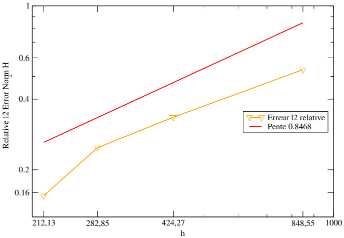
Table: Chemical reactions, (Equilibrium in blue) (Kinetic in red).

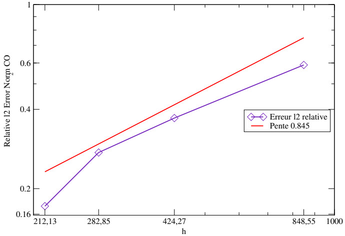
| Mineral | $log_{10}(K_s)$ [mol.m$^{-2}$.s$^{-1}$] | Surf. Area [m$^2$.m$^{-3}$] | Init. conc [mol.m$^{-3}$] |
|---|---|---|---|
| Anorthite | -12.0 | 88 | 87 |
| Calcite | -8.80 | 88 | 238 |
| Kaolinite | -13.0 | 17600 | 88 |

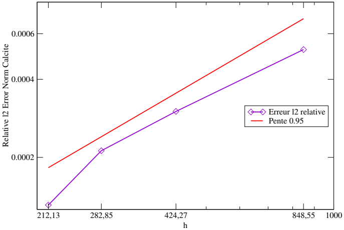
Table: Mineral, precipitation and dissolution parameters.

## Numerical convergence of some quantities of interest for test case I with their respective slopes at 100 years using the l2 relative error norm over all the domain.



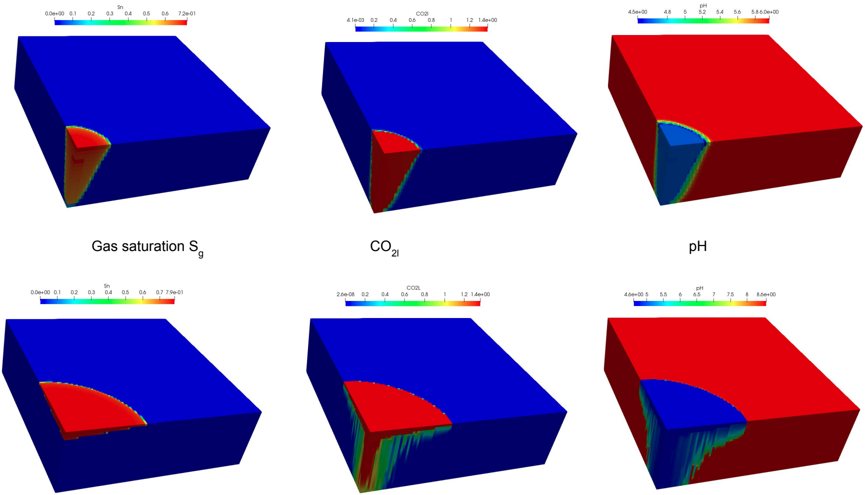




Relative l2 error $l^2$relative $= \sqrt{\dfrac{\sum_{i=1}^{i=NOE} (u_{ref}(i) - u_c(i))^2}{\sum_{i=1}^{i=NOE} u_{ref}(i)^2}}$,

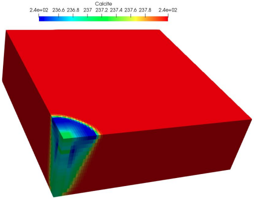
$u_{ref}$ : reference solution, $u_c$ coarse grid solution,
$NOE$ fine grid number of elements.

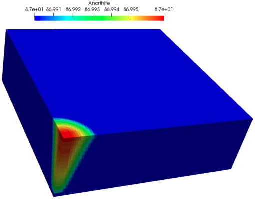
**10 000** cells : 25 $\times$ 25 $\times$ 16, $h = 848.55\ m$,
**80 000** cells : 50 $\times$ 50 $\times$ 32, $h = 424.27\ m$,
**180 000** cells : 75 $\times$ 75 $\times$ 32, $h = 282.85\ m$,
**640 000** cells : 100 $\times$ 100 $\times$ 64, $h = 212.13\ m$,
**5 120 000** cells : 200 $\times$ 200 $\times$ 128, $h = 212.13\ m$.
**reference solution**

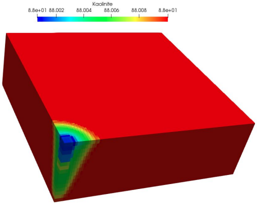



**Evolution of the some quantities of interest from 20 to 2000 years on a 320 000 cells.**

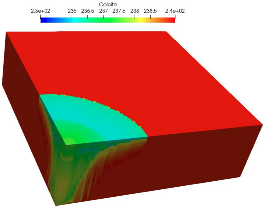
# 3D $CO_2$ injection in deep saline aquifer : Test case I

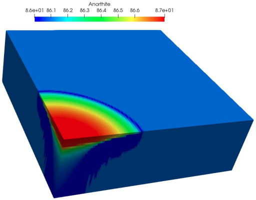


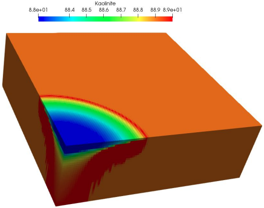




Calcite | Anorthite | Kaolinite



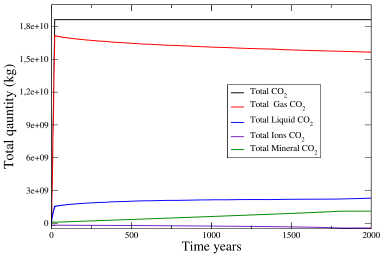



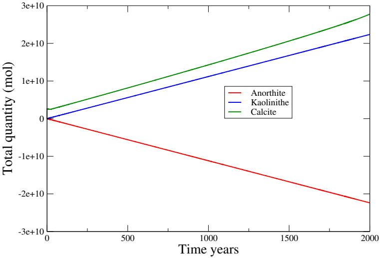




**Evolution of the some quantities of interest from 20 to 2000 years on a 320 000 cells.**

**The total quantity of $CO_2$ :**

$$
\begin{aligned}
T_{CO_2} &= CO_{(2}l) \quad \text{(dissolved)} \\
&+ CO_{(2}g) \quad \text{(gaz)} \\
&+ HCO_{3\_} + CO_3^{2-} \quad \text{(ions)} \\
&+ CaCO_3 \quad \text{(mineral)}
\end{aligned}
$$

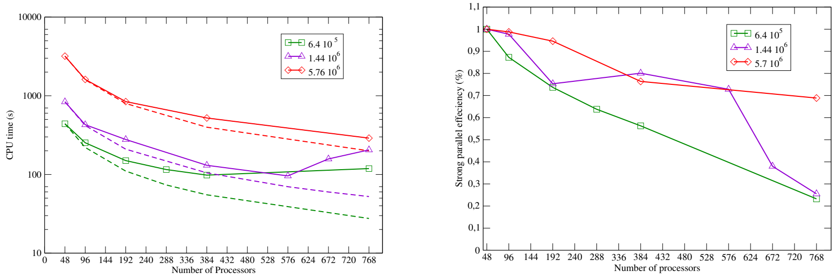


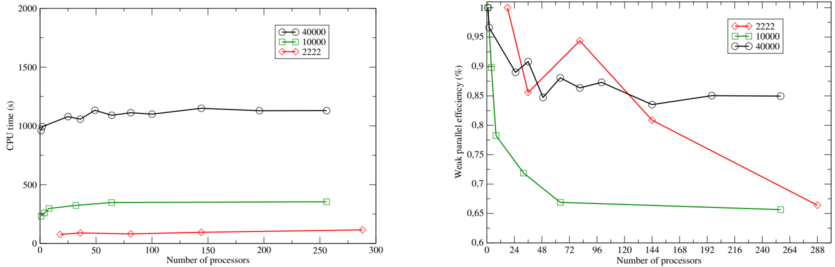

**Evolution of $CO_2$ (left) and mineral (right) total quantities over the domain over 2000 years**

Table: Final carbon distribution at 2000 years.

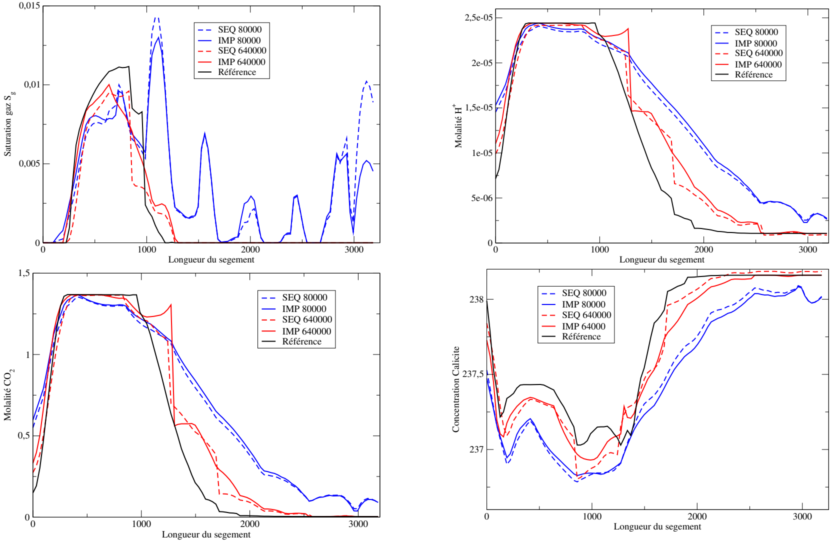
| In $CO_{2(g)}$ | In $CO_{2(l)}$ | In ions | In minerals |
|---|---|---|---|
| 84.02 % | 12.33 % | 0.2% | 5% |




**CPU time and strong parallel efficiency as a function of the number of processors.**

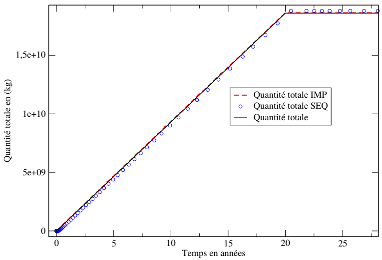


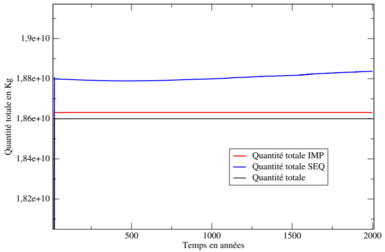

**CPU time and weak parallel efficiency as a function of the number of processors.**




**Comparison of results at the segment** [(0, 0, 0) (2250, 2250, 100)] **of the fully implicit scheme and operator splitting method using DSA for reactive transport problem [1] on differents mesh at 100 years.**

[1] E. Ahusborde, B. Amaziane, M. El Ossmani, Improvement of numerical approximation of coupled two-phase multicomponent flow with reactive geochemical transport in porous media, *Oil and Gas Science and Technology*, 2018.




**Evolution from 0 to 20 years** **Evolution from 20 to 2000 years**

**Comparison of $CO_2$ total quantity evolution, over the domain of the fully implicit scheme and operator splitting method using DSA for reactive transport problem [1]**

[1] E. Ahusborde, B. Amaziane, M. El Ossmani, Improvement of numerical approximation of coupled two-phase multicomponent flow with reactive geochemical transport in porous media, *Oil and Gas Science and Technology*, 2018.

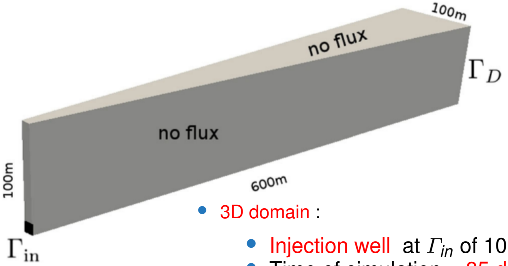
**CPU time (s) for the the fully implicit method (FIM) and operator splitting method (OPM).**

| Grid number of cells | Approach | CPU time | Iteration number |
|---|---|---|---|
| 320 000 | FIM | **6h 28min** | 892 |
| | OPM | **3h 34min** | 856 |
| 180 000 | FIM | 4h 15min | 888 |
| | OPM | 3h 7min | 856 |
| 80 000 | FIM | 4h 6min | 823 |
| | OPM | 3h 22min | 856 |
| 10 000 | FIM | 37min 30s | 246 |
| | OPM | 41 min | 326 |

- We have already reduced the CPU time up to **2x , 3x** compared to the simulations made by the **default strategies (timestep, reassembling)**
- The DSA approach performed better compared to SIA approach on single phase flow on particular test case (SHPCO2) test case
- However the operator splitting approach using the DSA approach for the reactive transport subproblem still performs better (sequential coupling of two implicit subproblems)
- More optimisations over the non-linear solver can be made and improvement the preconditioning and linear solvers.

- Test case presented in [1].

[1] F. Brunner, P. Knabner. A global implicit solver for miscible reactive multiphase multicomponent flow in porous media. Computational Geosciences, 23:127–148, 2019.




(1) $CO_{2(l)} \rightleftharpoons CO_{2(g)}$
(2) $CO_{2(l)} + H_2O \rightleftharpoons HCO_3^- + H^+$
(3) $\text{Calcite} + H^+ \rightleftharpoons Ca^{2+} + HCO_3^-$
(4) $\text{MinA} + 3\,H^+ \rightleftharpoons Me^{3+} + SiO_2$
(5) $\text{MinB} + 2\,H^+ \rightleftharpoons Me^{3+} + HCO_3^-$

- 3D domain :
  - Injection well at $\Gamma_{in}$ of $10m$ height
  - Time of simulation = 85 days
- Chemical reactions
  - 5 equilibrium reactions,
  - 3 precipitated minerals Calcite, MinA and MinB.

## Table: Input parameters for the test case II

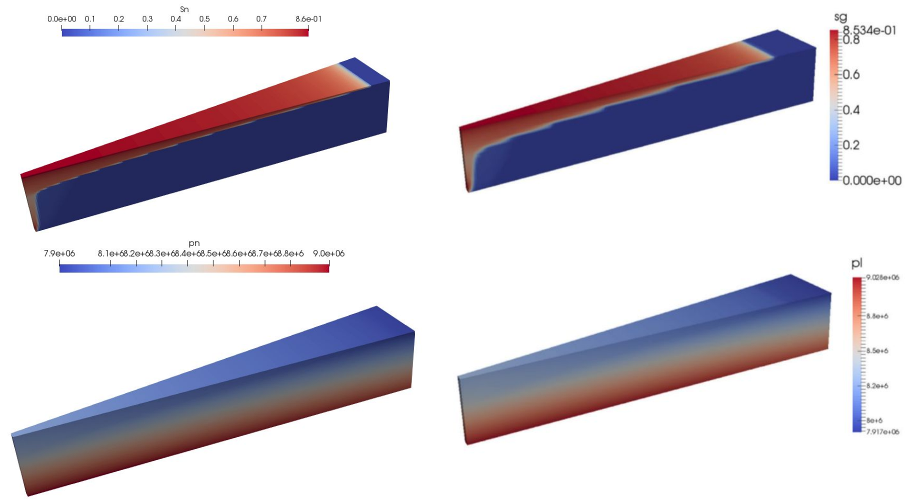
| | | | |
|---|---|---|---|
| Porosity | $\phi = 0.2$ | Absolute permeability | $K = 10^{-12} m^2$ |
| Capillary pressure | $P_c = 0$ | Relative permeability | Brooks–Corey<br>$S_l(res) = 0.0$ [-]<br>$S_g(res) = 0.0$ [-]<br>$\lambda = 2.0$ [-]<br>$P_{entry} = 1000.0$ Pa |
| Temperature | $T = 313.15$ K | | |
| Liquid diffusion | $D_m = 2.\ 10^{-9} m^2.s^{-1}$ | Gas diffusion | Model based on [1] |
| Liquid longitudinal dispersion | $\alpha_L = 0.1 m^2.s^{-1}$ | Liquid transversal dispersion | $\alpha_T = 0.01 m^2.s^{-1}$ |
| $CO_2$ injection rate | $2.10^{-2} Kg.m^{-2}.s^{-1}$ | | |
| Liquid density (T=3.13.15K) | $992 Kg.m^{-3}$ | Gas density | Model based on [1] |
| Liquid viscosity (T=3.13.15K) | $\nu_l = 6.526 Pa.s$ | Gas viscosity | Model based on [2] |

| | Molar mass $Kg.mol^{-1}$ | Initial concentration $mol.m^{-3}$ |
|---|---|---|
| $CO_{2(l)}$ | $4.4 \times 10^{-2}$ | $1 \times 10^{-2}$ |
| $H_2O$ | $1.8 \times 10^{-2}$ | 55333.33 |
| $HCO_3^-$ | $6.1 \times 10^{-2}$ | $1 \times 10^{-2}$ |
| $H^+$ | $1 \times 10^{-3}$ | $1 \times 10^{-3}$ |
| $Ca^{2+}$ | $4 \times 10^{-3}$ | $1 \times 10^{-1}$ |
| $Me^{3+}$ | $1.5 \times 10^{-2}$ | $1 \times 10^{-4}$ |
| $SiO_{2(l)}$ | $6 \times 10^{-2}$ | $1 \times 10^{-2}$ |
| Calcite | - | 0.1 |
| MinA | - | 0.2 |
| MinB | - | 0.0 |

[1] R. Span, W. Wagner, A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100 K at pressures up to 800 MPa, Journal of Physical and Chemical Reference Data 25, 1509–1596, 1996.

[2] A. Fenghour, W. A. Wakeham, V. Vesovic, The Viscosity of Carbon Dioxide, Journal of Physical and Chemical Reference Data 27, 31–44, 1998.

# 3D $CO_2$ injection in deep saline aquifer : Test case II




**Results comparison of some quantities of interest at 85 days : our results (9600 cells) (left) and the results in [1] (right).**

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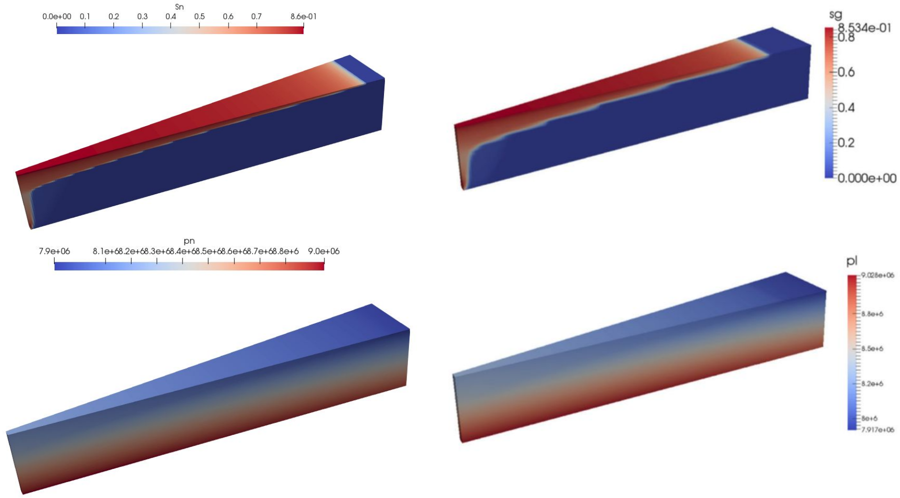


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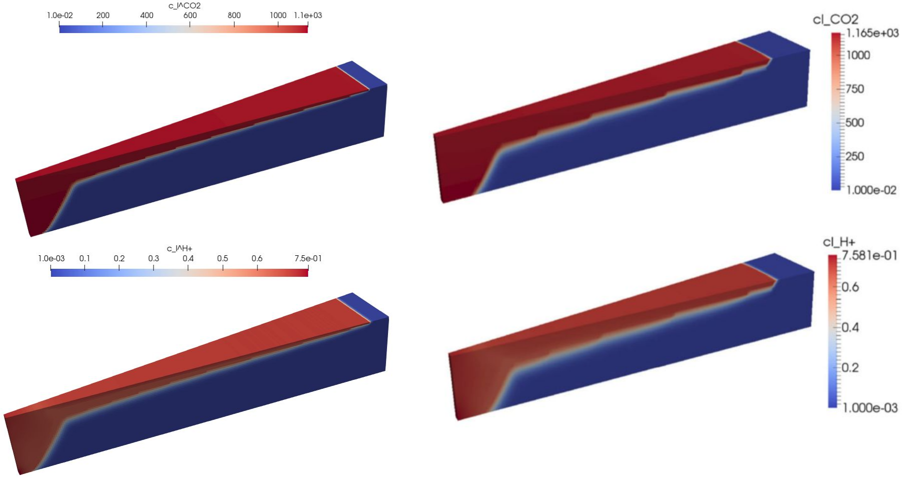


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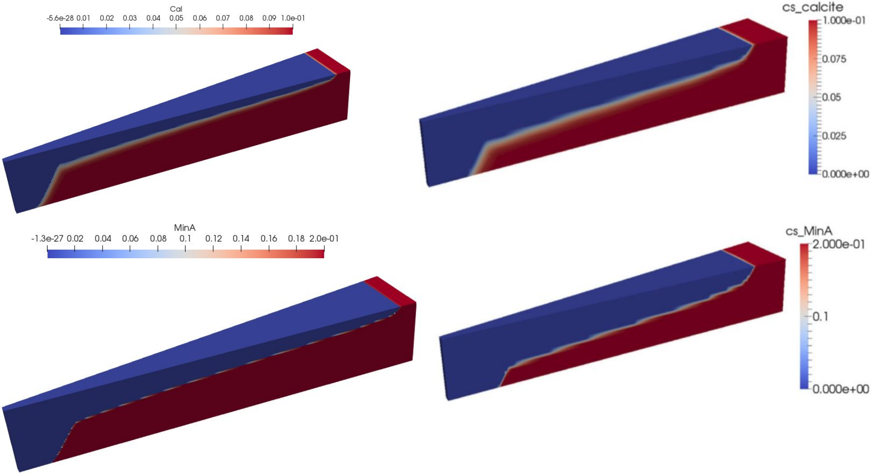


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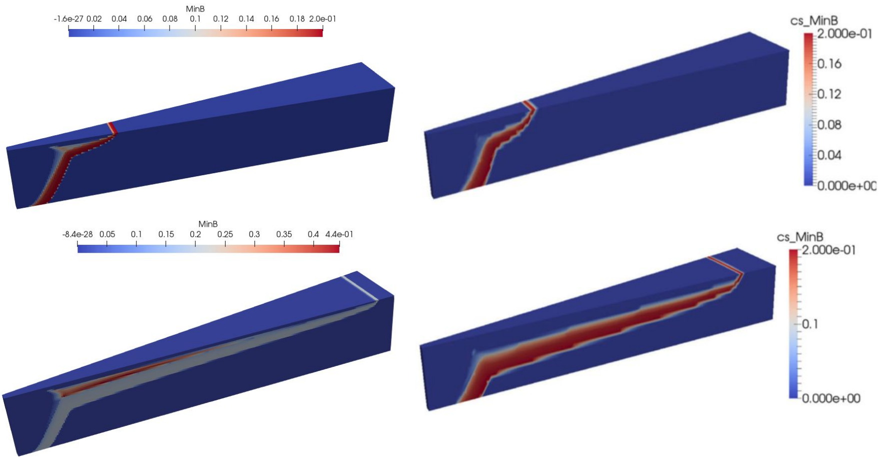
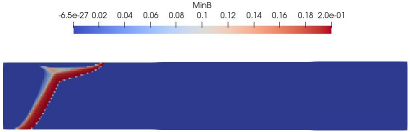
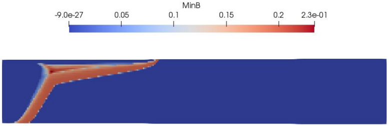



**Results comparison of MinB evolution from 20 days to 85 days : our results (9600 cells) (left) and the results in [1] (right).**

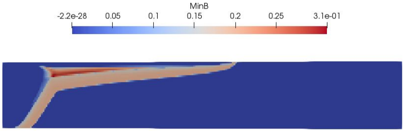
[1] F. Brunner, P. Knabner. A global implicit solver for miscible reactive multiphase multicomponent flow in porous media. Computational Geosciences, 23:127–148, 2019.



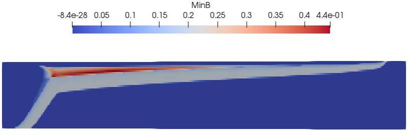

**20 days**




**30 days**




**60 days**

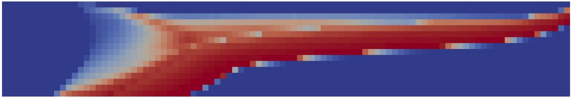



**85 days**

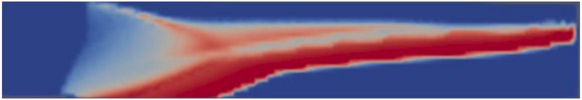
**MinB evolution from 20 days to 85 days on 9600 cells.**

[1] F. Brunner, P. Knabner. A global implicit solver for miscible reactive multiphase multicomponent flow in porous media. Computational Geosciences, 23:127–148, 2019.

# 3D $CO_2$ injection in deep saline aquifer : Test case II



**Our results on coarse mesh**



**Brunner & al. code** *(by Markus knodel)*

**Results comparison on coarse grid (600 cells) of MinB at 85 days with a 2D version.**


[1] F. Brunner, P. Knabner. A global implicit solver for miscible reactive multiphase multicomponent flow in porous media. Computational Geosciences, 23:127–148, 2019.

# Outline

1 Motivation and Goals
2 Reactive transport model
3 Numerical scheme
4 Validation & numerical results
5 Conclusion & Perspectives

# Conclusion & Perspectives

- Development of a fully coupled, fully implicit finite volume scheme for a two-phase multicomponent flow with reactive transport in porous media.
- Validation of our methodology and our implemented module *2pNc-react* on test cases for $CO_2$ injection in saline aquifers.
- Comparison of the the fully implicit method and the operator splitting approach on particular test cases.

- Validation of the *2pNc-react* module on 2D and 3D realistic test cases including $CO_2$ geological sequestration.
- Advanced comparison between the fully implicit method and the operator splitting approach.
- Reducing of the CPU time for the fully implicit method to make it more competitive the sequential approach by improving the non linear solver and the linear solver.

# Thank you for your attention :

*Questions ?*

This work was partially supported by the **Carnot Institute ISIFoR** project (Institute for the sustainable engineering of fossil resources).
We also thank the **DuMu**$^X$ and **DUNE** teams for their help during the development of our reactive transport module.
We also thank **CINES** (National Computing Center for Higher Education) to give us access to their computing resources facility. This work was granted access to the HPC resources of CINES under the allocations 2017-A0020610019 and 2018-A0040610019 made by GENCI.